Nanotech France 2018
NanoMaterials for Energy & Environment
NanoMatEn 2018 – NanoMetrology 2018

Joint International Conferences and Exhibition

27th - 29th June, 2018

Paris – France

Book of Abstracts

Organizer

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Nanotech France 2018, NanoMetrology 2018 and NanoMatEn 2018 Conference Program

June 26, 2018

15:00 - 17:00	**Registration**	**Registration Area**

June 27, 2018

Nanotech Plenary session I

Amphitheatre H

Session's Chairs:
Prof. Jacques Jupille, Institut des Nanosciences de Paris, France
Prof. James M Hill, University of South Australia, Australia

08:30 - 12:00	**Registration**	**Registration Area**
09:30 - 10:00	Hybrid Nanomaterials: Structural and Local Spectroscopic Studies via Advanced TEM R. Arenal	**Dr. Raul Arenal**, Zaragoza University, **Spain**
10:00 - 10:30	Nanocrystalline Alloy Structure for Remarkable Oxidation Resistance **R. Singh**	**Prof. Raman Singh**, Monash University, **Australia**
10:30 - 11:00	**Coffee Break / Posters Session I**	**Coffee Break Area**
11:00 - 11:30	Continuous approximation for interaction energy of adamantane encapsulated inside carbon nanotubes D. Baowan, **J.M. Hill** and W. Bacsa	**Prof. James M Hill**, University of South Australia, **Australia**
11:30 - 12:00	Disorder in graphene - from meter to atomic scale **P. Bøggild**	**Prof. Peter Bøggild**, Technical University of Denmark**, Denmark**
12:00 - 12:15	AFM PinPoint Nanomechanical Mode Using Probes with Different Stiffness W.Shi, G.Pascual, B.Kim, and **K. Lee**	**Mr. Keibock Lee**, Park Systems, **USA**
12:15 - 12:30	NFFA-EUROPE An open access resource for experimental & theoretical science **E. Travaglia**	**Dr. Elisabetta Travaglia**, CNR-IOM-Trieste, **Italy**
12:30 - 12:45	Research and innovation Dilemma on Nanotechnology **M.Bersani** and G. Casse	**Dr. Massimo Bersani**, Bruno Kessler foundation, **Italy**
12:00 - 14:00	**Lunch Break**	**Restaurant (Rue Basse)**

June 27, 2018

Session I.A: Nanomaterials Fabrication / Synthesis

Conference Room 561

Session's Chairs:
Prof. Jacques Jupille, Institut des Nanosciences de Paris, France
Prof. Peter Bøggild, Technical University of Denmark, Denmark
Prof. MariaPia Pedeferri, Milano Polytechnic Institute, Italy

14:00 - 14:30	Particle and Product Design by Top-down Processes **S. Mende**	**Dr. Stefan Mende**, NETZSCH Feinmahltechnik GmbH, **Germany**
14:30 - 14:45	Metallic Bismuth Nanoparticles : a Reproducible, Robust and Repeatable Synthesis via a Green and Safe Process **C. Gomez**, A. Pastor, A. Hassoun, G. Hallot, E. Brun, C. Sicard-Roselli, S. Laurent and M. Port	**Dr. Catherine Gomez**, Conservatoire National des Arts et Métiers, **France**
14:45 - 15:00	Functional Noncovalently Modifed Boron Nitride Nanotubes **Y. Martinez-Rubi**, Z. Jakubek, S. Zou, B. Ashrafi, M.B. Jakubinek, S. Denommee, K. Kim and B. Simard	**Dr. Yadienka Martinez Rubi**, National Research Council Canada, **Canada**

15:00 - 15:15	Facile Fabrication of Superhydrophobic Surfaces with Hierarchical Structures E. Lee and **K-H. Lee**	**Prof. Kun-Hong Lee** Pohang Univ. of Science & Technology, **Rep of Korea**
15:15 - 15:30	Solution-based synthesis of amorphous germanium nanopar-ticles from organogermanium halide precursors **B. Pescara**, K. A. Mazzio, K. Lips and S. Raoux	**Dr. Bruno Pescara**, Helmholtz-Zentrum Berlin for Materials and Energy, **Germany**
15:30 - 15:45	Synthesis of aqueous slurries with high concentration in polystyrene nanoparticles **D. Lopez-Pedrajas**, A. M. Borreguero, J. F. Rodríguez and M. Carmona	**Mr. Daniel López Pedrajas**, University of Castilla-La Mancha, **Spain**
15:45 - 16:00	Fabrication of nanocomposite thin films assisted by plasma polymerization, towards smart coatings **S. Wolak**, S. Jebali, K. Mougin, V. Roucoules and F. Bally-Le Gall	**Ms. Séverine Wolak**, Institut de Science des Matériaux de Mulhouse (IS2M) - CNRS/UHA, **France**
16:00 - 16:30	**Coffee Break / Posters Session I**	**Coffee Break Area**
16:30 - 17:00	Nanostructured anodic titanium oxides: production and engineered applications M.V. Diamanti, A. Brenna, M. Ormellese, B. Del Curto and **MP. Pedeferri**	**Prof. MariaPia Pedeferri, Milano Polytechnic Institute, Italy**
17:00 - 17:15	Synthesized In2-xSnxOy on ITO coated PET using Sol-Gel Method for Extended Gate FET-pH Sensor device. **S. Palit**, S. P. Bag, P. Garu, K. Singh, B. S. Lou, J. L. Her and T. M. Pan	**Ms. Sayani Palit**, Chang Gung University, **Taiwan**
17:15 - 17:30	Nanocrystals as high temperature local probes **G. Muraille**, E.A. Baquero, R.A. Swain, B. Chaudret, C. Nayral and F. Delpech	**Dr. Gaëlle Muraille**, University of Toulouse, **France**
17:30 - 17:45	Laser Nanopatterning of Colored Ink Thin Films for Photonic Devices **B. AlQattan**, D. Benton, A.K. Yetisen and H. Butt	**Mr. Bader AlQattan**, Unveristy of Birmingham, **UK**
17:45 - 18:00	Physical hybrid hydrogels with colloid-Cubosomes as crosslinker. F. Ferdeghini, Z. Guennouni, C. Le Cœur and **F. Muller**	**Dr. François Muller**, ECE-Paris Engineering School, **France**
18:00 - 18:15	Nonaqueous sol-gel synthesis and structural characterization of very small ZnO nanoparticles **A. Lemarchand**, F. Rémondière, J. Jouin, J. Manaud, P. Thomas and O. Masson	**Mr. Alex Lemarchand**, Limoges University, **France**
18:15 - 18:30	Surface Modification at Solid-Solid Interface to Enable Selective Adhesion **R. P. Jaiswal** and S. P.Beaudoin	**Dr. Ravi Jaiswal**, Indian Institutes of Technology-BHU, **India**
18:30 - 18:45	Improving the Sensitivity of Buckypaper Strain Gauges through Tailoring their Porosity **R. Hassan**, N. El-Mansoury, M. Ismail, K. El-Shamsy, O. El-Said, M. Arafa and A. Esawi	**Mrs. Rufaydah Hassan**, The American University in Cairo, **Egypt**

June 27, 2018

NanoMetrology 2018 - Session I.B: Nanomaterials characterization and properties

Conference Room 558

Session's Chairs:

Dr. Raul Arenal, Zaragoza University, Spain
Prof. Raman Singh, Monash University, Australia

14:00 - 14:15	Electrochemical Atomic Force Microscopy: In Situ Monitoring of Copper Electrodeposition on Gold Surface J.P. Pineda, M. Leal, G. Pascual, B. Kim and **K, Lee**	**Mr. Keibock Lee**, Park Systems, **USA**
14:15 - 14:30	Sub-Nanoscale topography standards for microscopy calibration: Manufacture, features and application **I. Busch**, O. Lenck , L. Daul, T. Dziomba, A. Felgner and L. Koenders	**Dr. Ingo Busch**, National Metrology Institute of Germany (PTB), **Germany**

14:30 - 14:45	Multi-scale assessment of soot using electron microscopy: applications on soot from bench-scale fire of polymers **G. Okyay**, S. Bellayer, F. Samyn, M. Jimenez and S. Bourbigot	**Dr. Gizem Okyay**, University of Lille, **France**
14:45 - 15:00	Investigation of the spin-orbit coupling effect of intrinsic and p-type 2D MoS2 by spectroscopic ellipsometry **B. Song**, H. Gu, Y-T. Ho, M. Fang and S. Liu	**Mr. Baokun Song**, Huazhong University of Science & Tech., **China**
15:00 - 15:15	Optical properties of Pb0.865La0.09(Zr0.65Ti0.35)O3 thin films studied by spectroscopic ellipsometry **H.Gu**, M.Li, C. Huang and S. Liu	**Dr. Honggang Gu**, Huazhong University of Science & Tech., **China**
15:15 - 15:30	Determination of the monolayer coverage of silica particles **A. La Rosa**, G. Durand, M. Alvarez, T. Justet and Alan Taylor	**Mr. Angelo La Rosa**, London South Bank University, **UK**
15:30 - 15:45	Friction Reduction on Anodized Alumina by Deposition of Ti Nanolayers **T. Matijošius**, L. Staišiūnas and S. Asadauskas	**Mr. Tadas Matijošius**, Center for Physical Sciences and Technology, **Lithuania**
15:45 - 16:00	Porous PDMS / CNF Nanocomposites for Sensing Applications W. Luo, **M.C. Saha** and Y. Liu	**Prof. Mrinal Saha**, University of Oklahoma, **USA**
16:00 - 16:30	**Coffee Break / Posters Session I**	**Coffee Break Area**
16:30 - 16:45	Tuning the electronic response of MoS2 by pressure induction **R. Torres-Cavanillas**, M. Morant-Giner, G. Escorcia, J. Dugay, M. Galbiati, S. Tatay, M. Giménez-Márquez, A. Forment-Aliaga, E. Coronado.	**Mr. Ramón Torres-Cavanillas**, Univesity of Valencia, **Spain**
16:45 - 17:00	Solution-processable inorganic hole injection layer to improve the performance of quantum-dot light-emitting diodes **S.J. Kang**	**Prof. Seong Jun Kang**, Kyung Hee University, **Rep. of Korea**
17:00 - 17:15	Highly Conductive, Mechanically Robust Ion Gels Based on Co-polymers and their Electrochemical Applications **H.C. Moon**	**Prof. Hong Chul Moon**, University of Seoul, **Rep. of Korea**
17:15 - 17:30	Enhancement in thermoelectric properties of Te-embedded Bi2Te3 by stong phonon scattering at interface **K. Jeong**, H. Choi, J. Chae, H. Park, J. Baeck, T. Hyeon Kim, J.Y. Song, J. Park, K-H. Jeong and M-H. Cho	**Dr. Kwangsik Jeong**, Yonsei University, **Rep. of Korea**
17:30 - 17:45	Multi-functional copolymer for coating on magnetite nanoparticle for use in bioconjugation **S. Paenkaew** and M. Rutnakornpituk	**Ms. Sujittra Paenkaew**, Naresuan University, **Thailand**
17:45 - 18:00	Poly(N-acryloyl glycine)-grafted magnetite nanoparticle conjugated with pyrrolidinyl peptide nucleic acid for selective enrichment of trace DNA samples **S. Khadsai**, N. Seeja, M. Rutnakornpituk, T. Vilaivan, M. Nakkuntod, W. Suwankitti and B. Rutnakornpituk	**Ms. Sudarat Khadsai**, Naresuan University, **Thailand**
18:00 - 18:15	Antibacterial activity of high-k oxides deposited by the ALD method- applications in biology and medicine **A. Słońska-Zielonka**, J. Cymerys-Bulenda, S. Gierałtowska, R. Pietuszka, B.S. Witkowski, K. Amaro, H. Buksiński, Z. Gajewski, M. M. Godlewski and M. Godlewski	**Dr. Anna Słońska-Zielonka**, Warsaw Univerity of Life Sciences, SGGW, **Poland**
18:15 - 18:30	Nanoparticles and Nanofibers/Polymer Conjugates for Antibacterial, Anti-corrosion and Drug Delivery Applications **W. Mamdouh**, J. Kegere, N. M. Elbaz, L. Ziko and R. Siam	**Prof. Wael Mamdouh**, The American University in Cairo, **Egypt**

June 27, 2018

NanoMetrology 2018 - Session on Mathematical Modelling in Nanoscience and Nanotechnology

Session's Chairs:
Prof.Natalie Thamwattana, University of Newcastle, Australia
Prof. Duangkamon Baowan, Mahidol University, Thailand
Prof. James M Hill, University of South Australia, Australia

Conference Room 458

14:00 - 14:30	Intercalating carbon nanotubes into graphene folds T. Dyer, **N. Thamwattana** and B. J. Cox	**Prof. Ngamta Thamwattana**, University of Wollongong, **Australia**
14:30 - 15:00	Energy behaviour of atomic force microscope cantilever system **D. Baowan**, K. Sumetpipat, B.J. Cox and J.M. Hill	**Dr Duangkamon Baowan**, Mahidol Univerisity, **Thailand**
15:00 - 15:15	Modeling of Polyoxometalates for Surface Fuctionalization: Nano-scale Interactions Controlling Macroscopic Features **G. De Luca**, M.Carraro, R. Amuso, R. Mancuso, J. Hoinkis, B. Gabriele, M. Bonchio and A. Figoli	**Dr. Giorgio De Luca**, University of Calabria, **Italy**
15:15 - 15:30	Modeling Realistic TiO2 Nanoparticles and Their Interaction with Water **D. Selli,** G. Fazio, G. Seifert and C. Di Valentin	**Dr. Daniele Selli**, University of Milano-Bicocca, **Italy**
15:30 - 15:45	Molecular Dynamics Simulation of Water-Graphene Nanofluid M. Mohammadi, M. Al-Wadhahi, A. M. Gujarathi, R. Al-Maamari and **G. R. Vakili-Nezhaad**	**Prof. G. Reza Vakili-Nezhaad**, Sultan Qaboos University, **Oman**
15:45 - 16:00	Dyadic Green Function based Model for Organic Light Emitting Diodes with Stratified Anisotropic Materials **X.H. Ke**, H.G. Gu, H.Jiang and S.Yuan Liu	**Mr. Xianhua Ke**, Huazhong University of Science and Technology, **China**
16:00 - 16:30	**Coffee Break / Posters Session I**	**Coffee Break Area**
16:30 - 16:45	Universality of Steric Effects of Electrolyte in Nano-confinement Rajni, I. S. Kang and **J. M. Oh**	**Dr. Jung Min Oh**, Institute for Basic Science, Center for Soft and Living Matter-Ulsan, **Rep. of Korea**
16:45 - 17:00	Solubilization of slovophobic polymer chains in interpolyelectrolyte complex cores of non-stoichiomeric co-assembled nanoparticles. Dissipative particle dynamics with explicit electrostatics **K. Procházka**, K. Šindelka, Z. Limpouchová and M. Lísal	**Prof. Karel Prochazka**, Charles University in Prague, **Czech Republic**
17:00 - 17:15	Determining the Schottky barrier in a metal/semiconductor interface by ab initio Ballistic Electron Emission Microscopy simulations **C. González**, P. de Andrés and F. Flores	**Dr. César González**, Autonoma University of Madrid, **Spain**
17:15 - 17:30	Molecular applications of nanomaterials: The case of ZnO and laser cooling **N.El-Kork**, C.Bradley, S. Mahmoud, M. Bechelany, P. Miele and M. Korek	**Dr. Nayla El-Kork**, Khalifa Univeresity of Science and Technology, **United Arab Emirates**
17:30 - 17:45	Properties of Ionic Liquid Mixtures **A.Vakilinejad**, Kh. Mahrami, M. Humaid and G. R. Vakili-Nezhaad	**Ms. Khansaa AlMahrami**, Sultan Qaboos University, **Oman**

June 28, 2018
Nanotech / Biotech Joint Plenary session II

Amphitheatre H

Session's Chairs:
Prof. Francesco Mutti, University of Amsterdam, The Netherlands
Dr. Olivier Sandre, Institut Polytechnique de Bordeaux, France
Dr. Jean-Olivier Durand, Institut Charles Gerhardt Montpellier, France
Dr. Winnie Edith Svendsen, Technical University of Denmark, Denmark

08:30 - 09:00	From antibodies to Metal Organic Frameworks: a Full Set of Enveloppes for metal cofactors in order to build up new artificial metalloenzymes **J-P.Mahy**, W. Ghattas, F. Avenier and R. Ricoux	**Prof. Jean-Pierre Mahy**, Paris-Sud University, **France**
09:00 - 09:30	Expanding and exploring natural sequence space – from protein engineering to chemo-enzymatic cascade reactions C. Mügge, Á. Gomez-Baraibar and **R. Kourist**	**Prof. Robert Kourist,** Ruhr University Bochum, Germany/ Graz University of Techology, **Austria**
09:30 - 10:00	Design and Evolution of New Biocatalysts for Organic Synthesis **N. J. Turner**	**Prof. Nicholas Turner,** The University of Manchester**, UK**
10:00 - 10:30	Practical biocatalytic solutions for the design of chemoenzymatic and multienzymatic concurrent processes **V. Gotor-Fernández**	**Prof. Vicente Gotor-Fernandez**, University of Oviedo, **Spain**
10:30 - 11:00	**Coffee Break / Posters Session II**	**Coffee Break Area**
11:00 - 11:30	Nanomedicines for the treatment of cancer and neurological diseases **P. Couvreur**	**Prof. Patrick Couvreur,** UMR CNRS 8612, **France**
11:30 - 12:00	Nanotechnology against viral deseases **F. Stellacci**	**Prof. Francesco Stellacci,** Ecole Polytechnique de Lausanne, **Swizterland**
12:00 - 12:45	Applications of Artificial Intelligence in Biotech and Nanotech research **M. Cristovao**	**Dr. Michele Cristovao**, Springer Nature, **Germany**
12:30 - 14:00	**Lunch Break**	**Restaurant (Rue Basse)**

June 28, 2018, 13:45 - 13:55
Conference Group Photo
At the conference registration desk (located at Rue Haute)
All conference participants are requested to be present for the Conference Group Photo

June 28, 2018
Session II.A: Nanotechnology for life science

Conference Room 109/110

Session's Chairs:
Dr. Stéphane Mornet, Bordeaux University, France
Prof. Rui Silva, University of Aveiro, Portugal
Prof. Giulio Caracciolo, Sapienza University of Rome, Italy

14:00 - 14:30	Brain Structure and Function Combine to Create the Characteristics of a Bio-Metamaterial **S.D.Morgera**	**Prof. Salvatore Domenic Morgera**, University of South Florida, **USA**
14:30 - 15:00	Nanostructures for biological and environmental applications **W.E. Svendsen**	**Dr. Winnie Edith Svendsen,** Technical University of Denmark, **Denmark**

15:00 - 15:30	Clickable' Recombinant Spider Silk and its Healthcare Applications **N.R. Thomas**, D. Harvey, R. Earlam, P. Bardelang, S.L. Goodacre and A. Cockayne	**Prof Neil R. Thomas,** University of Nottingham, **UK**
15:30 - 16:00	Surface nanoengineering of intravenously administered inorganic nanoparticles L. Adumeau, C. Vecco-Garda, G. Clofent-Sanchez, C. Genevois, F. Couillaud and **S.Mornet**	**Dr. Stéphane Mornet,** ICMCB (UMR 5026 CNRS - Bordeaux University - Bordeaux INP), **France**
16:00 - 16:30	**Coffee Break / Posters Session II**	**Coffee Break Area**
16:30 - 16:45	Vitamin A palmitate-loaded NLC for cosmetic application **S. AlZahabi** and A.R. Ramadan	**Ms. Sham AlZahabi,** American Uni. Cairo, **Egypt**

June 28, 2018

Session II.B: Nanomedecine- Bioimaging

Conference Room 111/112

Session's Chairs:
Dr. Valeria Grazú, University de Zaragoza, Spain
Prof. Wolfgang Ensinger, Technische Universitaet Darmstadt, Germany
Prof. Neil R. Thomas, University of Nottingham, UK

14:00 - 14:30	The iNAPO project: Biomimetic ion conducting polymer nanopores for bio-molecular and chemical sensing **W. Ensinger**, M. Biesalski, G. Buntkowsky, K. Hamacher, B. Laube, H. F. Schlaak, G. Thiel, Ch. Trautmann, N. van der Vegt and M. Vogel	**Prof. Wolfgang Ensinger**, Technische Universitaet Darmstadt, **Germany**
14:30 - 14:45	Confocal Laser Endomicroscopy Guided Photothermal/Photodynamic Therapy of Pancreatic Cancer **H. Li**, K. Yang and Y. Cheng	**Dr. Hui Li**, Shanghai Jiaotong University, **China**
14:45 - 15:00	Dual Metallofluorescent Nanoparticles for live cells assays **A. Delgado-Gonzalez**, E. Garcia-Fernandez, T. Valero, M.V. Cano-Cortes, M.J. Ruedas-Rama, A. Unciti-Broceta, A. Orte, R.M. Sanchez-Martin and J.J. Diaz-Mochon	**Mr. Antonio Delgado-Gonzalez**, University of Granada, **Spain**
15:00 - 15:15	Design of Polyelectrolyte Microcapsules Encoded with Excitonic Nanoparticles and Prospects of their Applications as Novel Bio-imaging and Theranostic Tools **G. Nifontova**, M. Zvaigzne, M. Baryshnikova, E. Korostylev, F. Ramos-Gomes, F. Alves, I. Nabiev and A. Sukhanova	**Dr. Galina Nifontova**, National Research Nuclear University MEPhI-Moscow, **Russia**
15:15 - 15:30	Development of new theranostic platforms based on carbon dots **M. Claudel**, J. Fan, F. Pons and L. Lebeau.	**Mr. Mickaël Claudel**, University of Strasbourg, **France**
15:30 - 15:45	Reduction of methemoglobin to oxyhemoglobin under influence of nanoparticles of perfluorocarbon emulsion and cytoflavin. **E.A. Manchenko**, E.K. Kozlova, A.M. Chernysh and V.A. Sergunova	**Mrs. Ekaterina Manchenko** V.A.Negovsky Scientific Research Institute of General Reanimatology-Moscow, **Russia**
15:45 - 16:00	Nanostructure as biomarkers for the diagnosis of donor blood during long-term storage. **V.A. Sergunova,** E.K. Kozlova, A.M. Chernysh and E.A. Manchenko	**Mrs. Victoria Sergunova**, V.A.Negovsky Scientific Research Institute of General Reanimatology-Moscow, **Russia**
16:00 - 16:30	**Coffee Break / Posters Session II**	**Coffee Break Area**
16:30 - 16:45	Novel Approach to Flow Label-Free Multiplex Biosensing via Photonic Crystal Surface Wave Detection Technique **I.O. Petrova**, V.N. Konopsky, Nabiev and A. Sukhanova	**Dr. Irina Petrova**, National Research Nuclear University MEPhI-Moscow, **Russia**
16:45 - 17:00	Feasibility of magnetic nanoparticles encapsulated inside carbon nanotubes for hyperthermia **R. Ghunaim**, S. Hampel, R. Klingeler and B. Büchner	**Ms. Rasha Ghunaim**, Leibniz Institute for Solid State and Material Research Dresden, **Germany**

17:00 - 17:15	Magnetic Nanozyme-Linked Immunosorbent Assay for Ultrasensitive Influenza A Virus Detection S. Oh, J. Kim, V.Tan Tran, D. Kyu Lee and **J. Lee**	**Prof. Jaebeom Lee**, Pusan National University, **Rep. of Korea**
17:15 - 17:30	Targeting and Killing of Leukemic Cells with Magnetic Nanowires **N. Alsharif**, J. Merzaban, T. Ravasi and J. Kosel	**Ms. Nouf Alsharif**, KAUST, **Saudi Arabia**
17:30 - 17:45	Bare Magnetic Nanoparticles for Protein Recognition **S. Schwaminger**, S. Blank-Shim, P. Anand, M. Borkowska-Panek, K. Fink, P. Fraga-García, W. Wenzel and S. Berensmeier	**Mr. Sebastian Schwaminger**, Technical Univ. of Munich, **Germany**

June 28, 2018

Focused Session on Nanotechnology for drug and gene delivery

Conference Room 561

Session's Chairs:

Dr. Olivier Sandre, Institut Polytechnique de Bordeaux, LCPO, France

Dr. Sonia Trigueros, University of Oxford, UK

14:00 - 14:30	Magnetic Iron Oxide Nanoparticles Grafted by a Thermosensitive Peptide Brush: Uptake by Tumor Cells and Cytotoxicity by Magnetic Hyperthermia **O. Sandre**	**Dr. Olivier Sandre,** Institut Polytechnique de Bordeaux – LCPO, **France**
14:30 - 15:00	Nano-Delivery Overcoming the major challenges in Drug and Gene delivey **S. Trigueros**	**Dr. Sonia Trigueros,** University of Oxford, **UK**
15:00 - 15:30	Mesoporous silica, periodic mesoporous organosilica, and mesoporous silicon nanoparticles for drug delivery and two-photon Photodynamic Therapy **J-O. Durand**	**Dr. Jean-Olivier Durand** Institut Charles Gerhardt Montpellier, **France**
15:30 - 16:00	Nanotherapeutics for Targeted Elastic Matrix Regenerative Repair in Vascular Disorders A. Camardo, S.Carney, N. Sharma and **A.Ramamurthi**	**Dr. Anand Ramamurthi**, Cleveland Clinic, **USA**
16:00 - 16:30	**Coffee Break / Posters Session II**	**Coffee Break Area**
16:30 - 16:45	Challenges on the development of nanotherapeutics: biophysical studies to guide formulation development E.Fernandes, T.B. Soares, H.Gonçalves and **M. Lúcio**	**Dr. Marlene Lúcio** University of Minho, **Portugal**
16:45 - 17:00	Biophysical characterization based on biomimetic nanosystems/drug interactions: a new strategy for a rational drug design process **E. Fernandes**, S. Bernstorff and M. Lúcio	**Mrs. Eduarda Fernandes,** University of Minho, **Portugal**
17:00 - 17:15	Diclofenac interaction with lipid nanosystems as membrane models: a bio-physical assessment of in vitro profiling **T.B Soares**, E. Fernandes, S. Bernstorff and M. Lúcio	**Ms. Telma Bezerra Soares**, University of Minho, **Portugal**
17:15 - 17:30	Novel oxide nanomaterials for drug delivery through the blood-brain-barrier **W. Lipinski,** M.M. Godlewski, J. Kaszewski, Z. Gajewski and M. Godlewski	**Mr. Waldemar Lipinski**, Faculty of Veterinary Medicine- Warsaw, **Poland**
17:30 - 17:45	SiO2 nanoparticles as a vehicle for delivery of nucleoside triphos-phate analogues into cells **S. Vasilyeva**, A. Shtil, I. Grin and D. Stetsenko	**Dr. Svetlana Vasilyeva**, Siberian Branch of the Russian Academy of Sciences, **Russia**
17:45 - 18:00	Synthesis of PHA nanoparticles for drug delivery: optimizing the size distribution via the effect of the surfactant **V. Amstutz**, N. Hanik and M. Zinn	**Dr. Véronique Amstutz**, University of Applied Sciences and Arts Western Switzerland, **Switzerland**
18:00 - 18:15	A report on synthesis of NIR light responsive nanoparticles-in-microparticles by a double emulsion method: Photothermal and drug delivery use in future **M. Dhanka**, D. S Chauhan and R. Srivastava	**Mr. Mukesh Dhanka**, Indian Institute of Technology Bombay, **India**

June 28, 2018

Focused session on Nanomagnetism - Part I

Conference Room 461

Session's Chairs:

Dr. Claude Fermon, Institut Rayonnement-Matière de Saclay (Iramis), CEA, France

Dr. Vincent Cros, Paris-Saclay University, France

09:00 - 09:30	Spin electronics based sensors for nanoparticle detection. **C. Fermon**, M. Giraud, F.D. Delapierre, G. Jasmin-Lebras, M. Roig, L. Fermon, J. Moulin, A. Solignac and M.Pannetier-Lecoeur.	**Dr. Claude Fermon**, Institut Rayonnement-Matière de Saclay (Iramis), **France**
09:30 - 10:00	The magnetic skyrmions: newcomers in spintronics **V. Cros**, W. Legrand, D. Maccarriello, J. Y. Chauleau, K. Garcia, S. Collin, K. Bouzehouane, N. Jaouen, N. Reyren and A. Fert	**Dr. Vincent Cros**, Paris-Saclay University, **France**
10:00 - 10:30	d-zero Magnetism in Nanostructures **J. M. D. Coey**	**Prof Michael Coey**, Trinity College Dublin, **Ireland**
10:30 - 11:00	**Coffee Break / Posters Session II**	**Coffee Break Area**
11:00 - 11:30	Coherence in electron spin chain: A potentional new kind of qubits C-E. Dutoit, J. Van Tol, M. Dressel, B. Barbara, A. Stepanov and **S. Bertaina**	**Dr. Sylvain Bertaina**, IM2NP - UMR 7334 CNRS, Faculté des Sciences et Techniques-Marseille, **France**
11:30 - 12:00	Magnon-based computing on the nano-scale **T. Brächer**	**Dr. Thomas Brächer**, Technical University Kaiserslautern, **Germany**
12:00 - 12:30	Ultrafast Lorentz Microscopy: A tool to study laser- and current-driven magnetization dynamics **M. Möller**, N.Rubian da Silva, J.H. Gaida, A.Feist, S. Schäfer, and C.Ropers	**Mr. Marcel Möller,** Göttingen University**, Germany**
12:30 - 14:00	**Lunch Break**	**Restaurant (Rue Basse)**

Workshop: SIESTA-PRO: Professional Software Ready for Industry

Conference Room 461

Session's Chairs:

Dr Monica Garcia Mota, Simune Atomistic Simulations, Spain

Prof. Pablo Ordejón, ICN2 (CSIC and BIST), Spain

14:00 - 15:30	**M. García-Mota and P. Ordejon** The workshop covers the following topics: - Introduction to SIMUNE and SIESTA - SIESTA-PRO: SIESTA code ready for the industry - SIESTA code: main technical features - hints to perform and accurate and well-converged siesta calculation - input file. Principal siesta input parameter - pseudopotential - basis set. The delta-test - analyzing the results. Post-processing siesta output - round table discussion and closing remarks	**Dr Monica Garcia Mota**, Simune Atomistic Simulations, **Spain** **Prof. Pablo Ordejón,** ICN2 (CSIC and BIST), **Spain**

Focused session on Nanomagnetism - Part II

Conference Room 461

Session's Chairs:
Dr. Claude Fermon, Institut Rayonnement-Matière de Saclay (Iramis), France
Dr. Vincent Cros, Paris-Saclay University, France

16:30 - 17:00	Magnetic Oxides-based Hetero-Nanostructured Ceramics: From Nanomaterial Engineering to Exchange-bias Coupling **S. Ammar**	**Prof. Souad Ammar**, Paris Diderot University, **France**
17:00 - 17:15	Strain-mediated all-magnetoelectric memory cell V.Preobrazhensky, L.Krutyansky, N.Tiercelin, **Y. Dusch**, P.Pernod and S.Giordano	**Dr. Yannick Dusch,** University of Lille, **France**
17:15 - 17:30	Probing Nanoscale Magnetic Properties Using a Pt-based Hall Device T.K. Hang Hang, M. Ribeiro, J. Hong Park and **T. Hee Kim**	**Prof. Tae Hee Kim**, Ewha Womans University, **Rep. of Korea**
17:30 - 17:45	Best of Two Worlds: Combination of Magnetic and Semiconducting Properties in (Ga,Mn)(Bi,As) Nanostructured Thin Films **K. Levchenko**, T. Andrearczyk, J. Sadowski, E. Lusakowska, J.Z. Domagala, M. Trzyna, R. Jakiela, I. Radelytskyi, J. Wrobel, T. Figielski and T. Wosinski	**Mrs. Khrystyna Levchenko**, Institute of Physics Polish Academy of Sciences, **Poland**

June 28, 2018

NanoMatEn 2018 - Session II.C: Nanomaterials for Energy / Nanoelectronics

Conference Room 508

Session's Chairs:
Prof Keon Jae Lee, KAIST, Rep. of Korea

09:00 - 09:30	Layered and 2D materials: electronic properties and structural instabilities from first principles **P. Ordejón**, B. Guster, M. Pruneda, R. Robles and E. Canadell	**Prof. Pablo Ordejón**, ICN2 (CSIC and BIST), **Spain**
09:30 - 10:00	Development of nanogenerators for mechanical energy harvesting and self-powered electronics X. Yang, L. Wang and **W.A. Daoud**	**Prof. Walid Daoud,** City University of Hong Kong, **Hong Kong**
10:00 - 10:30	Self-powered flexible electronic systems **K. Jae Lee**	**Prof Keon Jae Lee**, KAIST, **Rep. of Korea**
10:30 - 11:00	**Coffee Break / Posters Session II**	**Coffee Break Area**
11:00 - 11:30	Circularly Polarized Luminescent Polymer Film Fabricated with Chiral Nano-fibrils **H. Ihara**, M. Takafuji, Y. Kuwahara, K. Yoshida, H. Oishi, Y. Okazaki and R. Oda	**Prof. Hirotaka Ihara**, Kumamoto University, **Japan**
11:30 - 12:00	Nanomaterials for High Temperature Photonics P. Dyachenko, S. Lang, G. Shang, Q.Y. Nguyen, M. Chirumamilla, K. Knopp, G. Vaidhyanathan, S. Molesky, H. Renner, A. Yu Petrov, Z. Jacob, M. Störmer, T. Krekeler , M. Ritter, G. Schneider, and **M. Eich**	**Prof. Manfred Eich**, Hamburg University of Technology, **Germany**
12:00 - 12:30	Metal Selenides as Efficient Cathodes for Dye-Sensitized Solar Cells **Z-S. Wang**	**Prof. Zhong-Sheng Wang**, Fudan University, **China**
12:30 - 14:00	**Lunch Break**	**Restaurant (Rue Basse)**

Session's Chairs:
Prof Keon Jae Lee, KAIST, Rep. of Korea
Dr. Olivier Schneegans, Paris Saclay University, Centrale Supélec, France
Prof. Walid Daoud, City University of Hong Kong, Hong Kong

14:00 - 14:15	Efficient and Stable Flexible Perovskite Solar Cells with Nano-Engineered Solution-Processed NiO Hole-Transporting Layers C.-H. Hou, J.-J. Shyue, W.-F. Su and **F.-Y. Tsai**	**Prof. Feng-Yu Tsai**, National Taiwan University, **Taiwan**

14:15 - 14:30	Back-Contact Perovskite Solar Cells **U. Bach** and X. Lin	**Prof. Udo Bach**, Monash University, **Australia**
14;30 - 14:45	Control of Structural Ordering of InGaAs/AlGaAs Quantum Dots in MBE and Application to Intermediate Band Photovoltaics **Y. Okada**, A. Matsuoka, Y. Shoji and R. Tamaki	**Prof. Yoshitaka Okada**, University of Tokyo, **Japan**
14:45 - 15:00	Photochemical deposition of ZnS buffer layers for Cu(In,Ga)Se2 thin films solar cells via reusable solutions **S. Gallanti**, N. Loones, M. Bouttemy, A. Etcheberry, D. Lincot and N. Naghavi	**Dr. Serena Gallanti**, ECE Paris Engineering school, **France**
15:00 - 15:15	Optical up-conversion erbium-doped nanoparticles as coaters for solar cells efficiency improvement A. Hajjiah and **N. Shehata**	**Dr. Nader Shehata**, Alexandria University, **Egypt**
15:15 - 15:30	Ionic liquids confined in carbon nanotubes membranes: a route for a better electrolyte? **F. Ferdeghini**, Q. Berrod, P. Judeinstein and J.M. Zanotti	**Dr. Filippo Ferdeghini**, ECE-Paris Engineering School, **France**
14:30 - 14:45	Design of Different Polymer Electrolytes for Lithium Battery Application **A. Bozkurt**	**Prof. Ayhan Bozkurt**, Dammam University, **Saudi Arabia**
15:45 - 16:00	Size-dependent charge storage of graphene flakes **K F. Chong** and G. A. M. Ali	**Dr. Kwok Feng Chong**, Pahang Malaysia University, **Malaysia**
16:00 - 16:30	**Coffee Break / Posters Session II**	**Coffee Break Area**
Session's Chairs: **Dr. Olivier Schneegans, Paris Saclay University, CentraleSupélec, France** **Prof. Walid Daoud, City University of Hong Kong, Hong Kong**		
16:30 - 16:45	On the mechanism of dehydrogenation of MgH2 **S.S.V. Tatiparti** and S. Shriniwasan	**Prof. Sankara Sarma Tatipari**, Indian Institute of Technology Bombay, **India**
16:45 - 17:00	Tunnel Barrier Optimization for Room Temperature Operation of Single Electron Transistor R. Shah and **R. Dhavse**	**Dr. Rasika Dhavse**, SVNIT Surat, **India**
17:00 - 17:15	Storage Memory and Selector Functions in Silicon nitride Memristor **S.Kim**, M-H. Kim, T-H. Kim, S. Bang, D. Keun Lee,2 Y-J. Choi and B-G. Park	**Prof. Sungjun Kim**, Chungbuk National University, **Rep. of Korea**
17:15 - 17:30	Reduced Thermal Conductivity of Nanotwin Random Layer Structures: Effect of twin boundary for phonon localization **N. P. Samaraweera**, K. L. Chan and K. Mithraratne	**Mr. Nalaka Samaraweera**, The University of Auckland, **New Zealand**
17:30 - 17:45	Piezo-phototronic effect in III-Nitrides semiconductors and applications **W. Hu**	**Prof. Weiguo Hu,** Beijing Institute of Nanoenergy and Nanosystems- Chinese Academy of Science, **China**
17:45 - 18:00	Piezopotential Modulated Graphene Semiconductor Devices **Q. Sun**, Z.L.Wang and J. H. Cho	**Prof. Qijun Sun**, Beijing Institute of Nanoenergy and Nanosystems- Chinese Academy of Sciences, **China**
18:00 - 18:15	Environmental Impact Assessment of Triboelectric Nanogenerator Materials for Energy Harvesting M. A. Parvez Mahmud, **N. Huda**, S.H. Farjana and C. Lang	**Dr. Nazmul Huda**, Macquarie University, **Australia**
18:15-18:30	Piezophototronic Based Sensors and Applications **J. Zhai**	**Prof. Junyi Zhai,** Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Science, **China**

June 28, 2018

NanoMetrology France 2018 - Focused Session: Metrology of nanoparticles (NP) in Complex Media

Conference Room 558

Session's Chairs:

Dr. Carine Chivas-Joly, National Metrology and Testing Laboratory (LNE), France

09:15 - 09:30	**Opening session** - Introduction and presentation of the activities of the nanoMetrology Club by Presidents **Brice Gautier** and **Georges Favre** - New items "Metrological Characterization of Nanomaterials in Complex Media" by **Doru Constantin**, **Etienne Dague** and **Carine Chivas-Joly**	
09:30 - 10:00	Detection and quantification of engineered and natural nanoparticles in small sub-watersheds of Seine River **J. Wang**, E .Alasonati, P. Fisicaro and M. Benedetti	**Ms Jialan Wang**, National Metrology and Testing Laboratory (LNE), **France**
10:00 - 10:30	Following nanoparticles in complex turbid media **A.Mikhailovskaia**, J. Crassous, A. Salonen and D. Langevin	**Dr. Alesya Mikhailovskaia**, L'École supérieure de physique et de chimie industrielles, **France**
10:30 - 11:00	**Coffee Break / Posters Session II**	
11:00 - 11:30	Investigations of the hazard assessment of selected nano-objects used as additives for EVA-matrix nanocomposites **C. Chivas-Joly**, J. Pourchez, G. Sarry, L. Leclerc, C. Longuet, S. Delcour and J-M. Lopez-Cuesta	**Dr Carine Chivas-Joly**, National Metrology and Testing Laboratory (LNE), **France**
11:30 - 12:00	Designing plasmonic hard shells to control the self-assembly of gold nanorods into supercrystals **C. Hamon,** C.Goldmann and D. Constantin	**Dr. Cyrille Hamon**, Paris Sud University, **France**
12:00 - 12:30	Metrology of Nanoparticles with Small Angles X-Ray Scattering (SAXS) : from simple cases to nanoparticles in complex media **O. Taché**, V. Geersten, E. Barruet, O. Spalla and A. Thill	**Mr. Olivier Taché**,Univ Paris Saclay / LIONS NIMBE CEA, **France**
12:30 - 13:00	Infrared nano-imaging for intra-cellular cancer research and analysis of drug delivery **W. S. Hart**, A. Beckley, J. R. Brandt, S. Sundriyal, A. Zubiaurre, H. Amrania, M. J. Fuchter, E. O. Aboagye and C. C. Phillips	**Mr. William Hart**, Imperial College London, **UK**
12:30 - 14:00	**Lunch Break**	**Restaurant (Rue Basse)**
14:00 - 14:30	Probing lipid membrane nano-mechanics F. Bories, **D. Constantin**, P. Galatola and J.-B. Fournier	**Dr. Doru Constantin**, LPS, CNRS, Univ. Paris-Sud, Paris Saclay Univ., **France**
14:30 - 15:00	Nanoparticle concentration measurement is essential and, fortunately, quite easy to achieve **C. Roesch**	**Dr. Camille Roesch**, Izon Science Europe Ltd, **France**
15:00 - 15:30	Physicochemical characterization of nanomedicines and metrology: Evaluation of size and zeta potential **F. Varenne**, J. Botton, J.-B. Coty and C. Vauthier	**Dr. Fanny Varenne**, University Clermont Auvergne, **France**
15:30 - 16:00	Assessing the interactions between a single dendrimer and (bio)surfaces using atomic force microscopy **A. Beaussart**, C. Caillet, I. Bihannic and J.F.L. Duval	**Dr. Audrey Beaussart**, CNRS, University of Lorraine, **France**
16:00 - 16:30	**Coffee Break / Posters Session II**	**Coffee Break Area**

June 29, 2018
NanoMatEn2018 - Session III.A:
Nanotechnology for Environmental Application / Water Treatment

Conference Room 508

Session's Chairs:
Prof. Marco Stoller, Sapienza University, Italy
Prof. Marie-Odile Simonnot, University of Lorraine, France

08:30 - 09:00	Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale **J. Arbiol**	**Prof. Jordi Arbiol**, ICREA and ICN2 (CSIC and BIST), **Spain**
09:00 - 09:30	TreAting contamination through NanoremedIAtion: the TANIA project **M.O. Simonnot**, N. Enjelvin, C. Vuidel, C. Chêne and J.L. Morel	**Prof. Marie-Odile Simonnot**, University of Lorraine, **France**
09:30 - 09:45	Physicochemical characterization of nanoparticles-containing spray coating generated by atomization process O.Fichera, **J. Mejia**, J. Laloy , L. Alpan , S. Lucas and J-M. Dogné	**Dr. Jorge Mejia**, University of Namur, **Belgium**
09:45-10:00	Bridging homogeneous and heterogeneous catalysis through MOF support platforms and other efforts to obtain new class of highly active recyclable catalysts. **S.T. Madrahimov**	**Dr. Sherzod T. Madrahimov**, Texas A&M University Qatar, **Qatar**
10:00 - 10:30	**Coffee Break**	**Coffee Break Area**
10:30 - 10:45	Carbide core-shell nanostructures for oxygen reduction reaction **Z. Zhang**, A. Sadeghi, N. Brodusch, R. Gauvin, S. Ye, J. Gostick, J. E Barralet and G. Merle	**Mr. Zishuai Zhang,** McGill University, **Canada**
10:45 - 11:15	Case studies of different wastewater treatment processes by means of nanotechnologies **M. Stoller**	**Prof. Marco Stoller**, Sapienza University, **Italy**
11:15 - 11:45	Nanotubular and nanoporous titanium dioxide films for photocatalytic applications B.E. Sanabria, A. Strini, L. Schiavi, **M.V. Diamanti** and MP. Pedeferri	**Prof. Maria Vittoria Diamanti**, Milano Poltechnic Institute, **Italy**
11:45 - 12:00	Nanocomposites for the Removal of Radioactive Cesium from Water and their Applications **C. Roh**	**Prof. Changhyun Roh,** Korea Atomic Energy Research Institute (KAERI), **Rep. of Korea**
12:00 - 12:15	Study of modified electrodes with silver and gold nanoparticles to determine heavy metals in polluted waters **K. Torres-Rivero,** A. Espriu-Gascon, J. Bastos-Arrieta, L. Torralba, M. Martínez and A. Florido	**Mrs. Karina Torres-Rivero**, Polytechnic University of Catalonia, **Spain**
12:15 - 12:30	Zn-ferrite nanoparticles, potential photocatalysts for water depollution: Why do we still need detailled structural characterizations **A. Jezzini**, T. Hamieh, J. Toufaily, A. Davidson, C. Jolivalt, L. Valentin, M. Selmane, G. Wallez, J.M. Greneche and R. Cole	**Ms. Aya Jezzini**, Sorbonne University, **France**
12:30-12:45	Synthesis of Polysulfone/Carbon Nanotubes-Polyamide Thin film Nano-composite Membranes for Forward Osmosis Applications **A.O. Rashed**, A.M.K. Esawi and A.R. Ramadan	**Mr. Ahmed O. Rashed**, The American University in Cairo, **Egypt**

June 29, 2018

NanoMatEn 2018 - Session III.B: Nanomaterials for Clean and Sustainable Technology

Conference Room 561

Session's Chairs:

Dr. Michael Holzinger, University Grenoble Alpes, France

09:00 - 09:30	Porous carbon nanostructures for biological energy conversion and the utility of glucose biofuel cells. **M. Holzinger**	**Dr. Michael Holzinger**, CNRS-University Grenoble Alpes, Departement of Molecular Chemistry, **France**
09:30 - 09:45	Ultralow lattice thermal conductivity and high thermoelectric performance of polycrystalline SnSe **I. Chung**	**Prof. In Chung**, Seoul National University, **Rep. of Korea**
09:45 - 10:00	Effect of the electrode polarization on the water properties in the system with and without glow discharge electrolysis **S. Sato** and M. Ohuchi	**Dr. Shuichi Sato**, Tokyo Denki University, **Japan**
10:00 - 10:30	**Coffee Break**	**Coffee Break Area**
10:30 - 10:45	Glucose Effect on Controlling TiO2 Physicochemical Properties for CO2 Reduction by UV/Vis Light Irradiation **N. U. M. Nor** and N. A. S. Amin	**Prof. Nor Aishah Saidina Amin**, University of Technology of Malaysia, **Malaysia**
10:45 - 11:00	Various Nanocatalysts for Catalytic Furfural Hydrogenation **K. An**	**Dr. Kwangjin An**, Ulsan National Institute of Science and Technology, **Rep. of Korea**
11:00 - 11:15	LaMnO3 perovskite/reduced graphene oxide nanocomposites for supercapacitor electrode application **Z. A. Elsiddig**, W. Zhang and J. Chen	**Mr. Zuhair A. Elsiddig**, Jiangsu Key Laboratory for Advanced Metallic Materials-Southeast University, **China**
11:15 - 11:30	Scattering Parameters and Dielectric Properties of Nano Barium Ferrite Microwave Absorber Composite **H. Al-Mattarneh** and M. Dahim	**Prof. Hashem Al-Mattarneh**, King Khalid University, **Saudi Arabia**
11:30 - 11:45	Surface Oxygen Vacancy Assisted Visible Light-induced Photocatalytic Dye Degradation and Photocapacitive Performance of CeO2-Graphene Nanostructures **M.E.Khan**, M.M. Khan and M.H.Cho	**Mr. Mohammad E. Khan**, Yeungnam University, **Rep. of Korea**
11:45 - 12:00	Biowaste-derived carbon functionalized with polyaniline: Recy-cling to multifunctional applications **S. Goswami**, S. Nandy, E. Fortunato and R. Martins	**Dr. Sumita Goswami,** Nova da Lisboa University, **Portugal**

June 29, 2018

Session III.C: NanoMedecine / Nanosafety

Conference Room 558

Session's Chairs:

Dr. Jean-Olivier Durand, Institut Charles Gerhardt Montpellier, France

Dr. Sonia Trigueros, University of Oxford, UK

09:00 - 09:30	Short, long term fate and biodegradation of IONPs in vivo **V. Grazú** and J. M. de la Fuente	**Dr. Valeria Grazú,** University de Zaragoza and CIBER-BBN, **Spain**
09:30 - 09:45	Nanoparticle delivery of drugs for Tuberculosis **I.L. Batalha**, A. Bernut, R.A. Floto and M.E. Welland	**Dr. Iris Batalha**, University of Cambridge, **UK**
09:45 - 10:00	Synthesis of Gold Nanovehicles for Con-trolled Drug Delivery Applications **R. Lopes Rodrigues**, F.Xie, A. Porter and M. Ryan	**Ms. Rosalia L. Rodrigues**, Imperial College London, **UK**
10:00 - 10:30	**Coffee Break**	**Coffee Break Area**

10:30- 11:00	Nanopattern improves chondrogenesis for cartilage regeneration. I.Casanellas, A. Lagunas, I. Tsintzou, Y. Vida, D. Collado, E. Pérez-Inestrosa, C. Rodríguez Pereira, J. Magalhaes and **J.Samitier**	**Prof. Josep Samitier Martí**, Institute for Bioengineering of Catalonia (IBEC), **Spain**
11:00 - 11:15	Characterization of the interaction of graphene oxide with the mammalian sperm membrane **J.Simões**, M.Ramal Sanchez, R. Zappacosta M. Ciulla, A.Di Stefano, A. Fontana, P. Lanuti, E.Ercolino, M. Marchisio, G. Capacchietti, L. Valbonetti, N. Bernabò and B. Barboni	**Ms Juliana Simões**, University of Teramo, **Italy**
11:15 - 11:30	A Potential Approach to Assess and Control the Potential Risks Related to Nanomaterials **C. Schimpel**, S. Resch and A. Falk	**Ms. Christa Schimpel**, BioNanoNet, **Austria**
11:30 - 11:45	Tuball ™ Single wall Carbon Nanotubes: Health, Safety & Environmental issues **G. Van Kerckhove**	**Mr. Gunther Van Kerckhove**, OCSiAl Europe Sarl, **Luxembourg**
11:45 - 12:00	Review of human health risk assessment models considering their input requirements and applicability suring nanomaterial product development results from the EU H2020 'CALIBRATE' project **T. Oosterwijk**, R. Franken, M. Heringa, I. Rodriguez, A. Saämanen, T. Kanerva, M. Dal Maso, M. Poikkimaki, K.A. Jenssen, C. de Jong-Rubingh, R. Stierum and W. Fransman	**Mr. Thies Oosterwijk**,TNO, Risk Assessment of Products In Development, **The Netherlands**

June 29, 2018

Session III.D: Nanomaterials for food applications

Conference Room 461

Session's Chairs:
Dr Clara Silvestre, ICTP/CNR, Naples, Italy
Dr. Giovanna G. Buonocore, ICTP/CNR, Naples, Italy

09:00 - 09:30	Nanotechnology in the food packaging sector: recent applications and future trends **A.Sanches Silva**	**Dr. Ana Sanches Silva**, National Institute of Agrarian and Veterinary Research, **Portugal**
09:30 - 10:00	Active biopolymer film or coating for food packaging application: structure-properties relationship and shelf life extension **E. Torrieri**	**Prof. Elena Torrieri**, University of Naples Federico II, **Italy**
10:00 - 10:30	**Coffee Break**	**Coffee Break Area**
10:30 - 10:45	PAA.PVA-PAMAM bio-nanocomposite films incorporating thymol for food packaging **G. Amariei**, K. Boltes, I. Iriepa, I. Moraleda, P. Letón and R. Rosal	**Ms. Georgiana Amariei** University of Alcalá, **Spain**
10:45 - 11:00	A novel antibacterial strategy based on oxide nanoparticles for medical and food-related polygraphy **J. Cymerys-Bulenda**, R. Pietuszka, A. Słońska-Zielonka, S. Gierałtowska, B.S. Witkowski, Z. Gajewski, M. M. Godlewski and M. Godlewski	**Dr. Joanna Cymerys-Bulenda**, Warsaw University of Life Sciences – SGGW, **Poland**

Posters Session I: June 27, 2018
Nanomaterials synthesis, characterization/Nanometrology and properties

Exhibition and Posters Hall

N.	Title	Author/Affiliation/Country
1	Preparation and Characterization of AlOOH-based Nanocrystalline Film on Aluminum Alloy **A. Serizawa**, K. Watanabe, T. Oda and T. Ishizaki	**Prof. Ai Serizawa**, Shibaura Institute of Technology, **Japan**
2	Dynamic behavior of water droplet on hydrophobic surfaces covered with two organic silane molecules with alkyl chain **T. Ishizaki**, S.Hisada and A. Takada	**Prof. Takahiro Ishizaki**, Shibaura Institute of Technology, **Japan**
3	Quantitative analysis of point and lattice defects in Si0.6Ge0.4 alloys with thickness variation using Terahertz Pump probe measurement **JH. Kim**, . KS. Jeong and MH. Cho	**Mr. Jong Hoon Kim**, Yonsei University, **Rep.of Korea**
4	A Combination of PVD and PECVD Techniques for Deposition of CrNx Coatings and Metal Oxide Top-Coats on Polymers M. A. Neto, M. S. Rodrigues, J. Borges, F. Vaz, M. Amaral, A. Ferreira, L. Godinho, M. A. Valente, L. C. Costa, M. P. F. Graça, A.V. Girão, F. J. Oliveira and **R.F. Silva**	**Prof. Rui Silva**, University of Aveiro, **Portugal**
5	Hydrophobic/oleophobic coating of polydimethylsiloxane from modified silica nanoparticles **C. Sanfona**, G. Borja, G. Romero, L. Bautista, D. Amantia, L. Aubouy, N. Ferrer, J. Rius and A. Canet	**Ms. Carolina Sanfona**, Leitat Technological Center, **Spain**
6	The corrosion studies of Ni/Al2O3 and Ni/Al2O3/PTFE composite coatings in anti-icing environments B. Kucharska and **J. R. Sobiecki**	**Prof. Jerzy Sobiecki**, Warsaw University of Technology, **Poland**
7	Adsorption and Penetration of Nano-dispersed Super Hydrophobic Colorants into High Molecular Weight Polyethylene **T. Kim**, E. Jeong, J. Bae, J.Lee, J. Park and J. Lee	**Prof. Taekyeong Kim**, Kyungpook National University, **Rep.of Korea**
8	Enhanced Barrier Property of Poly(vinyl chloride) Film by Nano-confinement effects of graphene oxide nanoribbons **H-J. Jin**	**Prof. Hyoung-Joon Jin**, Inha University, **Rep.of Korea**
9	Fabrication of polyaniline-graphene/polyvinyl alcohol nanocomposites for flexible gas sensor **J.Bhadra**, A. Popelka, A. Abdulkareem and N. Al-Thani	**Dr. Jolly Bhadra,** Qatar University, **Qatar**
10	Natural Polymer Gate Dielectrics for Low-voltage Organic Thin Film Transistors **S. Park** and T. Kyu An	**Ms.Sejin Park**, Korea National University of Transportation, **Rep. of Korea**
11	Gas molecule sensing of van der Waals tunnel field effect transistors **H.K. Choi**, J. Park, N. Myoung and Y-J. Yu	**Dr. Hong Kyw Choi**, Metal-Insulator Transition and Quantum Lab-Daejeon, **Rep.of Korea**
12	Preparation and Luminescence of (Ba,Sr)1.3Ca0.7SiO4:Eu2+,Mn2+, Dy3+ powders for Warm White Light-Emitting Diodes J. Kim and **Y.J. Kim**	**Prof. Young Jin Kim**, Kyonggi University, **Rep.of Korea**
13	Graphene Nanoflake Inks Fabrication, Characterization and Use in a Solar Energy Application **N. Hickman**, I. Kravchunovska and B. Guo	**Prof. Nicoleta Hickman**, Florida Polytechnic University, **USA**
14	Reliability of pre-deformed flexible-printed electrodes by silver nano-particle inks under temperature and humidity conditions **C. H. Kim**, J. Y. Kim and C. Kim	**Prof. Chung-Hwan Kim**, Chungnam National University, **Rep. of Korea**
15	Influence of dispersion solvent in catalyst ink of polymer electrolyte membrane fuel cell on Ionomer distribution J.H.Lee and **S. Geol Lee**	**Prof. Seung Geol Lee**, Pusan National University, **Rep. of Korea**
16	Influence of the TixAly/a-Si:H Interlayer on the Adhesion of DLC Coatings on Stainless Steel Substrates **W.S. Hincapie**, G. Capote, J.J. Olaya and V.J. Trava-Airoldi	**Mr. Williams Hincapie**, National University of Colombia, **Colombia**

17	Nanoporous anodic alumina membrane modified with Chitosan and copper nanoparticles and its use as three-dimensional matrix for the degradation of the industrial dye Methylene Blue **B. Duran**, S. Hevia and C. Saldías	**Dr. Boris Duran**, Pontifical Catholic University of Chile, **Chile**
18	Effects of Halloysite on Morphological and Properties of Poly(3-hydroxybutyrate-co-3-hydroxyvalerate)/ Poly(butylene succinate) Blends **C. Remili**, S. Kennouche, L. Zaidi, M. Kaci and J.M. Lopez-Cuesta	**Dr. Cherifa Remili**, Bejaia University, **Algeria**
19	Biofunctionalized nanoscintillator for medical applications **E. Mihóková**, K. Popovich, L. Procházková, I.T. Pelikánová, V. Čuba, I. Jakubec,K. Tomanová,1,2 R. Dědic,4 M. Nikl1	**Dr. Eva Mihóková**, Institute of Physics, Czech Academy of Sciences, **Czech Republic**
20	Properties evaluation of Cu-based composite material by electroless plating **J-H. Jang**, H-K. Park, J-H. Lee, J-W. Lim and I-H. Oh	**Dr. Junho Jang**, Korea Institute of Industrial Technology, **Rep. of Korea**
21	Property evaluation of Ti-based target materials and their nitride nanocomposites coating layer **J-H. Lee**, H-K. Park, J-H. Jang and I-H. Oh	**Mr. Jeong Han Lee**, Korea Institute of Industrial Technology, **Rep. of Korea**
22	Nano-formulations of encapsulating Essential Oils in polymeric nano-carriers with antioxidant and antibacterial properties **A. Shetta** and W. Mamdouh	**Dr. Amro Shetta**, The American University in Cairo, **Egypt**
23	New Synthetic Route for the Preparation of Highly Ordered Multilayer Metal Membranes S. Pinilla, T. Campo, J.M. Sanz, F. Márquez and **C. Morant**	**Dr. Carmen Morant**, Autonomous University of Madrid, **Spain**

Posters Session II: June 28, 2018
NanoBioMedecine / Nanosafety

Exhibition and Posters Hall

1	Conductance measurements in Laponite-stabilized internally self-assembled particles in water. **C. Barth**, T. Dégousée, S. Gallanti and F. Muller	**Dr. Céline Barth**, ECE-Paris Engineering School, **France**
2	Capture and growth of cells on the ligand modified polystyrene chips coated with agarose and agarose/gelatin **M.K. Lee** and J. Jeong	**Dr. Myung Kyu Lee**, Korea Research Institute of Bioscience and Biotechnology, **Rep. of Korea**
3	Selective Claudin-4 Targeting of Clostridium Perfringens Entero-toxin (CPE)-conjugated Poly-sialic acid Nanoparticles for effective pancreatic cancer therapy M.K. Shim, I.K. Cho, K. Kim and **J-H. Kim**	**Prof. Jong-Ho Kim**, Kyung Hee University, **Rep. of Korea**
4	Silver-Polyvinyl Pyrrolidone (Ag-PVP) Nanoparticles Exhibit Antibacterial Activity against Chlamydia muridarum in Mouse J774 Macrophages S.Dixit, S. R. Singh and **V.A. Dennis**	**Dr. Vida A. Dennis,** Alabama State University, **USA**
5	Numerical optimization of the carboplatin encapsulation into Boron Nitride nanotubes **J. Bentin** and F. Picaud	**Mr. Jeremy Bentin**, University of Bourgogne-Franche-Comté, **France**
6	A new neural-cell specific peptide for targeted delivery of drug-loaded nanoparticles **R. Huey**, D. Rathbone, P. McCarron and S. Hawthorne	**Ms. Rachel Huey**, Ulster University, **UK**
7	Cationized Polymer (dCatAlb) Encrusted Nanoformulation enhance the chemotherapeutic activity of Doxorubicin V. Jhonson, **N. Raval**, P.Gondaliya, V.Tambe, K.Kalia and R. Tekade	**Ms. Nidhikumari Raval**, National Institute of Pharmaceutical Education and Research, **India**
8	Self-assembled Polymeric Nanoparticles for Targeting Mitochondrial Complex II K. Kwon, G. Battogtokh, Y.-Y. Cho, J. Y. Lee, H. S. Lee and **H. C. Kang**	**Prof. Han Chang Kang**, The Catholic University of Korea, **Rep. of Korea**
9	Customized D2B-gold coated Nanoparticles: promising therapeutic agents against prostate cancer. M. Sarkis, G. Minassian, H. Naim, G. Fracasso, J.D. Holmes, K. Rahme and **E.Ghanem**	**Dr. Esther Ghanem**, Notre Dame University, **Lebanon**
10	Exploitation of the liposome-biomolecular corona for early detection of pancreatic cancer D. Pozzi, L. Digiacomo, S. Palchetti, F. Giulimondi, M. Cartillone, C. Cascone, R. Coppola, D. Caputo and **G. Caracciolo**	**Prof. Giulio Caracciolo**, Sapienza University of Rome, **Italy**
11	Enhanced Gene Transfection by Multifunctional Properties of Polymeric Vitamins H. Cho, J. Y. Lee, Y.-Y. Cho, **H. S. Lee** and H. C. Kang	**Prof. Hye Suk Lee**, The Catholic University of Korea, **Rep. of Korea**
12	Preparation and physicochemical characterization of nanostructured iron(III) hydroxyphosphates as potential vaccine adjuvants **N. Angelova** and G. Yordanov	**Ms. Nadezhda Angelova**, Sofia University, **Bulgaria**
13	Gold nanoparticle-based colorimetric immunosensor for estradiol **A. Minopoli**, B. Della Ventura, C. Schiattarella, N. Sakač and R. Velotta	**Mr. Antonio Minopoli**, University of Naples "Federico II", **Italy**
14	Big Instrument- and Chaotropic Detergent-Free Assay for Ultra-sensitive Biomolecule Nucleic Acid Isolation and Detection Via Binary Nanomaterial **H. F. Liu**, F. Zhao, E. Y. Lee and Y. Shin	**Ms. Huifang Liu**, University of Ulsan, **Rep. of Korea**
15	Fabrication of Highly Sensitive Ammonia Sensor: Potential Use for Diagnosis Purpose **T.N. Ly** and S. Park	**Mr. Tan Nhiem Ly**, Dongguk University, **Rep. of Korea**
16	Rapid and Sensitive Detection of pathogen diagnosis based on Microfluidic Enrichment with a Label-free Nanobiosensing Platform **T.N.T. Dao**, J. Yoon, C. Eun Jin, B. Koo, E. Yeong Lee,, K. Han, T.Y. Lee and Y. Shin	**Ms. Nguyen Dao**, Uslan University, **Rep.of Korea**

17	Development of X-shaped DNA as an immune adjuvant for the cancer immunotherapy through dual activation of TLR9 and inflammasomes J.E. Koo, H.E. Lee, S.H. Eom, H.C. Kang, Y-Y. Cho, H.S. Lee and **J.Y. Lee**	**Dr. Joo Lee**, The Catholic University of Korea, **Rep.of Korea**
18	The Studies of Interaction Between Influenza Viruses and Surface of Nanocomposite PolyGraphene. **A.S. Botin**, V.N. Buravtsev, V.T. Ivanova, Ya.E. Kurochkina, L.A. Baratova, A.V. Timofeeva and T.S. Popova	**Dr. Alexander Botin**, Peoples' Friendship University of Russia, **Russia**

Posters Session II: June 28, 2018

NanoMaterials for Energy and Environment / Nanoelectronics / NanoPhotonics

Exhibition and Posters Hall

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19	Boron-doping effect on photovoltaic performances of silicon nanoparticle/organic polymer hybrid solar cells **K. Sato**, K. Furuya and N. Ikeda	**Dr. Keisuke Sato**, Tokyo Denki University, **Japan**
20	Enhanced performance of non-fullerene ternary organic solar cells **Y-Y. Yu** and T-W. Tsai	**Prof. Yang-Yen Yu**, Ming Chi University of Technology, **Taiwan**
21	Polysilsesquioxane-Derived Hybrid Gel Polymer Electrolytes for Lithium Ion Batteries A.S. Lee, J.H. Lee, C.M.Koo and **S.S. Hwang**	**Dr. Seung Sang Hwang**, Korea Institute of Science and Technology, **Rep.of Korea**
22	Novel modulating the concentrations of zinc oxide nanowires using electron beam **Y-S Cho** and H. Ji	**Mr. Young-Seung Cho**, Samsung Electronics/ Sungkyunkwan University, **Rep. of Korea**
23	Heterostructures of metal oxide/sulfide nanoparticles as efficient solar active photocatalysts **M. Madkour**, M. O. Amin and E. Al-Hetlani	**Dr. Metwally Madkour,** Kuwait University, **Kuwait**
24	The Synthesis & Analysis of Two Long Lasting Phosphorescent Compounds: SrAl2O4:Eu2+,Dy3+ **G. Alsaleem**	**Mrs. Ghayah Alsaleem**, University College Dublin, **Ireland**
25	CMOS Compatible Sensor for the Electrostatic Selectivity of Volatile Organic Compounds **N. Mahapatra**, A. Ben-Cohen, A. Henning, N. Swaminathan, H. Greenspan and Y. Rosenwaks	**Dr. Niharendu Mahapatra**, Tel Aviv University, **Israel**
26	Effect of Mg-doping on synthesis of lithium iron phosphate as cathode materials for lithium-ion batteries **W. C. Chien** and G. R. Zhuo	**Prof. Wen-Chen Chien**, Ming Chi University of Technology, **Taiwan**
27	Mustard Seed based Triboelectric Nanogenerator **S. Singh**, S.Muduli, R. Boomishankar and S.Ogale	**Mr. Sachin Singh**, IISER Pune, **India**
28	Endurance measurements of LixCoO2-based ReRAM cells V.S. Nguyen, V.H. Mai, A. Moradpour, P. Auban Senzier, C. Pasquier, K. Wang, M.J. Rozenberg,...and **O. Schneegans**	**Dr. Olivier Schneegans**, CNRS/ UPMC/Paris Saclay University, CentraleSupélec, **France**
29	Effect of nanofluidic electrolytes on the electrochemical reaction of vanadium redox flow batteries **J. Kim** and H. Park	**Mr. Jungmyung Kim**, Changwon National University, **Rep. of Korea**
30	Flexible thermoelectric devices for body temperature control **S. Han** and S. H. Lee	**Dr. Seungwoo Han**, Korea Institute of Machinery and Materials, **Rep. of Korea**
31	Ethanol steam reforming on Pd/ZnMgAl2O4 catalyst **J. H. Lee**, J. Y. Do, N. Park, T. J. Lee and M. Kang	**Mr. Jae Hyung Lee**, Yeungnam University, **Rep. of Korea**
32	Oxygen transfer capacity on a spinel typed CuxMg1-xMnyAl2-yO4 oxygen carrier **N. Son**, J. Y. Do, N. K. Park, J. I. Baek, H. J. Ryu and M. Kang	**Mr. Namgyu Son**, Yeungnam University, **Rep. of Korea**
33	Significant COS adsorption ability on K-AC composite and adsorption mechanism analysis **J. Kim**, J. Y. Do, N. K. Park, J. P. Hong and M. Kang	**Mr. Junyeong Kim**, Yeungnam University, **Rep. of Korea**
34	Spin Hall Effects in Antiferromagnets **S. Gulbrandsen**	**Mr. Sverre Gulbrandsen**, Norwegian Univ. of Science and Tech., **Norway**

35	Preparation and characterization of poly(vinyl chloride)-montmorillonite clay composite membranes for water purification **M.M. Alghamdi**, A.A. Zahar and B.M. Aseery	**Dr. Majed M. Alghamdi**, King Khalid University, **Saudi Arabia**
36	Pavement Material Incorporated Nono Fly Ash Filler M. Dahim and **H. Al-Mattarneh**	**Prof. Hashem Al-Mattarneh**, King Khalid University, **Saudi Arabia**
37	Use of SiO2 Nanoparticles for Vanadium and Niquel separation from crude oil **V. Vargas**, J. Castillo, R. Ocampo Torres, C-P. Lienemann and B. Bouyssiere	**Dr. Vicmary Vargas**, Central University of Venezuela, **Venezuela**
38	Biopolymer nanofiber doped with nanospinels by electrospinning and microbiological assays E. Vanegas, **C. Cruzat**, D. Peña, R. Arrue, N. Novoa, G. Pauta, D. Ponce and O. Peña	**Dr. Christian Cruzat**, University of Cuenca, **Ecuador**

Nanotech Plenary session I

Hybrid Nanomaterials: Structural and Local Spectroscopic Studies via Advanced TEM

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Abstract:
In the last two decades, transmission electron microscopes (TEM) have undergone a large number of improvements allowing ~ 100 meV (even few tens of meV) energy resolutions for a sub-nanometer electron beam. These performances offer new possibilities for probing the optical, dielectric and electronic properties of nanomaterials with unprecedented spatial information, as well as for studying the atomic configuration of nanostructures. I will present a selection of recent works taking advantage of these new capabilities [1-15]. These works will concern the study of the atomic structure & configuration of nanostructures (including doped carbon nanotubes and bio-nanomaterials), as well as opto-electronic properties studies carried out via electron energy loss spectroscopy (EELS) measurements of different kind of nano-objects (inorganic nanotubes and metallic nanoparticles). These works will illustrate the study of properties with extreme spatial resolution enabled by a Cs probe corrected STEM combined with the use of a monochromator.

Keywords: hybrid 1D-2D nanomaterials, transmission electron microscopy, plasmonic nanostructures, HR(S)TEM, EELS, electron tomography.

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Nanocrystalline Alloy Structure for Remarkable Oxidation Resistance

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Abstract:

Fe-Cr alloys are among the most commonly used materials in various energy systems. Their oxidation resistance is one of the critical criteria in selection of a given alloy type. This presentation will demonstrate the remarkable improvement in oxidation resistance of Fe-Cr alloys due to their nanocrystalline structure.

Metals and alloys possess much larger fraction of grain boundaries (i.e., high energy area) in their nanocrystalline (NC) than on their microcrystalline (MC) state. Grain boundaries being high energy areas, the metal with NC structure may suffer greater corrosion rate. However, the nature of the influence of NC and MC structures depends on the type of corrosion and environment-material system.

On the basis of the mechanism of the profound role of alloy grain size in oxidation of Fe-Cr alloys, the presenter's group has validated his own hypothesis that the oxidation resistance of a nanocrystalline Fe-Cr alloys should be considerably superior to a microcrystalline of same composition {1}, as shown in Figure 1. While this presentation will provide an overview of the validation, it will also provide recent data showing the combined effect of nanocrystalline alloy structure and alloying with Al, for still superior resistance to high temperature oxidation of Fe-Cr alloys.

Keywords: Fe-Cr alloys, oxidation, secondary ion mass spectroscopy (SIMS).

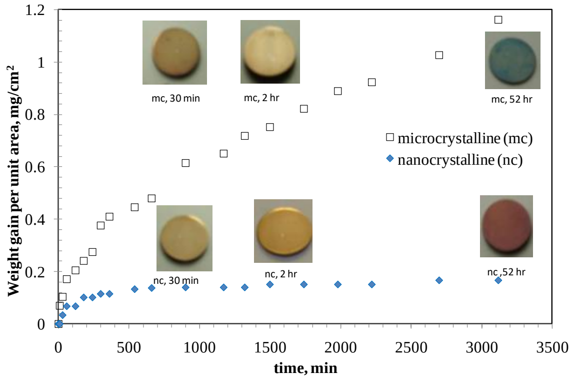

Figure 1: Considerably lower weight gain of NC Fe-10%Cr alloy showing reamarkably superior oxidation resistance of the NC alloy (than MC alloy of same composition) [1].

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Continuous approximation for interaction energy of adamantane encapsulated inside carbon nanotubes

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Abstract

Linear forms of crystalline diamond constitute a new one-dimensional nanomaterial. They assemble within carbon nanotubes which serve as a template and by taking diamondoids as building blocks. Template synthesis of linear chain nanodiamonds have been considered recently using diamantine polymers [1]. The smallest building block of diamond is adamantane, which is the smallest unit with a diamond lattice. The interaction energy for two adjacent adamantane molecules and that of adamantane molecules encapsulated inside carbon nanotubes are investigated. The Lennard-Jones potential and the continuous approximation are utilized to derive analytical expressions for these interaction energies from a highly simplified model. The derived equilibrium distance is found to be within 3% of density functional calculations [2] and an equilibrium distance of 3.281 Angstroms between two adamantane molecules is determined. The smallest carbon nanotube radius b0 that can encapsulate the adamantine molecule and the radius of the tube bmax that gives the maximum suction energy, are calculated to depend linearly on the adamantane radius. For larger diameter tubes, the off axis position is predicted, and the equilibrium distance between the molecule and the tube wall is found to be close to the interlayer spacing in graphene.

Keywords: Adamantane, carbon nanotube, Lennard-Jones potential, interaction energy.

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Disorder in graphene: from meter to atomic scale

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Abstract:

Disorder in crystals is in its strictest sense any deviation from infinite, periodic repetition of the unit cell; all surfaces are, as such, manifestations of disorder. Graphene is a two-dimensional crystal where the true surface is its one-dimensional edges, but where every single atom in the "bulk" can be directly accessed. Graphene is not surprisingly very vulnerable to disorder.

I will discuss disorder in graphene at very different scales and how the disorder is expressed in electronic properties. For fabrication of large-area graphene, high quality is not just about high carrier mobility but also high uniformity – on all scales. In collaboration with P. Jepsen, DTU Fotonik, we use terahertz time domain spectroscopy to measure the electronic properties of graphene without physical contact (Fig 1a), and compare with multi-configuration electric measurements[1]. The absorption of THz radiation by graphene is governed by low-energy intraband transitions, that are directly coupled to the ac conductivity. A closer look at the conductivity spectrum reveals intereating details of carrier scattering on line-defects (grain boundaries) on the submicron scale. By extracting the scattering time, we can produce maps of the carrier mobility and carrier density, and study how the quality and uniformity depends on growth and transfer of large-scale graphene (Fig 1b).

These one-dimensional interfaces and edges of graphene are nearly devices in their own right; I will show how the atomic scale disorder of the edge disorder can have deep consequences for the electron transport properties of graphene devices; not just for ballistic nanoconstriction but even micron-scale devices. I will discuss three recent examples of the structure of edges plays a leading role; nanostructured superlattices, molecular memcapacitors and quantum Hall breakdown in nanoconstrictions[2], see Fig 1c.

Keywords: graphene, disorder, terahertz time-domain spectroscopy, metrology, van der Waals heterostructures, grain boundaries, edge roughness, edge engineering, molecular switches.

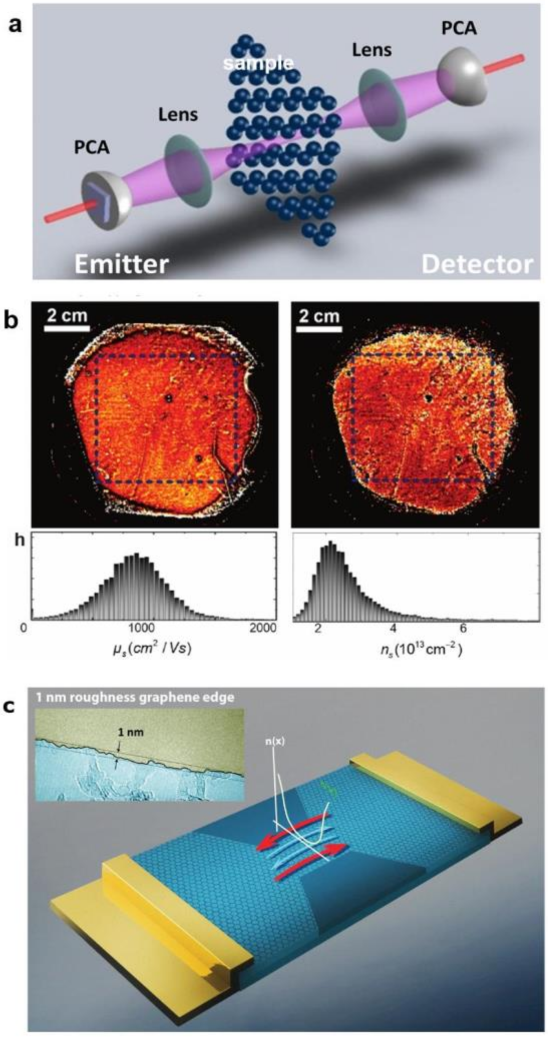

Figure 1: a) Terahertz time-domain spectroscopy of graphene. b) Large maps of carrier density and mobility of graphene derived from THz conductivity spectra. c) Illustration of graphene device where additional magnetic edge states appear when the edge roughness is lowered to 1 nm, suppressing the quantum Hall effect[2].

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AFM PinPoint Nanomechanical Mode Using Probes with Different Stiffness

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Abstract

Nanomechanical property measurement is one of the most popular functions of atomic force microscopy (AFM). Conventional nanomechanical measurement techniques are mainly based on AFM force-volume spectroscopy, which collects force-distance (F/D) curves at each pixel to calculate material elastic properties. However, these techniques have been recognized as being extremely slow, and it usually takes hours to acquire an elasticity map. Driven by the demand for a faster and more efficient technique, Park Systems developed PinPoint™ Nanomechanical Mode to provide a solution that is at least 100 times faster than traditional techniques. This mode enables acquisition of an elasticity map with a correlated topography image within minutes, and it represents a new application tool for collecting real-time topography and quantitative mechanical property maps of various materials, ranging from hard disks to soft tissues. To better access the capability of the PinPoint™ Nanomechanical Mode, we select three cantilevers with stiffness ranging from 0.2 N/m to 25 N/m and investigated their influence on the measured modulus values. In addition, for all three cantilevers, we also examine the influence of applied force on the resulted modulus. Findings show that cantilevers with smaller force constants will lead to smaller measured modulus values, and vice versa. With the same cantilever, a larger applied force results in a larger measured modulus compared to that obtained with smaller force values. The most important finding is that, with PinPoint™, the relative modulus difference/ratio within a sample can be accurately acquired regardless of the force constant of the cantilever or the applied setpoint force values.

NFFA-EUROPE An open access resource for experimental & theoretical science

E. Travaglia[1] and the NFFA-Europe collaboration

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Abstract:

NFFA-EUROPE is an open access platform, granted by the EU for 48 months from September 1st, 2015, to carry out comprehensive projects for multidisciplinary research at the nano-scale extending from synthesis to nano-characterization to theory and numerical simulation.

Advanced resources, made available by the 20 NFFA-EUROPE partners, specialized on growth, nano-lithography, nano-characterization, theory and simulation and fine-analysis with Synchrotron radiation, Free Electron Laser (FEL) and Neutrons are integrated to de-velop frontier research on nanoscience and to enable European scientists from diverse disciplines to access state of the art and unique methods and tools.

NFFA-EUROPE enables coordinated access to nanoscience laboratories co-located at the large-scale infrastructures for fine analysis, or linked to High-Performance Computing (HPC) facilities as well as Joint Research Activities (JRA) and Networking Activities (NA).

The access management structure optimizes the services to the users to pursue scientific excellence as well as industrial and technological innovation. Proposals can be submitted through the single entry point at the NFFA.EU portal to apply for all NFFA-EUROPE methods and instruments, and a panel of international experts is in charge of the peer-review selection to ensuring the scientific excellence and/or innovation potential of the accepted proposals. Moreover, the experts of the Technical Liaison Network (TLNet) dialogue with and assist the user from the proposal submission to the technical feasibility check and to the personalized access programme optimizing the use of the NFFA-EUROPE infrastructure. additional information is available at www.nffa.eu.

Keywords: multidisciplinary research, distributed research infrastructure, lithography and patterning, growth and synthesis, theory and simulation, characterization.

Figure 1: NFFA-EUROPE (www.nffa.eu) integrates 19 Partners, half of which are nano-foundries that are co-located with Analytical Large Scale facilities.

Research and innovation Dilemma on Nanotechnology

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Abstract:

The Horizon 2020 program represents a paradigm shift with respect to the past introducing a strong focus on innovation. In fact, two of the three pillars of the European program and numerous instruments are aimed to promote and develop innovation processes. Despite the resources committed by the H2020 program and various national and regional programs, the effects on society and the productive system are in many cases below expectations. An emblematic case is that of nanotechnologies, which have the potential to strongly affect vital fields such as healthcare, energy, environment and manufacturing. To unlock potential benefits at the most, it is necessary to reduce the 'valley of death' and enhance the track record in transforming breakthroughs into commercially valuable innovations.

Meeting these challenges involves understanding the internal (to the innovation process) and external (related to the surrounding environment) bottlenecks of the innovation cycle. Europe is therefore in need of studies aiming at developing an analytical framework for offering a novel perspective on innovation in nanotechnologies and for strengthening their systemic economic impact.

In the present talks is based on the analysis of the situation following two main way the studies undertaken by EC and the evaluation of specific case. The European scenario on nanotechnology innovation is pointed out as well the main challenges and obstacles are analyzed in order to stimulate a participating discussion and promote further studies to support the EU innovation processes on nanotechnology field.

Session I.A:
Nanomaterials Fabrication / Synthesis

Particle and Product Design by Top-down Processes

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Abstract:

Wet grinding machines, like agitator bead mills, are used in different industries for the production of inks and paints, pigments, dyes, pharmaceutical and cosmetic products, minerals, ceramics and many additional applications.

For the comminution down to the nanometer size range or for the dispersion of nano-sized particles the use of finer and finer grinding beads is necessary. Furthermore for the avoidance of changes in the crystal structure of the product smooth conditions for “Mild Dispersion” processes are very important.

First comprehensive investigations about grinding in agitator bead mills were done by Weit [1] and Stehr [2]. These investigations show that the comminution progress mainly depends on the specific energy input Em, which is the total energy supplied to the grinding chamber related to the product mass. Further studies published (among others Joost [3], Thiel [4], Bunge [5], Mankosa et al. [6], Stadler et. al. [7] and Roelofsen [8]) show that besides the specific energy input the grinding media size has a great influence on the comminution result. The specific energy consumption can be reduced considerably by accommodating the grinding media size to the comminution problem. In a product particle size range down to 1 µm the comminution behavior of agitator bead mills can essentially be described by the parameters specific energy Em, stress number SN and stress energy SE (s. Kwade [9]).

In the sub-micron particle size range the behavior of the product suspensions is more and more influenced by increasing particle-particle-interactions. Due to these interactions often spontaneous agglomeration of product particles occurs and the viscosity of the product suspension increases [10]. If product particle sizes smaller than 1 µm are reached, these interactions can lead to an interrelation between agglomeration, desagglomeration and comminution, thus no further comminution progress results in spite of increasing energy input. Fundamental theoretical and experimental investigations about grinding and crack formation in solids have been undertaken by Schönert [11]. Based on this work he estimates the possible minimum particle size for breakage to be in a range of 10 to 100 nm depending on the physical properties of the material.

Research by Mende, Stenger and Sommer [12, 13, 14] shows that it is possible to comminute, for example, zinc oxide, titanium dioxide and quartz down to below 10 nm. During this research the product suspensions were composed by adequate formulations in such a way that a reagglomeration of primary particles by electrostatic or steric interaction was eliminated.

The contribution gives an overview about grinding and mixing equipment from the laboratory scale to the production scale. Furthermore, the differences between real comminution and desagglomeration processes as well the choise of the right machine depending the product requirements will be discussed by the use of further real experimental results.

Keywords: Grinding, Disperision, Micronization, Top-Down, Comminution, Desagglomeration

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Metallic Bismuth Nanoparticles: a Reproducible, Robust and Repeatable Synthesis *via* a Green and Safe Process

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Abstract:

Bismuth is a highly biocompatible and inexpensive metal with a high atomic number, which confers an important X-rays opacity.[1] While bismuth oxide[2] or bismuth sulphide[3] have been extensively studied in imaging, little is known about metallic bismuth nanoparticles. The latter are more attractive for X-rays imaging because they do not contain oxygen or sulfur so a high quantity of metal atoms is contained inside the NPs. Few synthesis of Bi NPs are described by following a top down approach or a bottom up approach *via* a thermal decomposition of bismuth or a reduction[4, 5, 6] in organic solvent[7, 8] or in polyol.[9] A new robust, efficient and green process is reported here to obtain bismuth metallic nanoparticles. The procedure, which has been optimized to get a reproducible synthesis, will also tend to minimize chemical hazards to health and environment.[10] By applying the green chemistry principles,[11] Several experimental parameters have been studied such as reaction time, reactants stoichiometry, temperature and purification steps number.

Figure 1: Figure illustrating the advances towards both green process such as sonication and purification method to get metallic bismuth nanoparticles.

Few activation techniques have been compared (heating,[12] sonication) but also intensification process (batch, continuous flow). Two purification methods (centrifugation and ultrafiltration) were tested to isolate thin black powders of D-glucose-coated bismuth nanoparticles. Several analytical techniques were used to characterize products (structures, sizes and morphology) such as Infrared analysis, Dynamic Light Scattering (DLS) and Transmission Electron Microscopy (TEM).

Keywords: bismuth, nanoparticles, green process, reduction, glucose, sonication, millifluidic, ultrafiltration.

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Functional Noncovalently Modifed Boron Nitride Nanotubes

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Abstract:

Boron nitride nanotubes (BNNTs) are structurally analogs to carbon nanotubes (CNTs). Both have remarkable mechanical properties and thermal conductivity. However, BNNTs are electrical insulators and transparent in the visible region, have high neutron absorption cross-section due to the presence of boron, and have higher thermo-oxidative and chemical stability than CNTs. All these characteristics make BNNTs promising for the fabrication of advanced composites with corresponding functionalities such as for cooling of electronic components, neutron shielding and flame resistance. Studies on BNNT have been limited, mainly because only small quantities of BNNT had been produced. Advances in BNNT production[1] have facilitated the study of BNNT chemistry, composites and applications.

Similar to CNTs, BNNTs are not significantly soluble in common solvents unless their surface is chemicaly modified, which is expected to facilitate BNNT applications by enhancing dispersion and interfacial interactions with a matrix. The assessment of BNNT sample purity and crystallinity is also important since both parameters play a significant role in the performance of nanomodified matrices. Conjugated polymers have been shown to noncovalently modify and exfoliate BNNTs.[2] Here we evaluate the role of the conjugated polymers, specifically polythiophenes and polyfluorenes as functional dispersants for BNNTs. This noncovalent methodology is used for the fabrication of superhydrophobic films with conjugated polymers bearing hydrophobic alkyl chains. By using the appropiate pattern in a filtration membrane, the individualized functionalized-BNNTs can be recoverd by filtration as superhydrophobic nano-micro patterned films. On the other hand water soluble conjugated polymers are effective at improving the interaction between BNNTs and a polyurethane matrix, which leads to significant improvements in the Young's modulus as compared to pristine purified BNNTs. In another example of the functionality of this strategy, we explore a method to assess the relative purity of BNNT samples based on the strong, specific interaction between BNNTs and the conjugated polymer rra-P3HT[2] and the associated color-change and absorption spectra (Figure 1). The method is shown to be satisfactory for accessing the relative purity of BNNT samples obtained by different purification protocols. A correlation between the purity assessment results and the trends in mechanical enhancement of the respective BNNT-polyurethane composites is also demonstrated.

Keywords: BNNTs, purity assessment, nanocomposites, superhydrophobic films

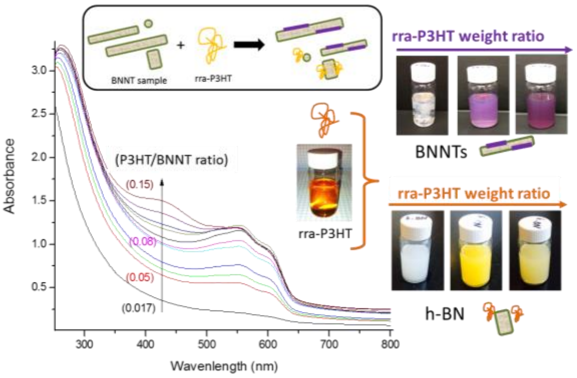

Figure 1: rra-P3HT conformational changes due to self-assembly on BNNTs and associated UV-vis absorption spectra at different rra-P3HT/ BNNT weight ratios

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Facile Fabrication of Superhydrophobic Surfaces with Hierarchical Structures

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Abstract:
Hierarchical structures are a common feature of hydrophobic surfaces found in nature. Hydrophobicity with hierarchical structures is known as Lotus-effect, and many artificial superhydrophobic surfaces mimick this structure. In this research, we will introduce a fast, clean, and simple one-step method to fabricate hierarchical structure on the surface of SUS304 plates. Hierarchical structure with 10 ㎛ scale micro-roughness and 100 nm scale nano-roughness were created after direct microwave irradiation under low-vacuum carbon dioxide atmosphere. The surface nanostructures were composed of hematite with 3.7% chromium content. This structure showed superhydrophobicity with water contact angle up to 179˚ after coating with octadecyltrihloroilane (ODTS). This fabrication method is expected to be easily scaled-up; a scanning microwave device can be used, which is readily available.

Keywords: superhydrophobic surfaces, plasma reaction, direct microwave irradiation, hierarchical structure, hematite nanostructure fabrication.

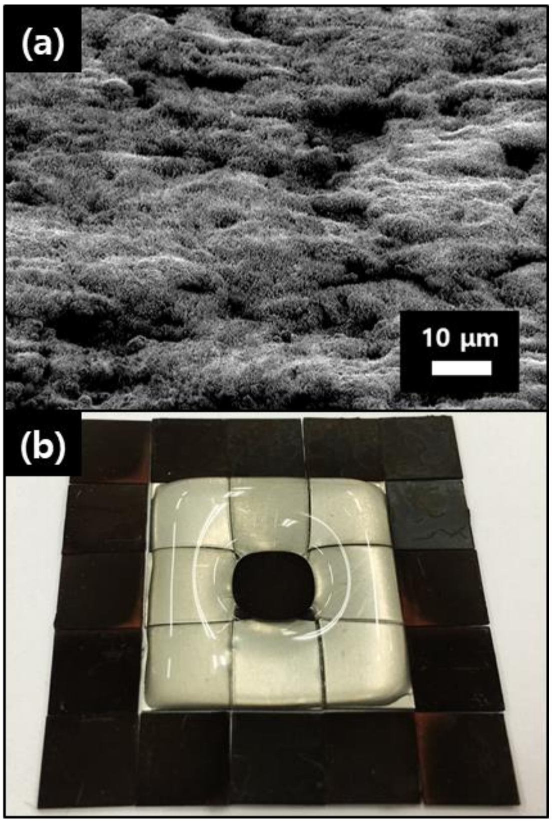

Figure 1: (a) Fabricated hierarchical structure after microwave irradiation at 1500 W for 10 minutes on the SUS304 plate. (b) superhydrophobic surface obtained after ODTS coating. The black plates are superhydrophobic surfaces, and the gray plates are bare SUS304 plates which have hydrophilic surfaces.

Solution-based synthesis of amorphous germanium nanoparticles from organogermanium halide precursors

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Abstract:

Semiconductor nanoparticles (NPs) are gaining increasing interest in many fields, ranging from renewable energy to biological imaging. This is due to the size dependence of their properties that arise in the quantum confinement regime, such as the development of the band gap with changing size. In this frame, germanium (Ge) is particularly appealing because of its intrinsic properties, such as its large Bohr radius (24 nm),[1] which renders quantum confinement effects observable at relatively large sizes. It has proven challenging to synthesize these materials with high quality and low cost, in addition to concerns revoling around synthetic scalability, safety, and environmental impact. Herein, we investigate a synthetic scheme that combines benign reagents such as sulfur and primary amines to promote the reduction of organometallic Ge (IV) precursors to form Ge NPs at relatively low temperatures (300 °C). We propose a reaction mechanism and examine the effects of solvent, sulfur concentration, and organogermanium halide precursors. We are able to identify H_2S as the primary reducing species and show multiple reaction pathways where it is produced *in-situ* from the interaction of elemental sulfur and primary amines. In addition, we observed an inverse relationship between the quantity of sulfur and the particle size. Halogen cleavage from the organogermanium precursor was found to be the rate-determining step. These synthetic details allow for control over the particle size and morphology. While we demonstrated the synthesis of Ge NPs, the reaction mechanisms elucidated can be extended to other members of the group IV family, in addition to other classes of nanoparticles that rely on precursors with similar properties.

Keywords: Nanoparticles, Amorphous, Crystalline, Germanium, Sulfur, Colloidal synthesis.

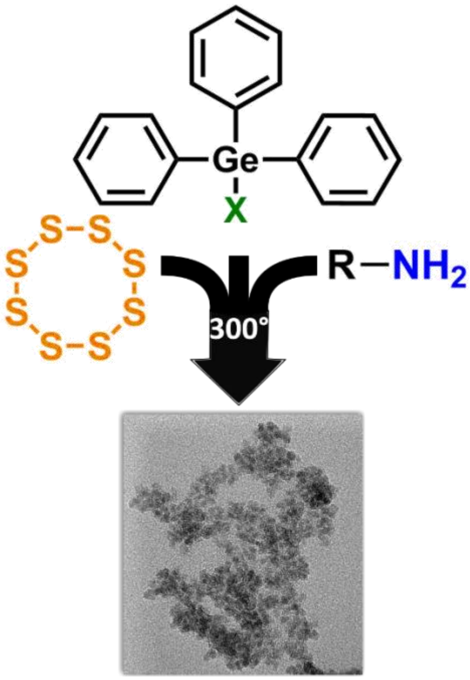

Figure 1: the fundamental questions tackled in this study revolve around the reaction mechanism for the formation of germanium nanoparticles starting from and organogermanium halide precursor and sulfur in an amine solvent/capping agent solution.

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Synthesis of aqueous slurries with high concentration in polystyrene nano-particles

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Abstract:

A slurry is a fluid that is formed by a stable dispersion of a solid in a liquid (commonly water or glycerol). The slurry can be pumped or it flows under the gravity effect. This fluid allows the manipulation of liquids stead of bulk solids. The most important applications are related with the development of concrete support or paints [1], or as thermal fluids [2]. On the other hand, the polystyrene (PS) is one of the most used polymers due to its elasticity, and good chemical and mechanical resistances and thermal and electrical properties. It has lots of different applications such as cover for electrical apliances, packing, toys, household utensils, etc.

In the present works, it has been synthesized a slurry with high concentration in polystyrene nano-particles in aqueous phase, by means of the suspension polymerization technique. In this method, silicon gel synthesized in-situ, containing vinils and OH groups, has been utilized like suspension agent. Beside, in order to increment the nano-particles production, it has been combined with sodium dodecylsulfate (SDS). The slurry and a SEM photo of PS nanoparticles are shown in Figure 1. It can be observed that this material present a spherical morphology and a particle size ranged between 21 and 190 nm. Through this technique it was possible to produce slurries with up to a 50 wt% of polystyrene nano-particles. One of the most important parameter related with the slurries is the viscosity in order to know the energy consumption during the pumping. This viscosity depends on the solid concentration, as well as of the fluid temperature. Results showed that they presented a behave like a no-Newtonian fluid, although they are completely stable and pumpable, according to the ζ potential results and the viscosity values. The maximum observed viscosity was 0.0662 Pa·s at a temperature of 25 ºC, in a share rate of 400 s^{-1} and the value of ζ potential is 76.7 mV, both for a solid concentration of 40 wt%.

Keywords: nano-particles, silicon gel, suspension polymerization, slurry, polystyrene, sodiumdodecyl sulfate (SDS).

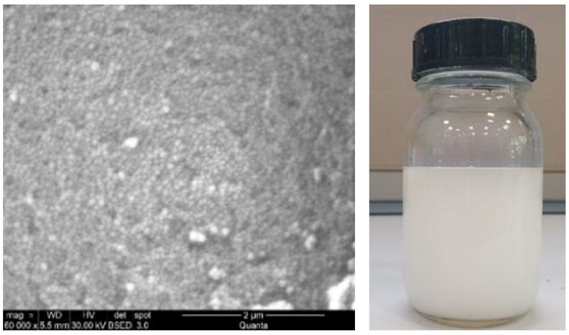

Figure 1: Scanning Electron Microscopy of the polystyrene nano-particles disperse in the slurry (left) and picture of once of the slurries synthesized (right)

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Fabrication of nanocomposite thin films assisted by plasma polymerization, towards smart coatings

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Abstract:

Nanoparticles made of noble metal as silver have been extensively used in various fields including biotechnology, catalysis and optics. Many studies dealing with colloidal solutions of nanoparticles aim at designing well-defined particle size and shape in order to control the properties of the solution. Fewer studies focus on the properties of nanocomposite coatings made of metallic nanoparticles embedded in polymer thin films.

Our group work on the design of smart (nanocomposite) coatings assisted by pulsed plasma polymerisation, which can be fabricated on many types of materials. A recent study has evidenced the effect of plasma duty cycle on silver nanoparticles loading within the polymer coating.[1]

In this study, we investigate more precisely the influence of the nature of the chemical groups present within the plasma polymer, the operating conditions of plasma polymerization as well as the synthesis protocol of nanoparticles in contact with the plasma polymer in order to control the size, shape and distribution of the nanoparticles within the nanocomposite coating.

Low-pressure plasma polymerization is used to fabricate functional polymer coatings of poly(maleic anhydride) and poly(allylamine). The plasma polymer is subsequently swollen in an aqueous solution containing the metal precursor before reducing and stabilizing metal nanoparticles with sodium citrate for instance, according to Turkevich method.[2] As illustrated in Figure 1, the size, shape and distribution of the nanoparticles within the polymer coating strongly depend on operating conditions and is mainly driven by the interactions between the chemical functional groups of the plasma polymer (carboxylate or amine groups) and the metal clusters.

XPS, TEM and AFM characterizations enable to understand and control the fabrication process and the morphology of the nanocomposite thin films. These results are a promising milestone for the design of original smart nanocomposite coatings whose properties vary with respect to the size and shape of the embedded nanoparticles. Anti-bacterial and optical properties of these coatings are currently under investigation.

Keywords:
Nanocomposite thin film, silver nanoparticles, plasma polymer, smart coatings, plasma-assisted process

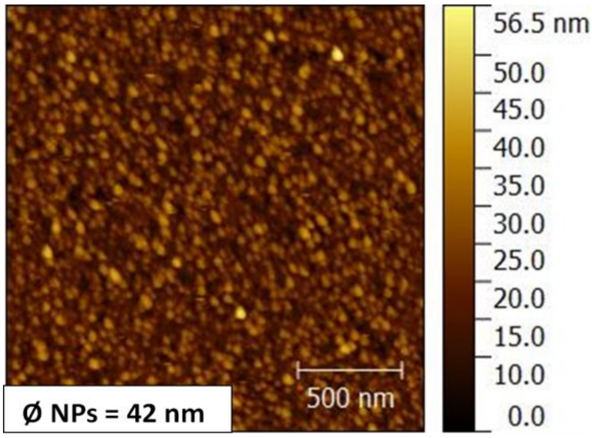

Figure 1: AFM image of a nanocomposite thin film made of Ag NPs embedded in poly(allylamine) plasma polymer.

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Nanostructured anodic titanium oxides: production and engineered applications

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Abstract:

The interest in titanium and its oxides keeps growing on account of their peculiar engineered properties, which find applications in several fields, from architecture to bioengineering, from automotive to photovoltaic cells and photocatalytic devices, as well as to produce self-cleaning surfaces. There are several anodic oxidation treatments currently applied to titanium, which allow to form nanostructured oxide layers suitable for their whole range of applications, depending on the process parameters employed in the growth of these oxides. The different procedures and parameters of anodic oxidation will be described, giving information on the main oxide characteristics achievable: thickness, morphology, structure and composition. An analysis of the fields of application associated with specific oxide characteristics will be provided.

The experimental data here presented will deal with the obtaining of three main classes of functional TiO_2 oxides, with particular reference to thin, transparent oxides. These films on one side show interference colors, which are of great interest not only in the design and jewelry field, but also as a means to investigate the kinetics of oxides formation through the indirect measurement of oxide thickness from the color achieved. On the other hand, electronic needs can also be addressed with such TiO_2 thin films which can show a memristive behavior, i.e., change resistivity as a function of current and voltage history across the oxide layer. This functionality is achieved by low voltage anodizing, which produces thin oxide films whose defective structure allows the mobility of oxygen vacancies to form conductive filaments in the generally resistive oxide.

Keywords: titanium dioxide, interference, color, memristor.

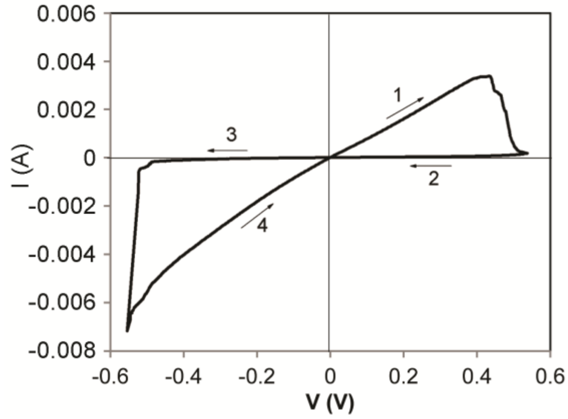

Figure 1: Memristive behaviour of a TiO_2 film grown on titanium by anodizing in H_3PO_4.

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Synthesized $In_{2-x}Sn_xO_y$ on ITO coated PET using Sol-Gel Method for Extended Gate FET-pH Sensor device.

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Abstract:

Indium tin oxide ($In_{2-x}Sn_xO_y$) films as a conductive transparent material have caused a great deal of interest due to their prominent electro-chemical behavior. We studied the sol-gel based $In_{2-x}Sn_xO_y$ oxide sensing membrane deposited on ITO-PET EGFET (1) device for bio-sensing applications. Herein, we used 15 mol % Sn doped in $In_{2-x}Sn_xO_y$ on ITO coated PET (2), a flexible substrate, to investigate the sensing performance. Sn doped $In_{2-x}Sn_xO_y$ layer on the top of the flexible substrate in extended gate FET (EGFET) (1) works as a sensing membrane of the electrochemical biosensor. $In_{2-x}Sn_xO_y$ was deposited using the sol-gel method due to its ease of fabrication, homogeneity, cost effective compared to other methods. The $In_{2-x}Sn_xO_y$–EGFET film annealed at 120°C displayed the sensitivity of 56.66 mV/pH with linearity 0.99 in the solutions from pH 2 to 12. The low defect film, obtains the low sheet resistance of 42.32 ohm/square. Thus, sol-gel based indium tin oxide- EGFET shows great promise in biochemical sensing applications.

Keywords: ITO coated PET, EGFET, sol-gel method, pH sensors, electrochemical biosensor.

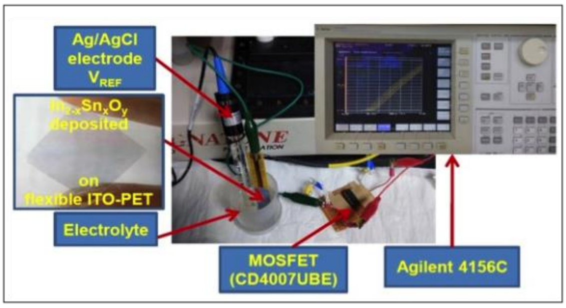

Figure a

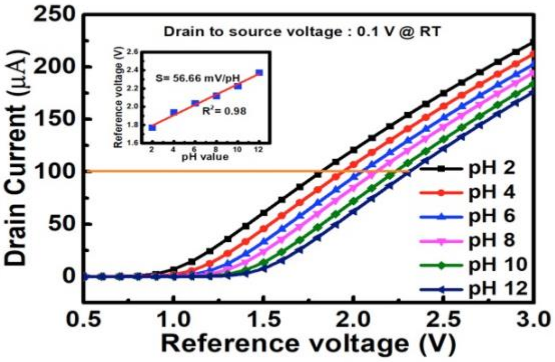

Figure b

Figure (a) Schematic view of the I-V measurement setup for the sol-gel deposited $In_{2-x}Sn_xO_y$ conductive oxide pH- EGFET sensor and (b) Response of I-V curves for $In_{2-x}Sn_xO_y$ EGFET sensor into the electrolyte having pH values ranging from 2 to 12.
Inset: Reference voltage as a function of the pH at room temperature.

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Nanocrystals as high temperature local probes

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Abstract:

The study of semiconductor nanocrystals (NCs) is a very active research field, due to the wide range of applications, related to light-emission and absorption, photodetection, solar cells, light emitting diode or tunable emitters for bio-labeling[1]. One area is the development of detection techniques with high spatial resolution enabled by the small size of nanomaterials. As a representative example, nanometer probes of temperature can be very useful to obtain an accurate local value of temperature, particularly in catalysis where the activity and selectivity are temperature dependent. In this context, semiconductor NCs are promising objects to provide this precision due to the temperature dependence of their optical properties. We present here the synthesis of different types of NCs (Cd_3P_2[1], InP@ZnS[2] and CdSe@CdS[3]), their capacities as nanothermometers for high temperatures (>340 K) and the conditions which have to be fullfilled for accurate measurements. Different parameters such as the wavelength, the intensity, the area and the full width at half maximum of emission were studied as a function of temperature. The studied temperatures ranges from room temperature to 540 K and the comparison between the different NCs is discussed.

Keywords: semiconductor nanocrystals, photoluminescence spectroscopy, nanothermometry, high temperatures probes

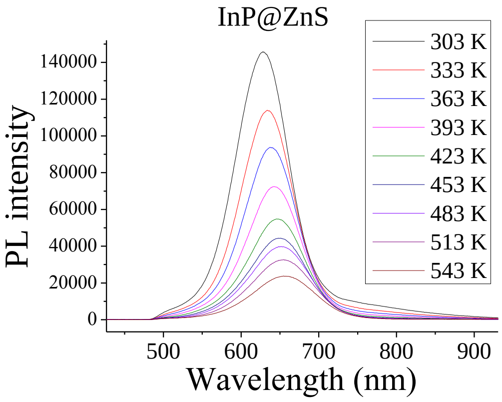

Figure 1: Figure illustrating the evolution of PL spectra of InP@ZnS in solution with temperature.

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Laser Nanopatterning of Coloured Ink Thin Films for Photonic Devices

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Abstract

Nanofabrication through conventional methods such as electron beam writing and photolithography is time-consuming, high cost, complex, and limited in terms of the materials which can be processed. Here, we present the development of a nanosecond Nd:YAG laser (532 nm, 220 mJ) in holographic Denisyuk reflection mode method for creating ablative nanopatterns from thin films of four ink colours (black, red, blue, and brown). We establish the use of ink as a recording medium in different colours and absorption ranges to rapidly produce optical nanostructures in 1D geometries. The gratings produced with four different types of ink had the same periodicity (840 nm); however, they produce distant wavelength dependent diffraction responses to monochromatic and broadband light. The nanostructures of gratings consisting of blue and red inks displayed high diffraction efficiency of certain wavelengths while the black and brown ink based gratings diffracted broadband light. These gratings have high potential to be used as low-cost photonic structures in wavelength-dependent optical filters. We anticipate that the rapid production of gratings based on different ink formulations can enable optics applications such as holographic displays in data storage, light trapping, security systems, and sensors.

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Physical hybrid hydrogels with colloid-Cubosomes as cross-linker

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Abstract:

Due to their high-water content, hydrogels are very promising for the biocompatible applications. However, these systems show very poor mechanical properties because of the large amount of water. This limitation has been overpassed by synthetizing the polymer chains in presence of inorganic nanoparticles (NPs). These latter act as physical cross-linkers and enhance remarkably the mechanical properties[1].

We recently extended the formulation of such a system by using lipid liquid crystalline (LC) phases stabilized by hectorite nanoplatelets[2,3]. As many polymers can be adsorbed on the platelets' surfaces, we could exploit this affinity to form a tridimensional polymeric network using the emulsion's drops as cross-linkers (Fig.1). These systems are very interesting for drug delivery-based applications since molecules both hydrophobic and hydrophilic can load the LC phases.

The goal of this work is the investigation of the correlation between the mechanical and structural properties of Polyacrylamide-based hydrogels cross-linked by the LC stabilized emulsion.

We performed dynamic mechanical analysis (DMA) and rheology measurements in order to determine the effect of the crosslinking on the mechanical properties of these systems at the macroscopic scale. We observed a remarkable enhancement of the Young and Shear moduli due to the interaction between the polymer chains and the emulsion's drops.

We completed our study by performing neutron and X-rays small angles scattering measurements in order to observe the effects of the mechanical deformation on the hydrogels' structural organization at the nm scale. We observed that the mechanical stress has a remarkable impact to emulsion's structure. First in the low-medium deformation range, the emulsion's drops shape seems to become anisotropic evolving from sphere to an ellipsoid in the direction of the stress. Furthermore for elevate deformation (at the elongation rate higher than 100%) the mechanical stress seems to induce an anisotropy at the lipid LC phase.

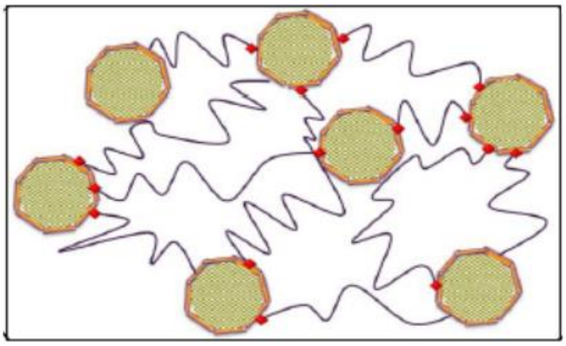

Figure 1: Schematic representation of the hydrogels cross-linked by the LC emulsion. The emulsion's drops are composed by the lipid LC phase (checked circles), which is surrounded by the nanoplatlets (brown cylinders). The polymers chains (dark lines) can be adsorbed on the NPs surface forming a 3D network.

Keywords: hectorite, nanoemulsion, polymer, hybrid hydrogels, lipid, drug delivery.

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Nonaqueous sol-gel synthesis and structural characterization of very small ZnO nanoparticles

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Abstract:

For a few decades, metal oxide nanoparticles are involved in a variety of applications and devices [1]. Zinc oxide in particular has been of high interest due to its excellent catalytic properties but also its potential use as antibacterial agent. A growing interest has risen in the synthesis of particles with a size lower than 5 nanometers since the structure of such small objects is not fully understood. Indeed, such materials present strong structural distortions in comparison to the bulk when the size decreases below the value of a few nanometers [2]. The aim of this work is to synthesize very small ZnO nanocrystals and to study their local structure. It is then of crucial importance to be able to obtain high quality particles of uniform size and shape. ZnO nanoparticles were obtained by two different non-aqueous sol-gel synthesis routes based respectively on the alcoholysis [3] or on the basic hydroxylation at low temperature in the presence of a strong complexing agent [4] of the zinc acetate precursor. The synthesized powders have been characterized by classical X-ray diffraction (XRD) and transmission electronic microscope (TEM) to estimate the phase purity and the average particle size. The results show that crystalline ZnO particles of uniform size and shape were synthesized with tunable sizes ranging from 2 nm to 6 nm. Selected samples with defined size have been analyzed by the atomic-pair distribution function (PDF) method in order to determine the nanocrystals local structure and its evolution with size. The experimental PDFs obtained from laboratory X-ray total scattering (Figure 1) clearly reveal important modifications in the nanoparticles structure induced by the nanoparticle size. Investigations are in progress to quantify the distortions of the structure and to produce pertinent structural models.

Keywords: nonaqueous sol gel synthesis, ZnO nanoparticles, pair distribution function, structural characterization, modelisation.

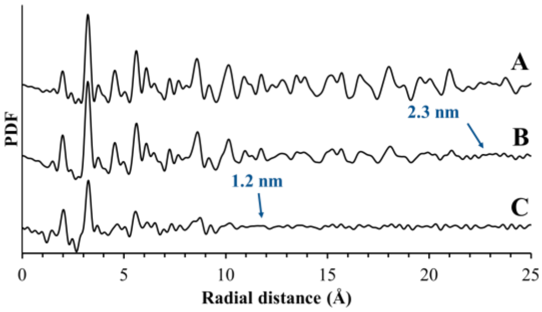

Figure 1: Evolution of the experimental ZnO nanoparticle PDFs with size

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Surface Modification at Solid-Solid Interface to Enable Selective Adhesion

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Abstract:

The understanding of the adhesion behavior of micron-/nano-scale particles at a solid substrate is of a great concern to many industrial applications. The contact adhesion at the solid-solid interface is primarily driven by the London - van der Waals (L-vdW) forces [1]. The L-vdW forces between a particle and a substrate strongly depends on the surface topography and the chemical properties of the interacting bodies [1-3]. In this study, the net adhesion forces were measured between micron-/nano-scale particulate bodies and a series of substrates with nano-scale surface morphology using atomic force microscopy (AFM) in dry and aqueous environments. The L-vdW forces acting between the interacting bodies were modeled by applying the volume element integration method on the solid-solid interface of the constructed mathematical surfaces. The adhesion forces predicted by the developed model were then validated against the experiments. Next, the physical (e.g. particle size and surface morphology) and chemical (e.g. interfacial chemistries) modifications in the target substrate were proposed to mitigate adhesion. The developed mathematical model was utilized to evaluate effect of the proposed surface modifications. The topographical modifications were found to be reducing the L-vdW forces by decreasing the contact area at the solid-solid interface. The compositional variations in the substrate were seen to be inducing a lateral drift (in addition to the normal L-vdW forces) in the approaching particle. The lateral L-vdW forces acting on the approaching particle was found to be maximum at the chemical interface. Finally, this study suggests that the topographical and chemical modifications in the substrate can be utilized as a tool to steer the path of an adhering micron-/nano-scale particle to facilitate a selective adhesion.

Keywords: Particle Adhesion, Surface modification, London - van der Waals Forces, Selective Adhesion.

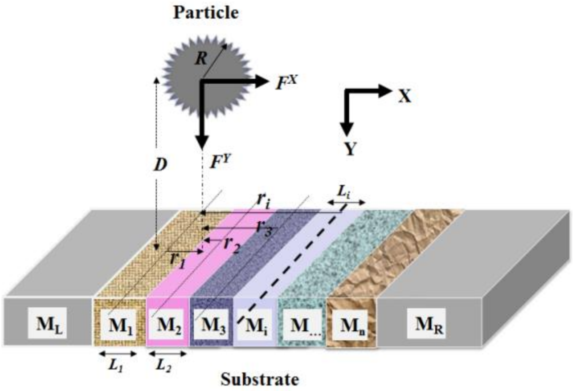

Figure 1: A schematic of particle (radius *R*) adhering to a rough and chemically inhomogeneous substrate. The substrate consists many chemical interfaces created by the patterns of different materials.

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Improving the Sensitivity of Buckypaper Strain Gauges through Tailoring their Porosity

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Abstract:

Many structural health monitoring applications require the use of strain gauges that are capable of measuring extremely small strains. Carbon nanotube (CNT)–polymer composites and Bucky papers (BPs) have previously been investigated as potential strain gauges owing to their superior strain sensitivity over conventional strain gauges. In the current work, BPs were prepared using two techniques: one involving the use of Triton X-100 as a surfactant and thus necessitating a long and thorough washing procedure and the second involving sonication at a low temperature without the use of a surfactant. The electrical resistance was evaluated at different positions in both BPs. It was found that the BP produced by the surfactant-free technique possesses lower electrical resistance. In addition, scanning electron microscopy (SEM) analysis confirmed that this technique produces more uniform BPs with fewer clusters.

Different treatment methods were used to densify the surfactant-free BPs and the effect on the strain sensitivity was investigated. The methods employed included: (1) subjecting the BPs to the vapour of a boiling solvent, which was reported by other researchers to cause densification of CNT structures [1-2], (2) annealing the BPs by heating them to 200˚C for 1 hour and (3) subjecting BPs to a 5 KN compaction force. Experimental design was used to study the effect of the interaction of the various variables on the gauge factor. The gauge factor was evaluated using a special setup involving a steel cantilever onto which the BP samples were attached. The change in resistance was measured as force was applied. Initial results show a dependence of the gauge factor on the treatment method used with compaction giving the best gauge factor exceeding by more than 6 times untreated BPs. On the other hand, the boiling solvent, although causing noticeable densification in some regions of the sample, did not result in enhancement in the gauge factor.

In conclusion, this study showed that enhancing the gauge factor of BP strain gauges is possible through employing additional treatments that are affecting the interconnectivity between the individual CNTs and thus affecting their overall electrical performance. Further experiments are underway to identify the best treatments that can give the highest possible gauge factor.

Keywords: carbon nanotubes, buckypaper, electrical strain gauge, structural health monitoring, porosity.

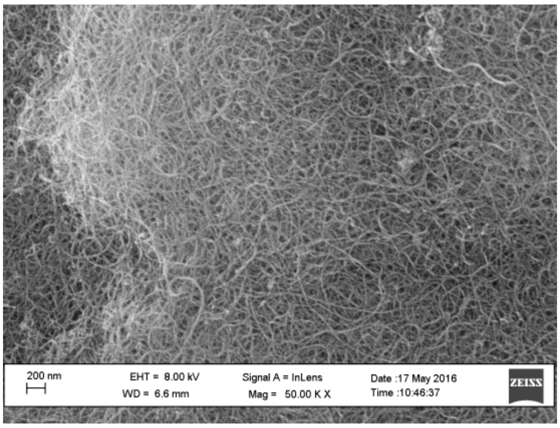

Figure 1: Surface of a BP subjected to a 5 KN compacting force showing a uniform and smooth morphology and noticeable densification.

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Session I.B:
Nanomaterials Characterization and Properties

Electrochemical Atomic Force Microscopy: In Situ Monitoring of Copper Electrodeposition on Gold Surface

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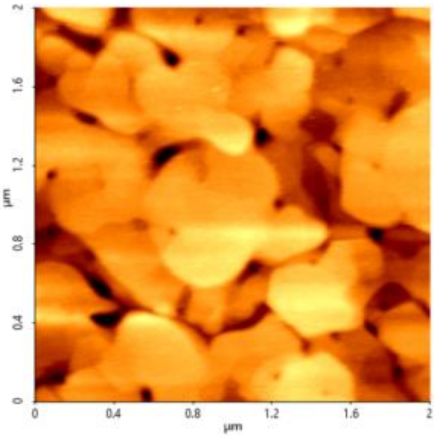
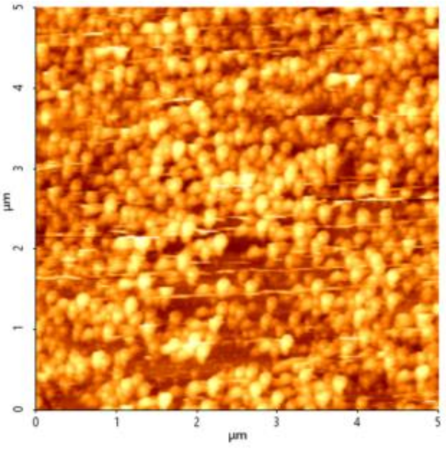
Abstract:

In recent years, understanding electrochemical processes such as electrodeposition (also known as electroplating) has become relevant for various technologies including microelectronics, nanobiosystems, and solar energy conversion due to its wide range of applications [1,2]. Electrodeposition is a conventional process that utilizes electrical current flowing through an electrolyte solution to modify surface properties, either chemical or physical, to make the material suitable for specific applications [3]. This technique is commonly done to enhance electrical conductivity, improve corrosion resistance and heat tolerance, and to make products more aesthetically appealing. A good deposition mainly depends on the substrate's surface morphology [4]. Thus, a technique that can measure this characteristic and monitor electrodeposition at nanoscale is greatly needed. There are several methods that have been employed for this kind of surface characterization. Examples include scanning electron microscopy (SEM) and scanning tunneling microscopy (STM). These techniques allow measurement of nanoscale structures however, some of them are ex situ, require a high vacuum environment, and/or are not applicable for monitoring continually changing processes because of inherently high time consumption during image acquisition [2,5]. To overcome these shortcomings, electrochemical atomic force microscopy (commonly known as EC-AFM) was introduced. This technique allows users to perform in situ imaging and visualization of changes to sample surface morphology under prescribed electrochemical environments at nanoscale [6]. In this study, the reversible deposition and dissolution of copper nanoparticles onto a substrate made of gold thin film in the (111) orientation (Figure 1) was successfully demonstrated. The morphological changes of the gold substrate before and during copper deposition and after copper dissolution were clearly observed in situ using a Park NX10 atomic force microscope system. A current-voltage (CV) curve was simultaneously acquired using a potentiostat during the experiment.

Keywords: atomic force microscopy, current-voltage curve, electrochemical atomic force microscopy, electrochemistry, electrodeposition, in situ imaging, nanoscale characterization, surface morphology



(a)



(b)

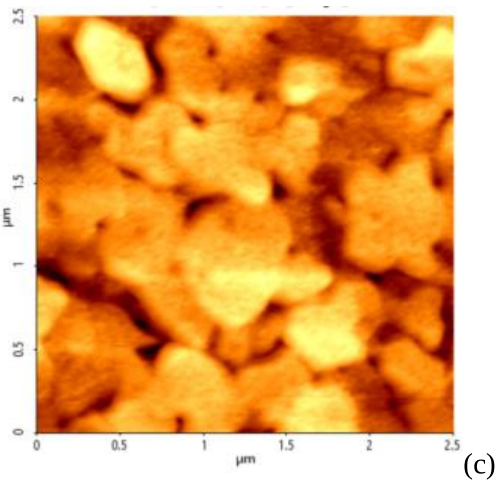
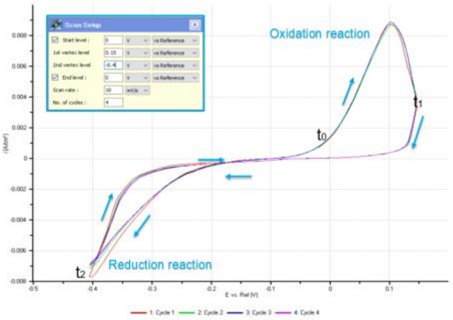


Figure 1: EC-AFM topography images of (111) oriented gold thin film working electrode before (a) deposition with scan size 2 µm x 2 µm, during (b) peak deposition with scan size 5 µm x 5 µm, and after (c) dissolution of electrodeposited copper nanoparticles with scan size 2.5 x 2.5 µm.


Scan Setup

☑ Start level : 0 V vs Reference
1st vertex level 0.15 V vs Reference
2nd vertex level -0.4 V vs Reference
☑ End level : 0 V vs Reference
Scan rate : 10 mV/s
No. of cycles : 4

Figure 2: Current-voltage curve obtained using cyclic voltammetry run during the deposition and dissolution of copper nanoparticles. The negative peaks demonstrate the reduction state where copper is deposited and the positive peaks demonstrate the oxidation reaction state where copper is dissolved. The shape of the curve suggests the entire process is reversible.

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Sub-Nanoscale topography standards for microscopy calibration: Manufacture, features and application

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Abstract:

For the success of standards for nanotechnology, their applicability and overall costs are of decisive importance in addition to the characteristic parameters that can be achieved in principle, such as size range, resolution and uncertainty.

In the field of nano-standards, the last two requirements represent a particular challenge. The dimensions of the probe and the calibration artifact are often of the same order of magnitude. Result: The measuring signal is a complex convolution of instrument and sample properties. A safe deployment, an essential prerequisite for a reliable use, can usually only be achieved with significant time and measuring effort. In addition, substantial technical and scientific expertise is required from the user to guarantee the reliability of the results or calibration.

In this paper topographic standards are presented which allow the calibration of the z-axis of microscopes (e.g. AFM) with the aid of sub-nanometer steps and additionally atomically flat surfaces to characterize flatness of image fields accordingly.

For the production of these standards, principles of self-organization are applied making use of the symmetry properties of silicon crystals. With these standards a calibration of ultra high resolution microscopes, operating at nano and sub-nanometer level, with a resolution in the sub-nanometer range with an uncertainty of several tens of picometers can be realized; representing a reduction of more than one order of magnitude compared to classical standards for this application.

In addition, this approach offers further advantages for the user, since simple separation of sample and instrument properties can be achieved here, i.e. the requirements for the successful application of these standards can be significantly lowered. This is made possible by a-priori information on the standards resulting from symmetry properties of the silicon crystals, thus enabling automated data evaluation.

Furthermore the costs for the production of traceable standards can also be significantly reduced, since the lattice parameters of silicon can be used as an invariant of nature to achive traceability.

Keywords: step height standards, self-organisation, Silicon, single crystal, AFM, optical microscopy.

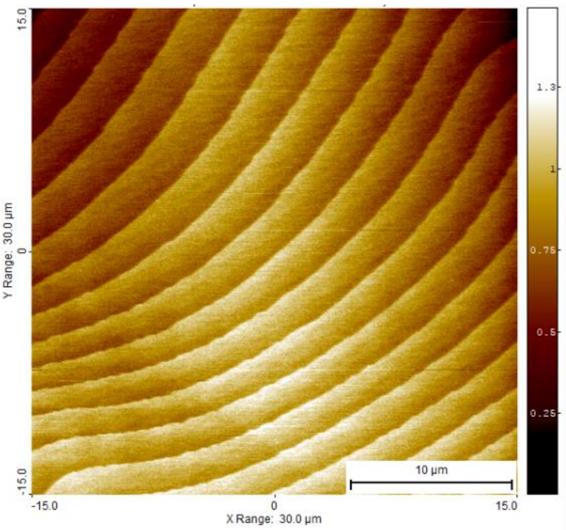

Figure 1: Image of a step height standard with single atomic stepping. The picture is made with an atomic force microscope (AFM). The area is 30 µm x 30 µm, the z-Range is 2 nm. Each line is representing a single atomic step with the lattice spacing of the (111) lattice plane. The standard has been formed by a self-organisation process.

Multi-scale assessment of soot using electron microscopy: applications on soot from bench-scale fire of polymers

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Abstract:
Soot is a degradation product of material burning, having the multi-scale fingerprints of the conditions in which it is formed. Micron sized aggregate morphology is dependent on residence times and burning rates, whereas particle size and nanoscale order reflects the burning source and temperature rates. In this work, we will present comparison of techniques for ex-situ analysis of soot probed in-flame from flaming combustion of natural and synthetic polymers, by means of SEM/STEM (Scanning electron microscope in transmission mode) and TEM.

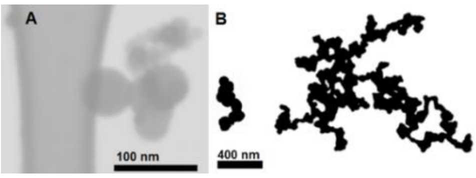

Figure 1: **A.** STEM image of soot agglomerate. **B.** Binarized images from STEM recordings [1].

STEM was practical for aggregate measurements and rapid screening due to the faster handling of multiple samples. STEM and TEM recordings were analyzed by manual and semi-automated techniques (Fig.1). Nonetheless, 2D measurements can lead to errors in aggregated media. 3D morphology was then analyzed by TEM (Fig.2) thanks to the volume data provided by tomography reconstruction. Advantages and disadvantages of techniques will be emphasized such as the limitations of STEM resolution, of TEM reconstructions, downsides of the image computation for overlapping particulates in aggregated media (i.e. both physical overlapping and projection artifacts [2]). Finally, some high resolution assessments will be made (Fig.3), based on our previous studies on nanoscale order indicating promising results in terms of scenario identification for bench-scale fire [1]. To conclude, we will introduce some numerical modeling aspects (material-radiation interaction) which are fed by microscopy measurements [2] and discuss the uncertainties. The work will allow the discussion of prospective insights with the community, on the measurement of carbonaceous materials and on the implications for other techniques used, e.g. for particle counting and monitoring in complementary domains as environment and toxicity.

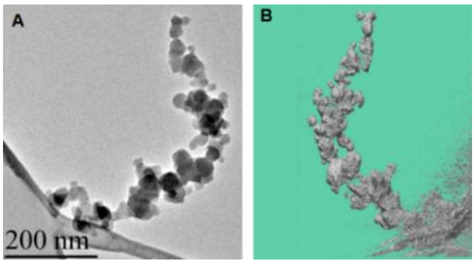

Figure 2: **A.** TEM image of soot. **B.** Corresponding tomography reconstruction from stack of rotated images (-60° to +60°).

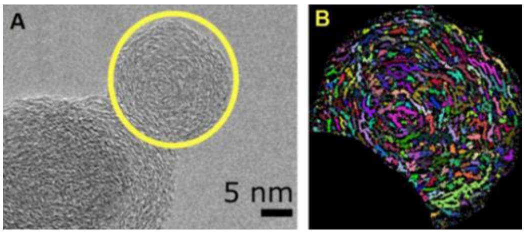

Figure 3: **A.** TEM recording of particles at high magnification. **B.** Corresponding image analysis to highlight the nanoscale order [1].

Keywords: soot, multi-scale, electron microscopy, tomography, aggregates, fractals.

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Investigation of the spin-orbit coupling effect of intrinsic and *p*-type 2D MoS_2 by spectroscopic ellipsometry

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Abstract:
2D MoS_2 films have been widely introduced into various photoelectric devices, such as solar cell, photodetector, and field effect transistor, benefiting from the layer-dependent bandgap, excellent on/off current ratios, strong spin-orbit coupling effect, valley-selective circular dichroism, and valley Hall effect[1]. The spin-orbit coupling effect occuring in 2D MoS_2 has great influences on the performance of related novel spintronics and valleytronics devices. Unfortunately, this exciting photoelectrical property is sensitive to sample thickness, temperature, and doping. Therefore, for the sake of optimal design and property improvement for 2D MoS_2 based devices, it is significant to systematically reveal the dependency of the spin-orbit coupling effect on the thickness and doping situation.

In this work, critical points (CPs) of intrinsic and *p*-type 2D MoS_2 were investigated by Spectroscopic ellipsometry[2]. An innovative approach called 2-step method is introduced to synthesize large-area and uniform intrinsic and Nb doped (*p*-type) 2D MoS_2 films. The uniformity, crystalline quality, and thickness of MoS_2 samples have been checked by AFM, micro-Raman spectrometer, and TEM. The dielectric functions of intrinsic and *p*-type MoS_2 with different thickness were extracted from the ellipsometric spectra over the energy range of 0.73 eV-6.42 eV. CPs of MoS_2 film were determined by the CP analysis theory. Critical points A and B shown in Fig. 1(a, b) are related to the spin-orbit coupling effect in MoS_2. And critical point C corresponds to complex many-body effects occurring between the K and Γ points of the Brillouin zone. However, there are no unambiguous interpretations for the intrinsic physical mechanisms of the D and E peaks so far. It's interesting that critical points A and B in intrinsic MoS_2 have combined into one critical point A+B in the Nb-doped MoS_2 as shown in Fig. 1(c, d). And this phenomenon can be explained by that the spin-orbit coupling effect is weakened by the doped impurity. The meaning of this feature is to provide an approach to control the spin-orbit splitting, which is promising in the design of novel spintronics devices based on 2D MoS_2.

Keywords: MoS_2, spectroscopic ellipsometry, critical points, spin-orbit coupling effect

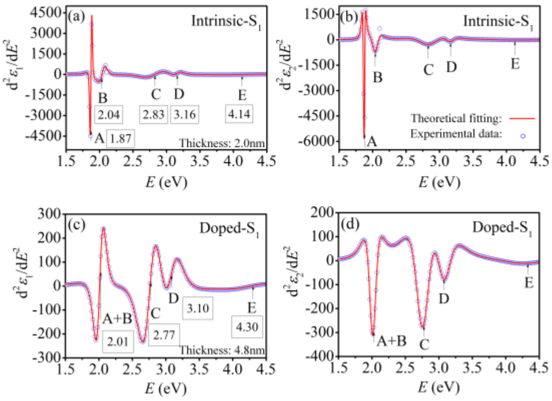

Figure 1: Results of critical point analysis for intrinsic and *p*-type MoS_2.

References:

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Optical properties of $Pb_{0.865}La_{0.09}(Zr_{0.65}Ti_{0.35})O_3$ thin films studied by spectroscopic ellipsometry

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Abstract:
The lanthanum-modified lead zirconate titanate (PLZT) is one of the most promising ferroelectric materials due to its virtue of transparency and electro-optic properties. In the last years, the study interest was mainly on the two dimensional PLZT thin films because of their potential of application into integrate optical devices. The optical properties of the PLZT films can be inherently tuned by control of the temperatures and pressures during growth. Thus, accurate characterization of the optical properties of the PLZT films is of great importance to guide optimal control of the fabrication process and further improve the performance of the optical devices. Spectroscopic ellipsometry has been developed as a powerful tool to characterize the optical properties of nanomaterials. In this work, optical properties of $Pb_{0.865}La_{0.09}(Zr_{0.65}Ti_{0.35})O_3$ (PLZT 9/65/35) thin films fabricated by pulsed laser deposition (PLD) are studied by a broadband Mueller matrix ellipsometer (ME-L ellipsometer, Wuhan Eoptics Technology Co., Wuhan, China) over a wide wavelength range of 200-1000nm. Figure 1 shows the spectra of the optical constants of the PLZT films at different deposition temperatures. A major peak can be observed in the spectra, and the position of the peak exhibits a slight red shift with the increasing of the temperatures. At the wavelength range of 300-1000nm, the refractive index gradually increases with the deposition temperatures, and the extinction coefficient is close to zero, which indicates the absorption can be neglected at long wavelength.

Keywords: spectroscopic ellipsometry, anthanum-modified lead zirconate titanate (PLZT), optical properties, deposition temperature

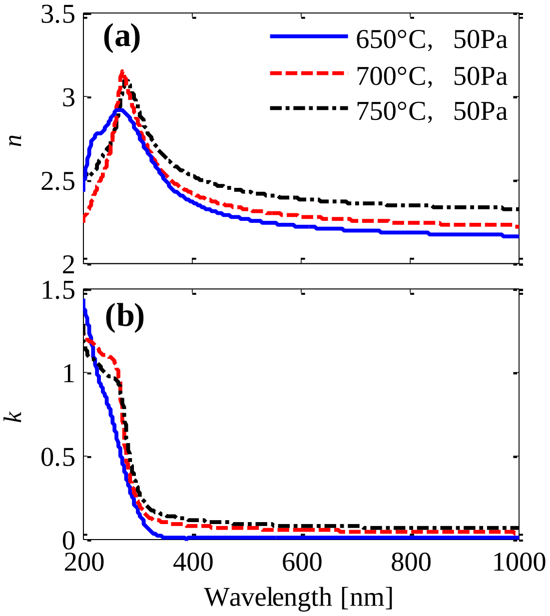

Figure 1: Optical constans of PLZT thin films versus different deposition temperatures.

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Determination of the monolayer coverage of silica particles

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Abstract:

Extreme weather conditions present significant challenges in several industrial sectors, such as automotive, wind energy, industrial cryogenics and aerospace.

Engineering solutions such as active de-icing by heating, pneumatic systems or by chemical bleed are the primary methods to deal with the issue of ice build-up. These add weight, cost and complexity, and the introduction of additional maintenance requirements.

Passive solutions are important for achieving long term-functional performance. However, an effective, durable passive anti-icing or deicing surface has been yet to be demonstrated, indicating significant developments are necessary.

Introducing enhanced chemical repellency and structured roughness into surfaces are two of the best candidates to achieve this main goal. Realizing these characteristics via the introduction of suitably functionalised silica nanoparticles represents an emerging approach that allows the modification of existing coatings and composite materials.

Selective and specific functionalization of these silica particles is crucial in order to achieve a monolayer coverage avoiding partially covered particles or a surfeit of unreacted silanes which may have undesirable impacts on the materials processing or ultimate properties.

The primary aim of this study was to establish methods to determine the degree of functionalisation and to then identify the monolayer coverage of tailored silica particles.

A model family of silica particles with diameter of approximately 35 nm was produced using a refined Stöber method. These silica particles were functionalized using n-propyltrimethoxysilane (NPTMS). A novel functionalization method was used to graft the silane to the silica particles. Particle size analysis using Dynamic Light Scattering methods was undertaken to determine the impact of the functionalisation on the average diameter and size distribution within the suspension. The functionalisation procedure led to a slight increase in the average particle diameter, but a marked narrowing of the distribution.

Drop Shape Analysis (DSA) was used to evaluate the repellency of a dried film of the functionalized silica particles deposited onto a glass slide. As the degree of functionalisation increases, the repellency of the film also increases to a maximum value followed by a plateau where increasing silane has little impact on the repellence. The influence of functionalization on the gelling behavior was also assessed. The gelation time was significantly influenced by the quantity of silane used in the functionalisation. A maximum gelation time was observed at approximately the same level of functionalisation at which the repellence started to level off.

These data indicate a clear point at which monolayer coverage of the TWI silica nanoparticles grafted with NPTMS can be inferred. This study provides the underpinning approach that allows the establishment of monolayer coverage and so optimize the coacervation of silica particles.

Keywords: silica particles, monolayer coverage, functionalization, novel properties.

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Friction Reduction on Anodized Alumina by Deposition of Ti Nanolayers

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Abstract:
Hard, protective alumina (Al_2O_3) coatings, which are obtained in sulfuric acid-based electrolytes by anodization at low temperatures, offer many advantages in food, automotive, high-tech, aerospace, biomed and other applications. Despite better hardness, surface friction is still one of the major challenges under dry sliding conditions. This is often solved by impregnation of polytetrafluoroethylene (PTFE) polymers, which act as barrier lubricants. However, application of PTFE is problematic due to the need for heating over 300°C. Therefore, new technologies to reduce friction of anodized Al would be very helpful in many applications.

In this study tribological effectiveness of metallic Ti nanolayers was evaluated on untreated and anodized alumina using two industrial alloys: 99.62% Al 1050 and 96.72% Al 6082. Tribometer in ball-on-plate reciprocating linear configuration was used for friction tests against chemically inert corundum balls. Untreated and anodized aluminum discs were used as substrates for Ti deposition by magnetron sputtering device. The test results on non-anodized alloys demonstrated that 0.5 µm Ti layers do not reduce friction at all. Even 2.3 µm Ti layers could not bring Coefficient of Friction (COF) below 0.4, see Fig. 1. In agreement with previous findings [1], anodized alloys without Ti layers had slightly lower friction than before anodization, however still well above COF 0.4. Deposition of 2.3 µm Ti layer made the alloy type or anodization irrelevant in terms of COF. However, 0.5 µm or thinner Ti nanolayers sputtered on anodized alumina have very positive effect on friction reduction and decrease COF below 0.2 (Fig. 1). As described previously [1], low friction was sustained in 16 nm and 75 nm Ti layers for at least 10 friction cycles, indicat-ing that no significant surface damage took place during initial stages of mechanical con-tacts. At 0.5 µm thickness, COF appeared somewhat higher, which suggests that this layer is too thick for tribological effectiveness. Nevertheless, the Ti layers of 2.3 µm thickness performed much worse than those of 0.5 µm or below. Consequently, a conclusion can be drawn that Ti nanolayers of less than 0.5 µm thickness have a great potential for industrial and medical applications, not only for their likely biocompatibility [2], but also for their tribological performance.

Keywords: anodization, alumina coatings, magnetron sputtering, titanium nanolayers, friction.

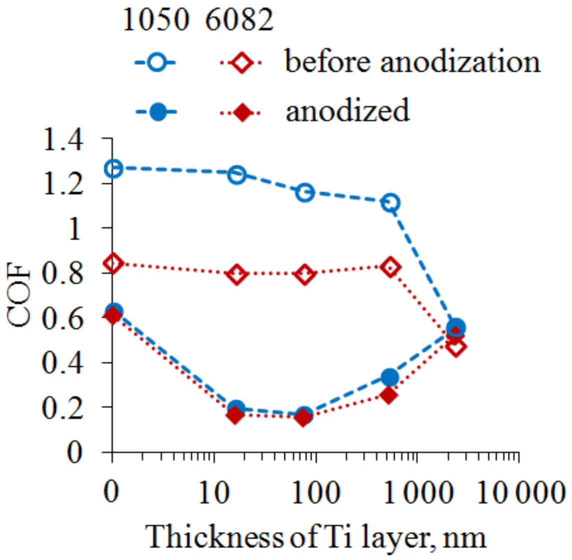

Figure 1: Influence of Ti layer thickness on Coefficient of Friction after 10 friction cycles (10 N load, 2 cm/s velocity) before and after Al anodization in sufuric/oxalic electrolyte at 15 °C, 200 A/m^2 anodic current density for 70 min.

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Porous PDMS / CNF Nanocomposites for Sensing Applications

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Abstract:
Highly stretchable and electrically conducting materials are of critical needs in emerging field of wearable electronics, prosthetics, robotic manipulation, and wearable health monitoring [1]. Polydimethylsiloxane (PDMS) elastomers are highly stretchable due to their large elastic deformation and have the ability to tailor their mechanical and deformation properties. Recent research has shown that the porous PDMS can further improve their stretchability compare to their solid (i.e., nonporous) counterparts [2]. Development of peizoresistance based sensors require that the porous PDMS be electrically conducting so that the change in resistance is proportional to the deformation. Carbon-derived nanomaterials such as carbon nanotubes (CNT), carbon nanofibers (CNF), and graphene as are excellent choice as conducting fillers. However, effective incorporation of carbon nanomaterials, such as CNF in porous PDMS nanocomposite still remains a challenge towards the development of highly flexible sensing materials and devices.

This paper reports the fabrication of highly flexible and electrically conducting porous PDMS/CNF nanocomposites using sugar particles as template. CNF are transferred in the pore walls of the porous PDMS via direct and indirect methods (See Figure 1). In the direct method, the sugar particles are first coated with CNF which ensure good adhesion between the CNF and the polymer during the fabrication process. In the indirect method, the raw sugar particles are used to make the porous PDMS followed by forced impregnation of CNF via ultrasonic agitation. Solvents with different CNF concentration are used to investigate the effectiveness of the CNF transfer in the pore walls of the porous PDMS. High resolution scanning electron microscope is used to investigate the CNF distribution with and around the pore walls. Mechanical properties and electrical conductivity are measured. The sensing ability of the porous PDMS/CNF nanocomposite is characterized under compression loading and their corresponding sensing functions are also evaluated.

Keywords: PDMS foam, carbon nanofiber, mechanical properties, compression behavior, electrical conductivity.

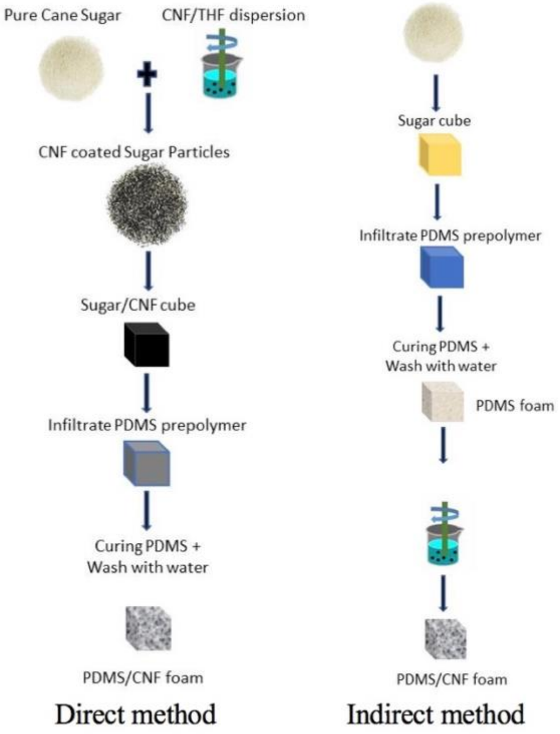

Figure 1: Schematic representation of two types of preparation method for porous PDMS/CNF nanocomposites.

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Tuning the electronic response of MoS_2 by pressure induction

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Abstract:

Layered two-dimensional (2D) transition-metal dichalcogenides (TMDs) have garnered intense attention as a result of their potential applications in optoelectronics, catalysis, electrochemistry and medicine. Their interest lies in the different electronic and optical properties that can be achieved based on different elemental composition and as a function of their number of layers. A representative example of TMDs family is MoS_2. It is an indirect band-gap semiconductor that turns to a direct-gap semiconductor when is exfoliated from bulk down to a monolayer, thus making it very interesting for electronic, optoelectronic and photovoltaic applications.

Another interesting property that recently has been focus of study for many groups, is the strain effect over MoS_2. Theoretical calculations show that the application of an external pressure over the flakes modifies the band-gap, changing their electrical behavior from semiconductor to metal[1]. Thus, the controlled and reversible application of this strain can be used as a tool to modulate MoS_2 properties and develop new hybrid 2D materials, towards the fabrication of multifunctional devices.

In this work we propose a new approach to induce a reversible strain change on MoS_2 flakes by means of their functionalization with molecular systems which volume can be tunned by the application of an external stimulus. In this context, spin-crossover materials (SCO) are ideal candidates. These SCO molecular materials can change the ground spin state between low and high spin state upon the exertion of various external physical or chemical stimuli, resulting in a variation of volume that could induce the strain over the flake[2]. We have achieved the decoration of MoS_2 flakes with SCO nanoparticles (NPs) of the well-known core-shell system $[Fe(Htrz)_2(trz)](BF_4)@SiO_2$; these NPs present a transition above roomtemperature with a broad hysteresis, 40 K, and experiment a change in volume of *ca.* 10 %.

This transition has a direct effect on MoS_2 electronic properties, as highlighted by transport measurements (Figure 1b).

Figure 1. TEM image of a MoS_2 flake decorated with NPs (top), and transport measurement of the same system (down).

Keywords: layered two-dimensional materials, Molybdenum disulfide, spin crossover, molecular material.

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Solution-processable inorganic hole injection layer to improve the performance of quantum-dot light-emitting diodes

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Abstract:

Solution-processable vanadium oxide (V_2O_5) was used as an inorganic hole injection layer (HIL) to improve the performance and stability of quantum-dot light-emitting diodes (QLEDs). Non-acidic and non-hygroscopic V_2O_5 solution was synthesized and spin-coated onto indium-tin-oxide (ITO)/glass substrate to serve as an HIL for QLEDs. QLEDs with a V_2O_5 HIL showed efficient hole injection and had improved luminous efficiency and life-time. Maximum luminous efficiency of QLEDs fabricated under ambient conditions were 2.96 Cd/A. Photoelectron spectroscopy measurements were conducted to construct an energy level diagram of the QLEDs, and we found that the gap states of V_2O_5 enabled efficient hole-injection from ITO into the devices through the V_2O_5 HIL. Interfacial energy level diagrams of TFB/ V_2O_5/ITO and TFB/PEDOT:PSS/ITO are summarized in Fig. 1(a) and (b), respectively. A gap state was observed at the HOMO region in the spectrum of V_2O_5 and it was located at 0.95 eV below the Fermi level, close to the HOMO level of TFB. Therefore, the gap state of V_2O_5 could play a significant role in hole injection from ITO into the emitting layer.

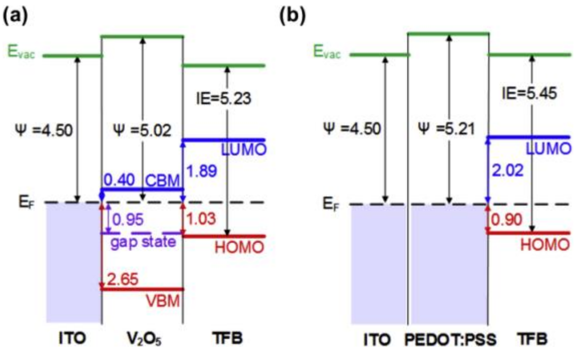

Figure 1: Interfacial energy level diagrams.

Therefore, QLEDs was fabricated with V_2O_5 HIL on a glass substrate as shown in Fig. 2. Luminous efficiency of QLEDs with a V_2O_5 HIL were superior to that of QLEDs with a PEDOT:PSS HIL. The maximum luminous efficiency of QLEDs with a V_2O_5 HIL was 2.96 cd/A, approximately 6-fold higher than that of QLEDs with a PEDOT:PSS HIL.

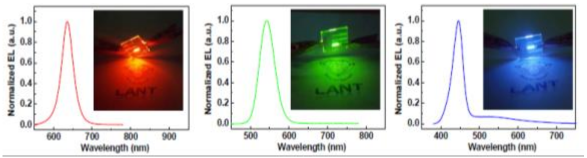

Figure 2: Fabricated QLEDs with V_2O_5 HIL.

These results suggest that solution-processable V_2O_5 is a feasible alternative to organic HILs for high-performance QLEDs.

Keywords: Quantum-dots, Light emitting dioide, interface electronic structure, photoelectron spectroscopy, hole injection layer

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Highly Conductive, Mechanically Robust Ion Gels Based on Copolymers and their Electrochemical Applications

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Abstract:

Polymer gel electrolytes (PGEs) have been employed in diverse applications including electrolyte-gated transistors, electrical skins, batteries, and electrochemical displays. However, a trade-off between two important properties of PGEs, ionic conductivity and mechanical property, is inevitable.

We propose a simple but effective strategy to prepare mechanically robust and highly conductive ion gels based on random copolymers, poly[styrene-*ran*-1-(4-vinylbenzyl)-3-methylimidazolium hexafluorophosphate] (P[S-*r*-VBMI][PF_6]). When we judiciously selected a composition of P[S-*r*-VBMI][PF_6] and the ionic liquid of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMI][TFSI]), the resulting ion gels exhibited large mechanical resilience (elastic modulus of 0.105 MPa) and high ionic conductivity (1.15 mS/cm). We employed this gel for electrochemical applications such as electrochromic devices (ECDs). The fabricated ECD based on the P[S-*r*-VBMI][PF_6]-gel operated at a low voltage bias (sub-1V), and showed a large transmittance contrast (ΔT) and good coloration/bleaching cyclic stability. We also examined device dynamics, at which diffusion-controlled behavior was observed. Moreover, by taking advantage of excellent mechanical property of the gel, we successfully demonstrated flexible ECDs on plastic. The device showed excellent bending durability against both tensile and compressive strains (Figure 1). The P[S-*r*-VBMI][PF_6]-based gel in this work offers a new solid-state electrolyte platform for flexible electrochemical devices such as ECDs, electrochemiluminescence (ECL) devices, and batteries.

Keywords: block copolymers, ion gels, ionic liquids, electrochemical displays, electrochemiluminescence, electrochromism, flexible electronics.

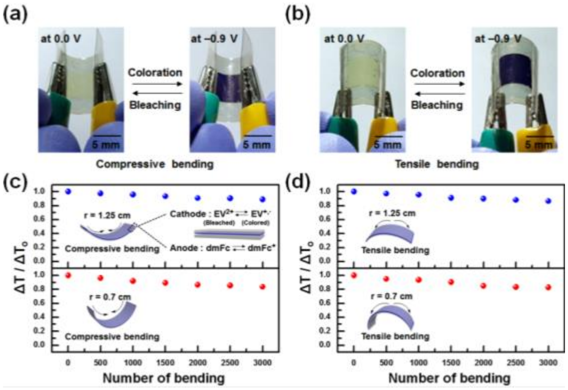

Figure 1: Photographs of ECDs bleached state and colored state under (a) compressive and (b) tensile bending. Changes in $\Delta T/\Delta T_o$ as a function of the bending number under (c) compressive and (d) tensile bending.

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Enhancement in thermoelectric properties of Te-embedded Bi_2Te_3 by stong phonon scattering at interface

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Abstract:

A comprehensive understanding of the nano-structural effects that cause reduction in thermal conductivity represents important challenges for the development of thermoelectric materials with an improved figure of merit ZT. Bismuth telluride (Bi_2Te_3)-based thermoelectric materials exhibit very low levels of thermal conductivity. In this study, a Te crystal-embedded Bi_2Te_3 (Te–Bi_2Te_3) thin film was formed by establishing a specific annealing temperature for a Te-rich Bi/Te multilayered structure with molecular beam epitaxiy (MBE) method. Modulations in structure and composition were observed at the boundaries between the two phases of Te and Bi_2Te_3. Furthermore, the samples contained regularly shaped nanometer-scale Bi_2Te_3 single grains. Therefore, we obtained a dramatic ZT value of 2.27 (+0.04, −0.08) at 375 K from the Te–Bi_2Te_3 thin film. Through comparison of Te-embeded Bi_2Te_3 and prous-Bi_2Te_3, we confirmed that strong interface phonon scattering between the Te–Bi_2Te_3 boundaries while electrically conductive plays an important role in inter-grain transport properties, which results in a reduction in the lattice thermal conductivity while electricl conductivity remained.

Keywords: Bi_2Te_3, Thermoelectric, nano-structure.

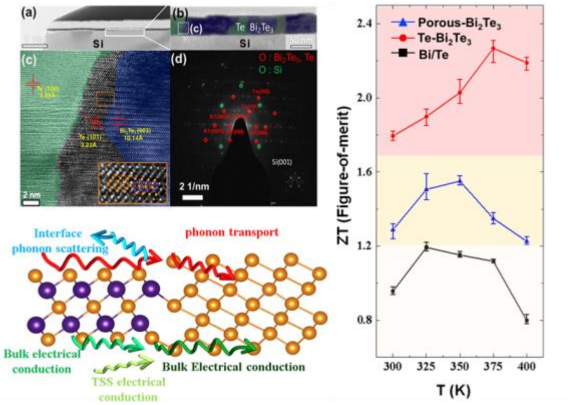

Figure 1: Figure illustrating TEM image of nanostructured Te-embedded Bi_2Te_3 structrue. By strong phonon scattering between Te and Bi_2Te_3 interface, while electon conduct without barrier, thermoelectric properties can be enhenced. Figure of merit in Te-embedded Bi_2Te_3 structrue is 2.27 (+0.04, −0.08) at 375 K

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Multi-functional copolymer for coating on magnetite nanoparticle for use in bioconjugation

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Abstract:

Surface modification of magnetite nanoparticle (MNP) with a multi-functional copolymer and its bioconjugation is presented herein. This copolymer was designed to possess multi-functions including 1) thermo-responsive poly(*N*-isopropyl acrylamide) (PNIPAAm) serving as a drug reservoir and for drug controlled release, 2) thiolactone moiety for covalent grafting onto MNP surface and also inducing the formation of MNP nanoclusters and 3) cationic poly(diethylaminoethyl methacrylate) (PDEAEMA) for improving its water dispersibility and for ionic adsorption with DNA. Fourier Transform Infrared Spectrophotometry (FTIR) results signified the existence of the copolymer in MNP nanoclusters. The copolymer-coated nanoclusters showed the significant increase in zeta potential from +16 mV to +28 mV after quaternization. This significantly improved dispersibility of the particle in an aqueous media and it was thus used as a cationic platform for adsorption with DNA through the electrostatic interaction. Thermo-responsive PNIPAAm coated in the nanoclusters collapsed at the temperature above its critical solution temperature, resulting in the shrinkage of the nanoclusters and thus eventually decreasing their hydrodynamic size (D_h). The shrinkage of the copolymer when heated to 45 ^{o}C would be utilized as a triggering mechanism for drug controlled release application. It was also found that the use of alkyl amines having various chain lengths ($R-NH_2$; where R is alkyl groups having C3, C8 and C12) in the nucleophilic ring-opening reactions of the thiolactone rings affected their magnetic separation ability, water dispersibility and release rate of doxorubicin model drug. These versatile copolymer-coated nanoclusters showed a great potential for use as a smart platform for bioconjugation and drug controlled release application.

Keywords: magnetite nanoparticle, multi-functional copolymer, thermo-responsiveness, drug controlled release**.**

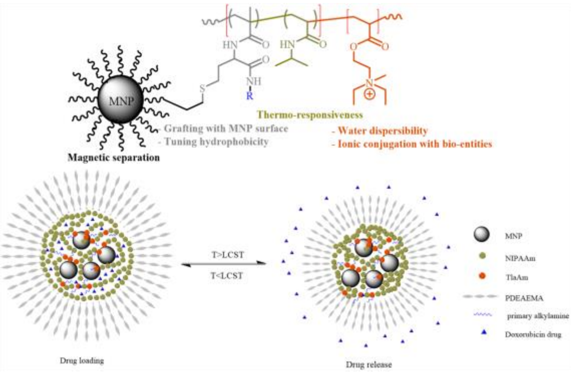

Figure 1: Illustrating the surface modification of magnetite nanoparticle (MNP) coated with the multi-functional copolymer and its use in controlled drug release.

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Poly(*N*-acryloyl glycine)-grafted magnetite nanoparticle conjugated with pyrrolidinyl peptide nucleic acid for selective enrichment of trace DNA samples

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Abstract:

Poly(*N*-acryloyl glycine) (PNAG)-grafted magnetite nanoparticle (MNP) was used as magnetic support for real deoxyribonucleic acid (DNA) preconcentration using pyrrolidinyl peptide nucleic acid (PNA) as a probe. The PNAG-grafted MNP was covalently conjugated with streptavidin, followed by immobilization with biotin-conjugated PNA via specific interaction between biotin and streptavidin. The particles with the size of 300-400 nm were well dispersible in water, had a good response to a magnet and had the capacity of 373 pmol PNA/mg MNP. The probe on the particle can discriminate between non-complementary and complementary DNA using fluorophore-tagged DNA as a model. Also, the particles were used for precontration of zein genes of maize in fresh produce and eight cereal products as real samples. After the desorption of the DNA adsorbed on the particle and then amplification with Polymerase Chain Reaction (PCR) technique, gel electrophoresis indicated that only the real samples having zein gene of maize can be adsorbed on the PNA-functionalized MNP, indicating the high specificity between PNA and complementary DNA. This PNA-functionalized MNP might be effectively used as nano-solid supports for DNA enrichment in real samples.

Keywords: magnetite, nanoparticle, nano-solid supports, pyrrolidinyl peptide nucleic acid, PNA probe, real deoxyribonucleic acid, enrichment, pre-concentration

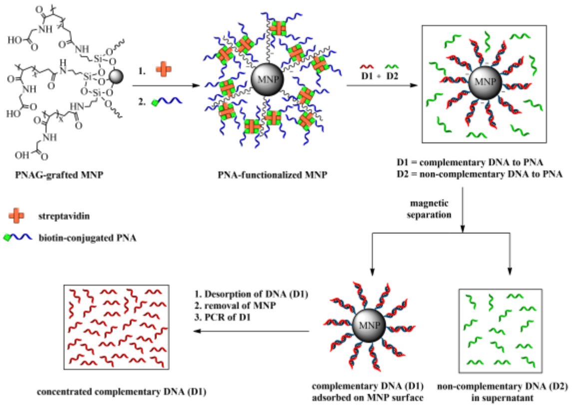

Figure 1: Description of DNA enrichment using PNAG-grafted MNP functionalized with PNA probe as nano-solid supports.

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Antibacterial activity of high-k oxides deposited by the ALD method - applications in biology and medicine

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Abstract:

Metal oxides (high-k oxides and zinc oxide) find their widespread applications in modern electronics. Recently, special attention has been paid to their antibacterial properties, due to which they can be also used in biology, medicine, and food industry. For mentioned application, atomic layer deposition (ALD) was the most suitable metod, becauce it allows to receive uniform coating of various materials, including temperature sensitive ones (e.g., perishable fabrics) and equipment and instruments (including implants) used in hospitals and in a food industry. In the currest study we investigated the antibacterial activity of various high-k oxides (HfO_2, TiO_2, ZrO_2, and Al_2O_3). As a positive reference the ZnO layer of known antibacterial activity was used. Antimicrobial susceptibility testing was performed according to the agar disk diffusion method, which is normally used to determine drug sensitivity. Tests were performed using bacterial strains both reference and wild serotypes, that can be commonly found in nature, mostly in the skin, mucous membranes and gastrointestinal tract in humans and animals, but also they in the air, dust, on the objects in the soil, water or effluent. According to the obtained results we can conclude that ALD-deposited metal oxides exhibit antibacterial properties, thus promising a range of potential applications in medicine, veterinary, broader health care, and food industry.

Keywords: atomic layer deposition (ALD), high-k oxides, antibacterial properties, biological and medical applications

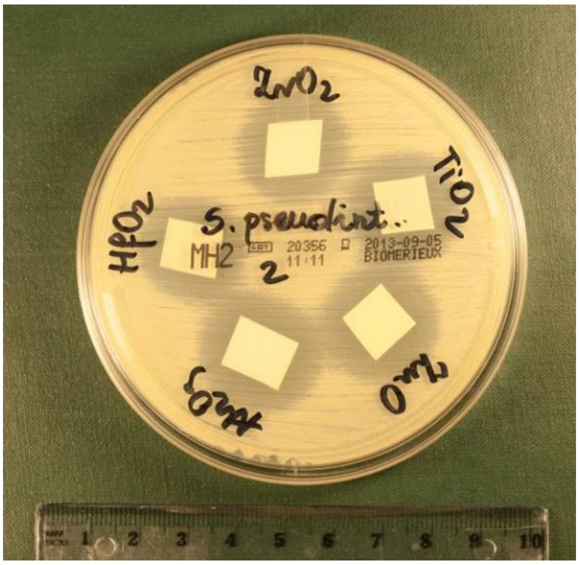

Figure 1: Figure illustrating the zones of bacterial growth inhibition formed around the paper disks coated with monolayers of metal oxides. *Stahpylococcus pseudintermedius* on Mueller-Hinton agar plates. The dark zones around the disks indicate the zone of bacteria growth inhibition where bacteria were sensitive to selected oxide layers.

Acknowledgments:

NCN DEC-2012/05/E/NZ4/02994, NCN 20/0139/N/ST3/04189, 05-1/KNOW2/2015

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Nanoparticles and Nanofibers/Polymer Conjugates for Antibacterial, Anti-corrosion and Drug Delivery Applications

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Abstract:

Bacterial infections in health facilities are one of the key challenges facing humanity today and this is worsened by the current trend of anti-biotic resistance and resistance to natural controls through different adaptive mutations. Currently, disinfection is done through the use of powerful chemical agents which come with harmful side effects to both human health and the environment. The present invention (NANO-Fib-TECH, a spin-off company of AUC) is focused on the fabrication of natural polysaccharide (chitosan) composite electrospun nanofibers mixed with other FDA approved materials (in some variations also with other fillers) and solubilize the produced nanofibers to be used as natural liquid disinfectant and antibacterial as well as anticorrosive agent. The main challenge in this invention was to fabricate a composite that has purely natural and FDA approved materials, and yet overcome the conventional disinfectans in the market which have major drawbacks, and more importantly is to make a liquid solution of the fabricated electrospun composite nanofibers to be applied directly in different surfaces such as floors, walls and machinaries without causing any side effects to the users.

Our latest results on designing novel core-shell silver/polymeric NPs composed of Ag core and three different polymeric shells which were loaded with a chemotherapeutic agent doxorubicin (DOX) will be presented. Notably, low dosage of core-shell DOX-loaded Ag/polymeric nanocarriers (NCs) exhibited a synergic anticancer activity, with DOX-Ag/PVP being the most cytotoxic. We believe that the prepared NPs-based combinatorial therapy showed a significant enhanced cytotoxic effect against breast cancer cells.

Latest results on radiolabeling AgNPs conjugations and evaluating their cytotoxicity and animal models results will be illustrated. Moreover, recent achievments on fabricating electrospun nanofibers and nanocomposites as Na-noscaffolds for wound dressings, prebiotic and anti-bacterial applications will be presented.

Keywords: antibacterial, electrospinning, nanofibers, Drug delivery, cancer, silver nanoparticles, core/shell combinatorial therapy, polysaccharides

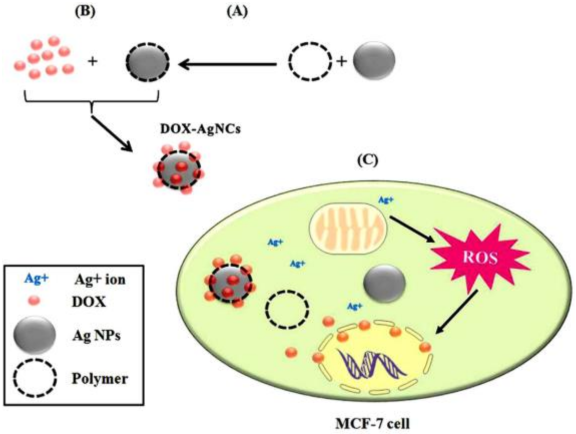

Figure 1: Scheme of the synergic cytotoxic effect of DOX-loaded Ag/polymeric NCs at very low doses of DOX on MCF-7 cells.

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Nano-formulations of encapsulating Essential Oils in polymeric nano-carriers with antioxidant and antibacterial properties

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Abstract:

Different Essential oils (EOs) were encapsulated in polymeric nanoparticles. The aim of EOs encapsulation was to convert the pure EOs into a heat stable and water soluble powder form with enhanced antioxidant and antibacterial activities. Encapsulation process relies on emulsification followed by cross linking method. Nanoparticles was investigated through different characterization techniques such as; Dynamic light scattering (DLS), Fourier transform infrared (FT-IR) spectroscopy, powder X-ray diffraction (XRD). Transmission electron microscopy (TEM) detected spherical shapes of nanoparticles with average size range below 100 nm. Thermogravimetric analysis (TGA) showed an enhancement in the thermal stability of encapsulated EOs by more than 1.7 folds. Encapsulation efficiency (EE %) and loading capacity (LC %) of the encapsulated EOs were in range of 22 - 82% and 2 - 23 %, respectively. The *in-vitro* release studies in two buffering solutions; acetate buffer and phosphate buffer saline showed an initial burst effect followed by a slow release for more than 72 hrs, providing sustained release profile. The study showed the ability of polymeric nanoparticles to preserve bioactive phenolic compounds in EOs. The antioxidant activity of encapsulated EOs was improved by about 2 folds. Finally, EOs loaded polymeric nanoparticles showed an enhancement in the antibacterial activity on both Gram positive and negative bacteria by about 39 - 57% and 1.8 – 3%, respectively.

Keywords: polymeric nanoparticles, Essential oils (EOs), in-vitro release, bioactive phenolic compounds, antioxidant activity, antibacterial activity.

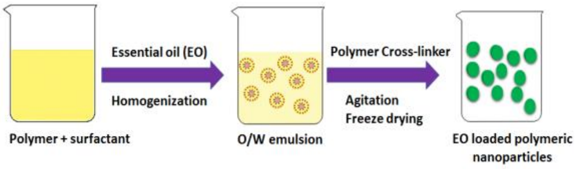

Figure 1: Figure illustrating the Essential oil encapsulation process.

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NanoMetrology 2018
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Intercalating carbon nanotubes into graphene folds

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Abstract:

Folding graphitic materials have the potential to create complex structures with new properties.
Intercalating molecules into these folds is an interesting method of one-dimensional functionalisation of a graphene sheet. Here, we investigate the incorporation of a single-walled carbon nanotube into folded graphene structures and between sheets of graphene. The optimal curved structure caused by both the elastic and van der Waals energies is examined using variational calculus. Results are shown to match with molecular dynamics simulations.

Keywords: graphene, carbon nanotubes, calculus of variations, elastic energy, van der Waals force.

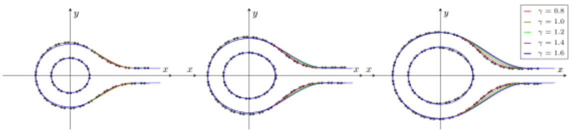

Figure 1: Minimising the elastic bending energy and van der Waals energy gives rise to the minimum energy configurations of curved graphene sheets wrapped around various sizes of carbon nanotubes. This figure shows overall agreement between the analytical solutions based on calculus of variations for different values of bending rigidities and results for molecular dynamics studies.

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Energy behaviour of atomic force microscope cantilever system

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Abstract:

Brief introduction on an atomic force microscope will be given. Here, we utilize mathematical modelling, comprising Lennard-Jones potential and techniques involving calculus of variations, to obtain the energy equations arising from the probe and the substrate, leading to the deflection equations of the cantilever. We assume a silicon tip and the substrate surface is assumed to be a graphene sheet. The geometry of cantilever tip is shown in Fig. 1. The spring constant and the bending behaviour of cantilever system will be discuss. Further, the comparison between bending energy and van der Waal energy is studied and it is shown in Fig. 2.

Keywords: mathematical model, calculus of variations, elastic energy, van der Waal energy.

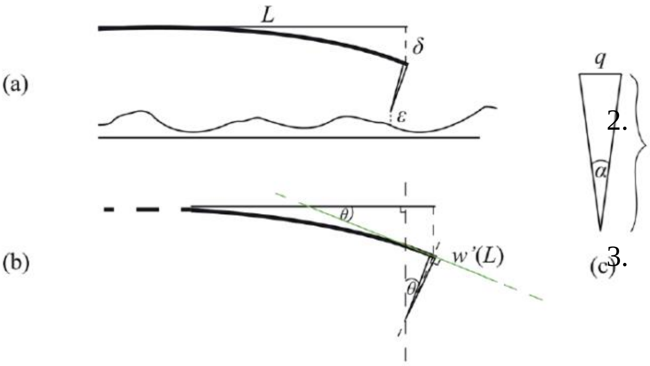

Figure 1: Geometry of cantilever.

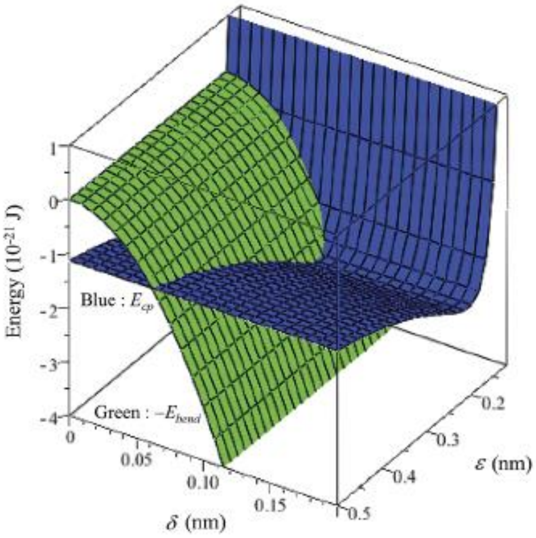

Figure 2: Comparison of bending and van der Waals energies.

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Modeling of Polyoxometalates for Surface Fuctionalization: Nano-scale Interactions Controlling Macroscopic Features

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Abstract

Owing to their tunable properties, polyoxometalates (POMs) are widely used in several fields. Surfaces of carbon nanotubes were modified with $Ru_4(SiW_{10}O_{36})_2^{10-}$ to obtain stable oxygen-evolving anodes for efficient water splitting (Toma *et al.*). Moreover, in the *VicInAqua* project, membrane pores were decorated with $Ru_4(SiW_{10}O_{36})_2^{10-}$ exploiting POM interaction with polymerizable surfactants in order to produce O_2 from H_2O_2 dismutation. Nascent O_2 promotes the pores cleanliness (Squarcina *et al.*) and self-cleaning membranes are thus made. $[PMo_{12}O_{40}]^{3-}$ showing high redox potential was also used for the preparation of antimicrobial coatings. Extenuating experimental tests are necessary to synthesize POM-based nanostructures, hence the nanoscale modeling can help their optimization. A quantum (DFT) and molecular mechanics modeling of the mentioned POMs is presented herein. The binding energies associated to the interactions between Ru based POM and surfactants were first evaluated in presence of Na^+ and Cl^- in order to clarify the effect of these ions on the stability of the surfactant-catalyst complex. To elucidate the effect of inert cations on the catalytic activity, the interaction between the hydrated Na^+ with the Ruthenium core was also modelled. The geometries of the surfactant-Ru_4POM complex are unknown, thus, the stablest structures were found. The solvated ions do not significantly modify the geometry of the complex as well as the POM-surfactants interactions, although a change in binding energies has been found. Interestingly, the hydrated Na^+, initially linked to the catalyst *via* water molecules H-bonds, after geometry optimization, binds directly to the POM atoms. This can lead to changes in the catalytic activity of the $Ru_4(SiW_{10}O_{36})_2^{10-}$.

Keywords: POMs-based nanostructures, *ab-initio* modeling, supramolecular chemistry.

Noncovalent interactions between $[PMo_{12}O_{40}]^{3-}$and ammonium surfactants, were also evaluated to check if an undesirable exchange with anions can take place. Energy balances were theoretically assessed, showing that the Br^- counterion, initially attached to the surfactants, cannot be exchanged in large extent with the $[PMo_{12}O_{40}]^{3-}$. As a result, the concentration of the surfactants at the water/polymer interface must be sufficiently high to prevent the POM release (*critical surfactant concentration*, De Luca *et al.*). To validate the theoretical findings, accurate measurements were carried out by using homemade coatings. Bromide concentration in the POM solution was followed at different times by gravimetrical analysis. The agreement between theoretical prediction and experimental data was remarkable, as this *ab-initio* modeling correctly accounted for the involved noncovalent short-range interactions Analogous predictions were achieved for the $[PMo_{10}V_2O_{40}]^{3-}$ POM.

Acknowledgment

The work performed has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 689427 for the project **VicInAqua**.

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Modeling realistic TiO_2 nanoparticles and their interaction with water

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Abstract:

Among all the synthesized nano titania, high curvature nano-systems, e.g. nanospheres (NSs) or nanorods, are of prominent interest for TiO_2 functionalization in photoapplications and biomedicine.[1] TiO_2 NSs are fundamental building blocks of technologies that operate in an aqueous environment, thus understanding their interaction with water is of extreme importance. Despite the great interest on TiO_2 nanoparticles and their interaction with water, quantum chemical studies have been, so far, limited to low index TiO_2 surfaces, due to the large size of realistic TiO_2 NSs. However, titania flat surfaces are far to be representative of the real highly curved surface of nanospheres. We present an innovative computational approach, which allows to tackle the complexity of realistic TiO_2 nanospheres (with a diameter of 2.2 nm) interacting with water multilayers (Figure 1), keeping a quantum chemical level of theory. First, we use an highly performing DFT-based semiempirical method, namely density functional tight-binding theory (SCC-DFTB), to obtain globally optimized NSs structure in vacuum.[2] Second, we set up new SCC-DFTB parameters to simulate the interaction between TiO_2 and water with an accuracy comparable to DFT.[3] Finally, the static and dynamic interaction of the NSs with water is studied at both DFT (only static) and SCC-DFTB (static and dynamic) level of theory.[4] This study gives a precious atomistic insight on the processes occuring at the TiO_2 NS/water interface and on the influence of the aqueous medium on the NS structural and electronic properties.

Keywords: TiO_2 Nanoparticles, SCC-DFTB, Hybrid DFT, Molecular Dynamics, Solid-Liquid Interface, Water Adsorption.

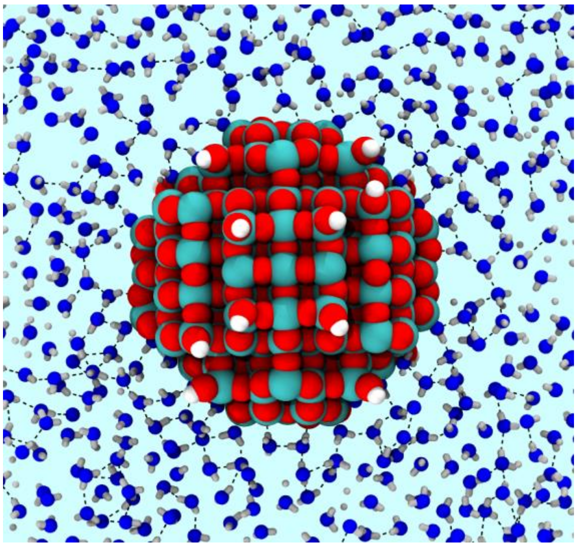

Figure 1: Representation of a TiO_2 spherical nanoparticle surrounded by water. The water molecules closer to the NS interact strongly with the surface, while far from it they resemble the structure of bulk water.

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Molecular Dynamics Simulation of Water-Graphene Nanofluid

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Abstract:
Nowadays, nanofluids due to their enhanced thermal properties are widely used in a variety of applications, such as electronic cooling, internal combustion engine cooling and lubrication, industrial cooling, industrial and comfort air conditioning and extraction of geothermal and solar energy. There are only a few recent studies available on viscosity and surface tension of nanofluids. In recent years, the family of carbon forms has increased considerably with the discovery of fullerenes, carbon nanotubes, and other related structures. In the graphene sheets, carbon atoms are located in a honeycomb lattice and are joined by covalent bonds. As in the case of carbon nanotubes, the graphene properties could be of great interest. Thus, our goal in this work was to study of the effect of graphene size on the water-graphene nanofluid viscosity using molecular dynamics (MD) simulation. We also investigate how nanoparticles alter the viscosity of nanofluids from microscopic viewpoint. Prior to the calculation the viscosity of the nanofluid, a validation of the computational strategy and the simulation model was tested and the results of the viscosity and density of water molecules with SPC/E, TIP3P and TIP4P potentials at 298 K were compared to the experimental data. It was found that the TIP3P potential gives better result for viscosity and in our further calculations we used TIP4P potential. Simulations were performed in the NVT ensemble. Long-range electrostatic interactions were handled using the Particle-Particle Particle-Mesh K-space (PPPM) solver. The cut-off distance was set to 10 Å, for short-range van der Waals forces. The simulations were conducted at room temperature (298 K) and atmospheric pressure with the Berendsen algorithm. The system was initially run for 300 ps under the NVT condition. Finally, the production steps of 2ns with the integral step of 1 fs were performed. For investigating the effect of nano particle size in the nanofluid viscosity we considered two graphene sheets sizes of 20*20 and 10*10 nm lengths. The results showed that all the graphene@water fluids have the higher viscosity than the base liquid water for all systems. It is also observed that the viscosity of the smaller-diameter particles is higher than that of the higher-diameter particles. Therefore, at a given temperature, viscosity decreases with the increase of graphene sheet size. The results of the simulations were in good agreement with the experimental data which shows graphene–water nanofluid viscosity decreases with an increase in the nanoparticles size. This behavior mainly comes from the strong interaction between graphene and water molecules and consequently stronger water-water interaction. Also it might be because of the hydrogen bonds. In general, a larger amount of the hydrogen bonds implies stronger intermolecular interactions among the molecules, which could result in an increase in the viscosity. Moreover, to obtain a better insight into the local structure and organization of the studied system, the site–site and center of mass radial distribution functions (RDFs) were studied. Usually, RDF is used to analyze the phase state of particles in a system. Here, the RDFs of oxygen and hydrogen atoms of water molecules are calculated. The obtained RDFs showed that distinct layers of water molecules are formed near the graphene sheet. The peaks due to the interactions between water molecules and graphene exhibit a strong interaction.

Keywords: nanofluid, dynamic viscosity, molecular dynamics simulations, radial distribution function, potential functions, graphene, carbon nanostructures.

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Dyadic Green Function based Model for Organic Light Emitting Diodes with Stratified Anisotropic Materials

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Abstract:
Organic light emitting diodes (OLEDs), with ultrathin thickness, color tunability and color quality, are attracting a lot of attentions in high quality light sources and displays. One of the main challenges in OLEDs research is to increase the outcoupling efficiency, and earlier strategies to address this issue assume all organic materials in the OLED structure are optically isotropic. However, during the past years, optical anisotropy has been observed and reported in both polymer molecules and small molecules OLEDs. These anisotropic materials exhibit the electric field dependent optical properties and furthermore have non-negligible impact on outcoupling efficiency of the OLED devices. Therefore, it is important to develop a proper optical model to accurately simulate the outcoupling efficiency of OLEDs with stratified anisotropic materials. A few of works have been done for birefrigent medium with principal axes coincident with the coordinate axis. In order to deal with more comprehensive cases, we propose a model that uniaxial and biaxial materials with arbitrarily tilted principal axes are taken into consideration in any organic layers. In this method, based upon dyadic Green function, the field of an arbitrarily orientated dipole in emission layer can be decomposed into a superposition of plane and evanescent waves. The scattering matrix method is extended and employed to obtain the reflection matrix. Consequently, the Purcell factor modified by interfaces between the stratified anisotropic layers can be calculated from the optical cavity model, and so that, the relevances between the outcoupling efficiency and the stratified material properties can be revealed.

Keywords: organic light emitting diodes, stratified anisotropic materials, optical simulation method, arbitrary tilted principal axes, dyadic Green function, Purcell factor.

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Universality of Steric Effects of Electrolyte in Nano-confinement

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Abstract:

The electric double layer (EDL) structure, which has a profound importance in many applications such as energy storage, biological application, and sea water desalination, is likely to be highly distorted in the nanoconfinement (including EDL overlapping), especially considering the finite size of the ion. It is known to deviate much from the conventional Poisson-Boltzmann model. In this study, we solve the EDL structure problem considering steric effect in various nanoconfinement, and analyze dynamic pressure, ion enrichment and electrocapillarity change in the various channels. The osmotic pressure is lessen dramatically by the ion saturation (corresponding to the tightly packed layers of ions), and, as a consequence, the electrical stress and the dynamic pressure exerting on the walls are modified in large extent. The dynamic pressure and ion enrichment are the sensitive function of steric factor, and the EDL structures of equilateral polygonal channels show a consistent tendency of increasing and converging from that of 1D channel to the circular one in the view of osmotic pressure, dynamic pressure and electrical stresses. However, the averaged dynamic pressure on the channel wall and the charge density in channel are almost independent of the cross section shapes of channels (Figure 1). It implies that the averaged electric field flux and the averaged electrical stress are preserved irrespective of channel shape. The universal properties of the steric effect of electrolyte in nanoconfinement will clarify our understanding on the EDL structure in various geometry and can be applied to many electrohydrodynamic and electrochemical applications.

Keywords: electric double layer (EDL), steric effect, the modified Poisson-Boltzmann model, nano-confinement, osmotic pressure, electrocapillarity, ion enrichment.

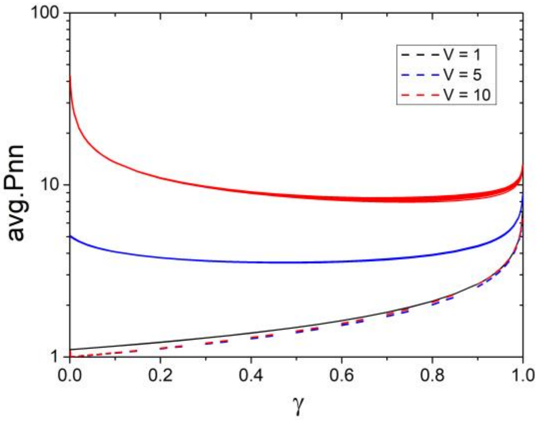

Figure 1: Steric factor dependence on the averaged dynamic pressure on the channel wall and for equilateral polygons (solid) and 1D channel (dashed) at various wall potentials.

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Solubilization of slovophobic polymer chains in interpolyelectrolyte complex cores of non-stoichiomeric co-assembled nanoparticles. Dissipative particle dynamics with explicit electrostatics

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Abstract:

We present results of our recent dissipative particle dynamics (DPD) simulations on the electrostatic co-assembly of double hydrophilic copolymers containing a polyelectrolyte (PE) block and a neutral water-soluble block with the oppositely charged PE homopolymers and on the solubilization of solvophobic polymer chains in cores of associates. DPD is a coarse-grained simulation technique which (in its original variant) employs three types of forces: (i) conservative force (soft repulsion), (ii) dissipative force (emulating friction) and (iii) random fluctuating force (emulating thermal motion).[1] If PE systems are studied, electrostatic interactions have to be included into the simulation scheme. There exist alternative approximate approaches, e.g., the "ion-free" approach[2] which do not include electrostatics into the DPD computational machinery. In contrast to the “ion-free” approach, we use DPD with explicit electrostatics[3,4] because we are of the opinion that the entropy of counterions and electrostatic correlation effects are properly taken into account only if the used DPD variant employs explicit electrostatics.

In the first part of our presentation, we will shortly outline the principles of DPD and problems connected with the implementation of electrostatics. In the second part of the presentation, we will present results of our recent simulations on the co-assembly and solubilization of solvophobic compounds. Results of simulations confirm general correctness of trends predicted by the "speciation diagram" proposed by van der Burgh[5], but they simultaneously show that the behavior of electrostatic co-assembling systems is more complex and the proposed scheme does not predict all details correctly.

Keywords: dissipative particle dynamics, electrostatic assembly, interpolyelectrolyte complexes, solubilization of polymers.

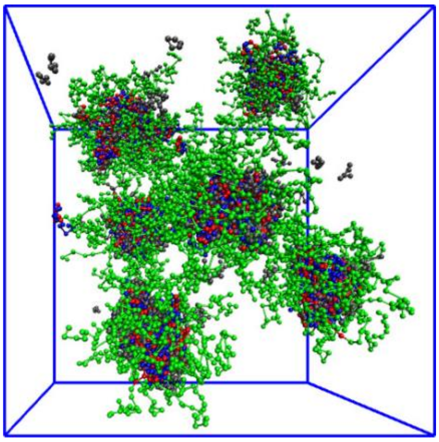

Figure 1: A typical snapshot of the simulation box showing the co-assembled nanoparticles with polymer chains (black) solubilized into the interpolyelectrolyte cores (red and blue); shell-forming chains – green.

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Determining the Schottky barrier in a metal/semiconductor interface by ab initio Ballistic Electron Emission Microscopy simulations

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Abstract:

A new theoretical model for the simulation of the electronic current in a Ballistic Electron Emission Microscope (BEEM) is presented. Based on the Scanning Tunneling Microscope (STM), BEEM measures the electronic current that collected after a metal-semiconductor interface placed far away from the metallic surface. This allows the study of the corresponding Schottky barrier formed in such interface. The previous proposed models took into consideration only a semi-infinite metallic part joined to the semiconductor by a semiclasical approach [1], while the revised method should be generalized to new interesting systems including thin films. Our layer-by layer procedure allows the simulation of both large or thing metallic regions using the Keldysh Green function formalism [2]. In a final step, a semi-infinite semiconductor is connected creating a realistic interface. The three parts of the problem (metal, interface and semiconductor) have been simulated using an accurate *ab initio* parametrization.

As a proof of concept, we have used out methodogy to analyze the Au(100)/Ge(100) interface shown in Figure 1a [3]. Our theoretical calculations reproduce precise Ultra-High Vacuum, low-Temperature experimental measurements on such a metal-semiconductor interface without using adjustable parameters. Although for a voltage (V) close to the Schottky barrier (V_{SB}) temperature effects become significant, we show that at T = 0 K the theoretical current follows closely the law $(V-V_{SB})^{2.1}$. The inclusion of the temperature effect leads us to identify two slightly different values for the Schottky barrier located at 0.67 and 0.75 eV that we associate to different patches forming the interface (see Figure 1b).

Keywords: BEEM, electronic transport, *ab initio* simulations, Schottky barrier.

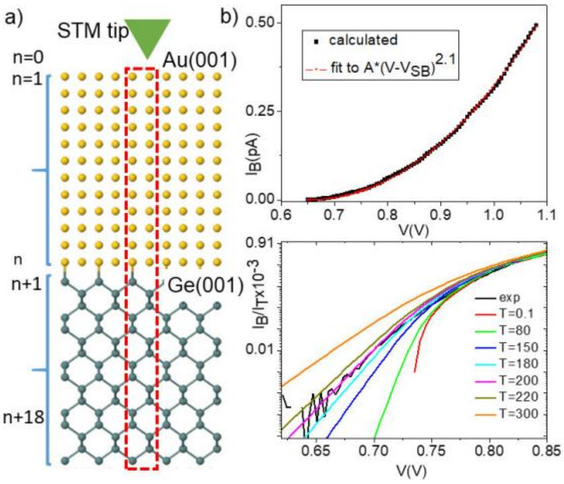

Figure 1: a) Ball and stick model of the Au(100)/Ge(100) interface (the red square shows the unit cell used in the *ab initio* simulation), b) in the upper part, the fit of the theoretical BEEM current to $(V-V_{SB})^n$ is shown, while in the lower part, the experimental I_B/I_T (BEEM divided by the STM current) curve is presented with the calculations including the Temperature effect.

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Molecular applications of nanomaterials: The case of ZnO and laser cooling

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Abstract:

Zinc Oxide nanoparticles have many applications in optoelectronics and biomedical sciences. Many of these applications rely on the fact that ZnO quantum dots exhibit quantum confinement effects i.e. their emission properties depend on their size (or the size of their bandgap more specefically.)

We have previously used ab-initio quantum calculations to propose a possible relationship between the energy gap between potential energy curves of the smallest possible unit of a ZnO nanoparticles. i.e the ZnO molecule, and the band gap within ZnO nanoparticles[1]. The Ab-initio calculations have been performed via the quantum chemical package MOLPRO [2], taking the advantage of the graphical user GABEDIT [3]. The Zinc atom was treated by using ECP10MDF basis set for s, p, d functions, while the oxygen atom was treated in all electronic scheme by using the AV5Z basis set for s, p, d and f functions.

Within the same type of framework, we investigate in this paper how one can use specific materials that are of high interest at the nanoscale, within molecular applications. In more detail, we will consider the case of laser cooling of ZnO molecules, and understand the feasibility of producing such cold/ultracold materials. One important parameter in the application of this technique is the calculation of the transition probabilities between different vibrational states of the potential energy curves, or the Franck-Condon Factor of the molecule in question. We base ourselves in this paper on results that we obtained through Franck-Condon factor calculations to discuss the possibility of usage of ZnO in laser cooling experiments.

Keywords: ZnO nanoparticle, Potential Energy curve, Laser Cooling, Franck-Condon Factor, Vibrational Levels, Diatomic Molecule, ab-initio calculations.

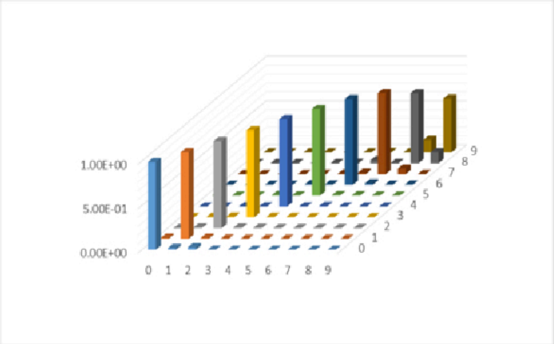

Figure 1: Figure illustrating the diagonal nature of Franck-Condon factor matrix for ZnO molecules, between different vibrational levels of the potential energy curves of two molecular states.

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Properties of Ionic Liquid Mixtures

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Abstract:

Ionic liquids (IL) have attracted considerable interest over the last few years especially in nano-technology field. Nanoparicles can be added to the ionic liquids to achieve required properties. They are defined as salts in liquid phase at a temperature less than 100°C or even at room temperature (RTIL). This is because one ion at least has a delocalized charge and one component is organic, which prevents the formation of a stable crystal lattice (1).

RTILs possess a unique array of physico-chemical properties that make them suitable in numerous task-specific applications in which conventional solvents are non-applicable or insufficiently effective. Such properties include: high thermal stability, high electrical conductivity, large electrochemical window, low nucleophilicity and capability of providing weekly coordinating or non-coordinating environment, very good solvents (2).

Ionic liquid properties are different from one ionic liquid to another ionic liquid. In order to have desired properties, mixing of different ionic liquids is needed to obtain enhancement properties. However, mixing process of ionic liquids requires reliable estimates of the mixture's physical properties such as refractive index and density. There are many semi-empirical mixing rules for liquid mixtures. This requires examining of these mixing rules with respect to ionic liquid mixtures and choose the best mixing rule for each physical property. Moreover, ideal mixture assumption simplifies the complexity of using ionic liquid mixtures. However, accuracy and validation of each rule need to be determined (3).

In the present work various binary mixtures of ionic liquids made from 1-butyl-3-methylimidazolium thiocyanate ([BMIM][SCN]), 1-butyl-3-methylimidazolium tetra- fluoroborate ([BMIM][BF4]), 1-hexyl-3-methylimidazolium tetra-fluoroborate ([HMIM][BF4]) and 1-hexyl-3-methylimidazolium hexa-fluorophosphate ([HMIM][PF6]) haven been studied. Density and refractive index of various binary mixtures have been measured and correlated with the most accurate mixing rules. For density prediction of the ionic liquid mixtures, ideal mixing rule was found to be very accurate with an average percentage deviation of 0.78%. Hence, it is well justified to assume such mixtures as ideal mixtures with the volume additivity behavior. Furthermore, all of the examined mixing rules for refractive indices of the studied mixtures accurately estimated the refractive indices of different binary mixtures. However, the most accurate empirical formula was found to be Heller's relation with an average percentage deviation of 0.24%.

Keywords: Ionic Liquids, Thermodynamic Properties, Excess Volume, Theory of Solutions, Refractive Index Mixing Rules, Applied Nanotechnology.

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Nanotech / Biotech Joint Plenary Session II

From antibodies to Metal Organic Frameworks: a Full Set of Enveloppes for metal cofactors in order to build up new artificial metalloenzymes

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Abstract:

In a global context of sustainable growth there is an urgent need for finding catalysts that would be able to work under eco-compatible conditions. This can be realized by combining the robustness and wide range of reactions of chemical catalysts, such as metal complexes with the ability of enzymes to work under mild conditions in aqueous medium and with high selectivity. This affords new hybrid biocatalysts, which we name artificial metalloenzyme or “Artzyme“ in which the metal complex is responsible for the catalytic activity and the protein by its chiral environment around the substrate induces the selectivity and also protects the metal cofactor from degradation.

A first generation of artificial metalloenzyme was prepared by inserting metal (Fe, Mn, Cu, Zn) complexes of various ligands including water soluble tetraarylporphyrins, phenanthroline, terpyridine or tris-pyridylamine, into various proteins such as monoclonal antibodies (generation of catalytic antibodies or AbZyMes), xylanase A, beta-lacto-globulin or neocarzinostatin, either non-covalently (Trojan-Horse and Host-Guest strategies) or by by covalent attachment through a linker arm. The obtained hybrid biocatalysts were found to be able to stereo-selectively catalyze reactions such as: the oxidation of organic compounds such as sulfides and alkenes by H_2O_2, the C-C bond creation through the stereoselective Diels-Alder reaction, the RNAse like hydrolysis of oligonucleotides (1-3)

More recent developments are turning towards the elaboration of totally artificial metalloenzymes. Three strategies are followed:

- First, metal complexes are inserted either covalently or not into a new family of artificial proteins based on a thermostable alpha-helical repeated motif αRepeat proteins (αRep). This has allowed the design of new artificial Diels Alderases (4).

- Second, enzymes such as microperoxidase 8, a minienzyme with peroxidase and monoxygenase activity, are inserted into Metal Organic Frameworks (MOF Mil 101) in order to get new artificial metallloenzymes that are able to catalyze in water the selective oxidation of dyes, sulfides and alkenes by H_2O_2 ((5)

- Third, Poly-oxo-metallates are associated with artificial polyimine polymer based reductases (6) to afford new hybrid catalysts that are able to catalyze the oxidation of organic substrates by O_2 in water).

New perspectives concerning the development of new artificial metalloenzymeq “in vivo“ for theranostic purposes will finally be introduced.

Keywords: stereoselective catalysis, metalcomplexes, hybrid biocatalysts, artificial metalloenzymes

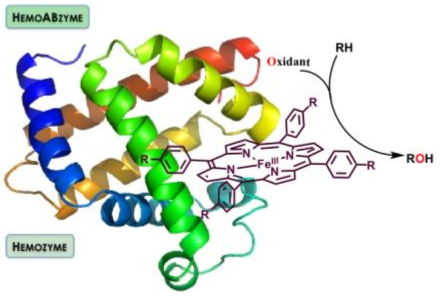

Figure 1: An artificial metalloenzyme that catalyzes the stereoselective oxidation of alkanes.

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Expanding and exploring natural sequence space – from protein engineering to chemo-enzymatic cascade reactions

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Abstract:

Cascade and one pot reactions represent an exciting and recent development in biocatalysis. There are, however, a range of technological and scientific challenges to be met *en route* to industrial scale. This includes particularly the compatibility of different catalysts and their reaction conditions, cross-reactivity and the overlap of substrate spectra. The assembly of catalysts from different sources therefore requires an interdiscinary approach the interface of organic synthesis, enzyme engineering and process engineering. In this talk, we will focus on the *in situ* coupling of biocatalysts to other catalysts in order to provide routes that would be difficult with the individual, separated reactions.

A first example deals with the combination of cofactor-free and cofactor-dependent decarboxylases with chemical synthesis. Decarboxylases constitute versatile biocatalysts with often outstanding selectivity. The release of carbon dioxide is a powerful driving force to shift thermodynamic equilibria. Yet, the substrate spectra of decarboxylases are often limited, either by mechanistic constraints or their natural role. Enzyme engineering is used to provide tailor-made enzyme variants with widened substrate scope and high selectivity. Coupling to metal-catalyzed reactions offers new routes towards *one-pot* cascade reactions for the synthesis of optically pure pharmaceuticals and bio-based high-value products [1].

A second example reports on the coupling of biocatalytic redox reactions to the cyanobacterial photosystem for cofactor regeneration with water as sacrificial substrate. While oxidoreductases catalyze a plethora of highly selective reactions, they demand a stoichiometric supply of petrol-based or agricultural co-substrates as electron donors. Photobiocatalytic water oxidation is a sustainable strategy for the supply of electrons for redox transformations without the need of organic electron donors and opens new possibilities in the biotechnological toolbox [2].

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Design and Evolution of New Biocatalysts for Organic Synthesis

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Abstract:

This lecture will describe recent work from our laboratory aimed at developing new biocatalysts for enantioselective organic synthesis, with a particular emphasis on the design of in vitro and in vivo cascade processes for generating chiral pharmaceutical building blocks. By applying the principles of 'biocatalytic retrosynthesis' we have shown that is now increasingly possible to design new synthetic routes to target molecules in which biocatalysts are used in the key bond forming steps [1].

The integration of several biocatalytic transformations into multi-enzyme cascade systems, both in vitro and in vivo, will be addressed in the lecture. In this context monoamine oxidase (MAO-N) has been used in combination with other biocatalysts and chemocatalysts in order to complete a cascade of enzymatic reactions [2-4]. Other engineered biocatalysts that can be used in the context of cascade reactions include □-transaminases [5], ammonia lyases [6], amine dehydrogenases [7], imine reductases [8], and artificial transfer hydrogenases [9]. We shall also present some very recent work regarding the discovery of a new biocatalyst for enantioselective reductive amination and show how these enzymes can be used to carry out redox neutral amination of alcohols via 'hydrogen borrowing' [10].

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Practical biocatalytic solutions for the design of chemoenzymatic and multienzymatic concurrent processes

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Abstract:

The design of chemo- and multienzymatic approaches provides an straightforward access to complex molecules, including the possibility to develop stereoselective reactions. One of the main advantages of these methods is circumventing the isolation and purification of sometimes unstable reaction intermediates. Overall, this usually leads to shorter reaction times and higher isolated yields, avoiding additional purification steps. In this context, enzymes provide elegant solutions by catalysing cascade and sequential (stereo)selective transformations towards the formation of a wide number of organic compounds.[1,2]

In this presentation, recent successful approaches will be presented, focusing on the production of products such as alcohols, amines, epoxides, lactams, lactones and others, by two different strategies:

a) An enzyme-catalyzed reaction followed by a chemical reaction based on the special reactivity of the reaction intermediate.
b) Two enzymes working in a selective manner, where a prochiral intermediate is later transformed into an optically active and valuable product.

Among different classes of enzymes, the behaviour and compatibility of alcohol dehydrogenases, ene-reductases, laccases and transaminases will be disclosed aiming to produce high added value products in a straightforward and general manner.[3-6]

The possibility to develop cascade transformations will be the main objective, considering the design of sequential approaches when reaction conditions are not compatible for both enzymes at the same time.

Keywords: biocatalysis, concurrent processes, laccases, lipases, organic synthesis, oxidoreductases, stereoselective synthesis, transaminases.

References:

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Broadspectrum Nanoparticles-based Antivirals

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[2] EPFL, Interfaculty Institute of Bioengineering, Lausanne, Switzerland

Abstract:

In this talk novel approaches to develop antiviral drugs will be presented. Specifically, nanoparticles capable of irreversibly damaging viruses will be presented. It will be argued that that the mechanism of action is that of exerting a pressure on the viral shell.[1] This property, combined with the fact that the particles have minimal toxicity to mammalian cells, has lead to promising in vivo results. In particular the case of herpes simplex 2 will be discussed. Other effects of nanoparticles on virus stability and infectivity will be presented.[2]

Keywords: nanoparticles, nanomedicine, antivirals, vaccines.

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Applications of Artificial Intelligence in Biotech and Nanotech research

M. Cristovao

Springer Nature, Germany

Abstract:
Sieving through scientific literature can at times be a daunting task. Everyday more and more scientific research articles are being published and as a researcher it is difficult to on the one hand, keep up to date with the newest research, and on the other find the right information for your research project. AI and machine learning are revolutionizing scientific research and Springer Nature is making use of these new tools to make scientific literature research more efficient. We have recently launched two new research solutions with the focus on life science/biotech and nano research – Springer Nature Experiments and Nano.

This talk will illustrate how researchers can benefit from these tools and how they provide fast and precise insight into the wealth of scientific knowledge, using knowledge graphs, smart article indexing and dedicated knowledge models.

Session II.A
Nanotechnology for life science

Brain Structure and Function Combine to Create the Characteristics of a Bio-Metamaterial

Salvatore Domenic Morgera[1,2,*]
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Abstract:

Unlocking the mysteries of brain structure and function are one of the grandest challenges of our time. This work will look at the latest research on the core phenomena involved in brain structure and function. The World Health Organization reports that more than one billion people worldwide, irrespective of age, sex, education, or income, suffer because of neurological disorders associated with brain health and autoimmune diseases involving interactions between the central nervous and immune systems. This compelling societal need provides more than ample motivation for research on understanding brain structure and function. In our view, understanding begins with the neurological networks of the brain and how the most elementary components, the nerve fibers, interact with each other. We discuss the recent discovery of the *endogenous electric near-fields* generated by the billions of nerve fibers in the brain[1]. Advances have elevated the importance of these endogenous fields to a leading role of primary phenomena, as opposed to the traditionally thought secondary role of epiphenomena[2]. We note that near-field phenomena form the basis for near-field communications (NFC), a smartphone/smartcard technology (albeit magnetic, in the smartphone application) that enables contactless information transfer and payment. The nanoscale dimensions between nerve fibers and the way populations of nerve fibers are geometrically arranged in different regions of the brain gives rise to what we call a *bio-metamaterial* and leads to the highly sophisticated spatial-temporal structure of the near-fields. Metamaterials are a class of electromagnetic materials not thought to occur in nature that are engineered on a length scale intermediate between the wavelength and the atomic scale. A scale much less than the wavelength implies that the structure of the brain may be invisible to its function (but responsible for it) embodied in the billions of action potentials, their timing, and the near-fields that they create. Locked away in the near-fields are the fine resolution details of brain structure. This work contains many new and fascinating results about brain structure and function. Our goal is to describe the spatial-temporal structures of the endogenous fields and use these to *rationally design* clinically accurate neurodevices for diagnosis and therapeutic treatment.

Keywords: brain mapping, brain structure, brain function, nerve fibers, near-field, electric-field, bio-metamaterial, metamaterial.

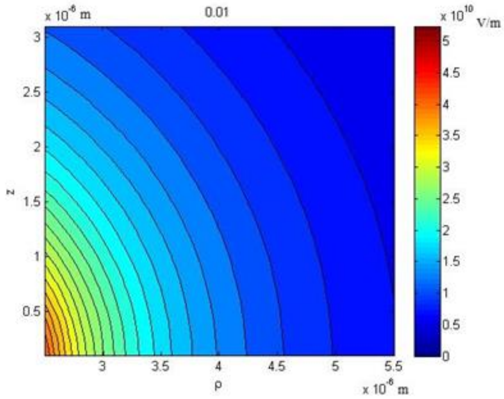

Figure 1: Snapshot of a video displaying both *in silico* and *in vitro* time-varying electric near-field level due to nerve fiber voltage-gated ion channels at a node of Ranvier.

References:

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Nanostructures for biological and environmental applications

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Abstract:

Nanostructures like nanoparticles and nanotubes have physical and electrical properties that make them ideal for use in sensor technology and chemistry. For example, nanoparticles have a high surface to volume ratio which gives them high reactivity, while silicon nanowires are one dimensional semiconductors that can change their electrical properties when affected by an electric field created from e.g. charged molecules in a biological sample.

Although technological progress has made nanoscale fabrication relatively affordable, there is still a need to reduce costs with only minimal compromise of yield and function. In this work we will present how use of in situ doped polysilicon on standard silicon wafers can replace the use of expensive SOI wafers for the fabrication of silicon nanowire based biological field effect transistors (bioFETs). Moreover, a simple underetching step can lead to nanoscale dimensions of these wires, without the use of nanolithographic techniques. We will show that the resulting FETs have an acceptable performance for use as biological sensors and discuss process yield and reproducibility.

We will also present our work with using zero valence iron nanoparticles encapsulated in alginate gel for cleaning water from nitrate, which can be found in common fertilizers. This preliminary work opens possibilities for online cleaning of water for known contaminants, by utilizing novel encapsulating structures for the NZVI.

Keywords: Silicon nanowires, in situ polysilicon doping, field effect transistors, biosensors, Zero valence iron nanoparticles, alginate

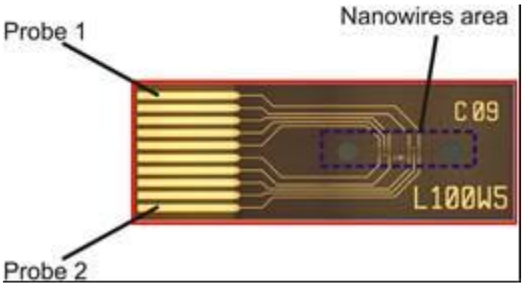

Figure 1: Top: silicon nanowire chip with 4 nanowire sensors made with in situ doped polysilicon [1]. Bottom: Alginate beads containing NZVIs. Each bead is 2mm in diameter [2].

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‘Clickable’ Recombinant Spider Silk and its Healthcare Applications

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Abstract:

Spider silk including recombinant forms is a biomaterial of significant interest for medical and other applications due to both its mechanical properties (tensile strength and toughness) and its biocompatibility.

We have recently reported the preparation of antibiotic and fluorophore functionalized silk fibres self-assembled from the miniaturized major spidroin protein 4RepCT derived from the dragline silk of the South African nursery web spider, *Euprosthenops australis*.[1] This has been achieved through the site specific incorporation of the un-natural, bio-orthogonaly functionalized amino acids L-azido-homoalanine (Aha) and L-homopropargylglycine (Hpg) in the mini spidroins.

The functionalized fibres were prepared by incorporating the bio-orthogonal amino acid in place of the three methionines in the 4RepCT protein. The Aha residues can be selectively and efficiently modified with ligands bearing alkyne groups using either a copper (I) catalysed azide alkyne cycloaddition (CuAAC) or strain promoted azide alkyne cycloaddition (SPAAC) ‘click’ reaction.

We have demonstrated that we can functionalize the silk proteins with fluorophores, peptides and with the broad spectrum antibiotic levofloxacin. The antibiotic has been attached via a glycerol ester that is cleaved either through a drop in pH or by esterases released by *E. coli* as they grow. The 4RepCT^{3Aha} proteins can be modified either prior to or after silk fibre assembly and the tensile strength of the resulting fibres is unaffected. This has allowed fibres decorated with two or more different ligands in defined ratios to be prepared. The antibiotic functionalized silk fibres prevent *E. coli* growth for at least 5 days demonstrating good potential for future use in medical dressings. Additional applications of the functionalised silks in regenerative medicine will also be presented.

Keywords: spidroin, spider silk, self-assembly, residue specific mutagenesis, bio-orthogonal, click chemistry, Huisgen cycloaddition, antibiotic, controlled release, protein scaffolds, tissue regeneration, stem cells, biomedical applications.

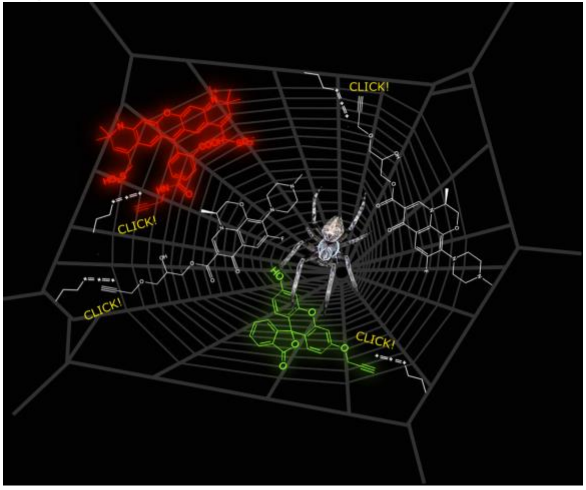

Figure 1: A cartoon showing some of the ligands we have functionalized spider silk with using bio-orthogonal ‘click’ reactions.

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Surface nanoengineering of intravenously administered inorganic nanoparticles

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Abstract:

Recent progresses in nanotechnology offer exciting opportunities in the development of promising nanomaterials for medicine and bioimaging. Among them, multifunctional nanoparticles offer plenty of applications because of their physical properties (optic, magnetic…) which allow their use as well as contrast agents, as cell labelling tools, as hyperthermia mediators and smart drug delivery systems (DDS). The common point between these nano-objects lies in their surface chemistry which has to be mastered in the aim to control their physico-chemical features in terms of non-specific binding, targeting efficiency, or drug release. This talk will stress on current surface modification strategies of multifunctional nanoparticles developed for biological applications through two topics:

- The nano-bio interface engineering using nanoparticles for in vivo imaging. Their small size, similar to that of biological entities, enables the labelling of biomolecules of interest. For instance, these nanomaterials can be used for in vivo active targeting labelling and cell tracking in the frame of diagnostic or therapeutic applications. All synthesis stages have to be controlled from the inorganic cores surface modification to the conjugaison of functional ligands such as antibodies. We experienced different application fields in biology as various as tumour labelling [1], monocyte and stem cells tracking [2,3], diagnosis of the instability of atherosclerotic plaques [4], etc.
- The development of long circulating fluorescent NPs i.v. administered, as markers of EPR effect of tumors, where the surface grefting density of PEG macromolecules have been optimized [5].
- Drug Delivery Systems (DDSs) remotely triggered by magnetic induction. In this field, functionalized magnetic nanoparticles used as heat mediators for self-regulated heat release were designed [6]. Another example of DDS based on multifunctional nanoparticles made of a mesoporous matrix allowing the transport of bioactive molecules containing superparamagnetic nanoparticles will be presented [7]. This type of system provides an interesting tool for increasing the efficacy of pharmaceuticals through improved pharmacokinetics and biodistribution.

Keywords: Bioconjugaison, targeting, long-circulating NPs, heat-triggered Drug Release Systems, Hyperthermia, mesoporous NPs, Magnetic NPs, Fluorescent NPs.

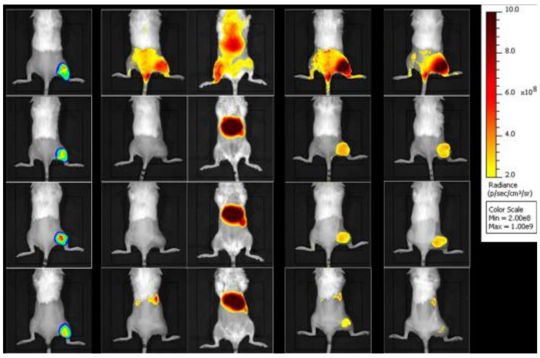

Figure 1: bioluminescence and reflectance NIR imaging of a representative mouse injected with fluorescent NPs of various surface grafting densities of PEG, observed at 1 h (right, prone position; left, supine position), 8 h and 48 h (prone position).

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Vitamin A palmitate-loaded NLC for cosmetic application

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Abstract:

Nanostructured lipid carriers (NLC) are a new generation of SLNs, with improved drug loading capacity, and stability. Their administration in topical based drug delivery has shown several advantages.[1] The potential use of vitamin A for skin therapy is widely known among dermatologists, and pharmacists. The side effects, however, of direct application induced by the vitamin, such as irritation, itching and scaling has limited their use.[2] The aim of this work is to understand the effects of the constituents of the lipidic carriers, on their release and skin permeation profiles for vitamin A.

Two NLC formulation with varying surfactant to solid lipid ratio were prepared using the hot homogenization method and compared with a SLN formulation. The effect of the variation in the constituting matrix of the nano-carriers was investigated and characterized.

The results show a wide variation in characteristics as a result of the change in the surfactant to solid lipid ratio. The NLC particle diameters were in the range of 220-240 nm, and PDI 0.24-0.25. The SLN had a larger diameter of 297 nm and PDI of 2.47. The significant value of the PDI is associated with the onset of gelling that is a disadvantage often exhibited by SLNs.[3] The release patterns in both in-vitro and ex-vivo showed differences in trends for the two formulations. The total release of the in-vitro trials was identical for the NLCs, and much lower for the SLN. The flux, however, varied among all. The formulation with the highest surfactant ratio showed the highest permeation across the membrane but possessed lower skin retention. DSC measurements showed a significant difference in the thermal behavior of the SLN as opposed to the NLCs, attributed to the crystalline structure of the lipids.

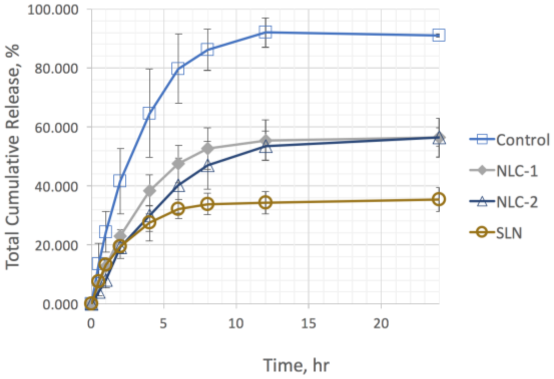

Figure 1. In-vitro release profiles of a control solution of RP and from lipidic nanocarriers, NLCs and SLN.

Keywords: Nanostructured Lipid Nanoparticles; Solid Lipid Nanoparticles; Vitamin A; Polymorphism.

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Acknowledgement:

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Session II.B:
NanoMedecine - Bioimaging

The iNAPO project: Biomimetic ion conducting polymer nanopores for bio-molecular and chemical sensing

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Technische Universitaet Darmstadt, Germany

Abstract:

The *iNAPO*-project is run by a group of materials scientists, biologists, chemists, physicist and electrical engineers. The aim is the development of biomimetic (bio)molecular sensors based on ion conducting nanopores in polymer foils. The basic principles of fabrication and working mechanism of such a nanosensor is described. PET foils are irradiated with a highly energetic single ion of a heavy element, auch as gold. The ion damage zone in the polymer is chemically etched into a conical pore, with the small aperture being in the nm range. The nanopore walls are functionalized with a biorecognition unit, i.e. a molecule which specifically reacts with a molecule to be analyzed. In an electrochemical cell, the foil acts as separation membrane, see Fig. 1. The electrolyte current *I* flowing through it is measured as a function of the applied voltage *V*. In the presence of specific analyte molecules, which bioconjugate with the biorecognition unit, these ionic currents are changed. Thus, a highly sensitive nanosensor is available. The preparation and working principle of the nanosensor is described. As an example, results on protein sensing are shown. In Fig. 1 the quantitative measurement of the protein Concanavalin A that specifically bioconjugates with mannose is depicted. The concept of the functionalized ion conducting nanopores can be applied to a large number of biorecognition couples. Within the project *iNAPO*, the potential of this technique will be further explored. In a step further, it is planned to embed protein-based nanopores with even better selectivity into polymer membranes. Eventually, the membranes will be incorporated in electronic micro sensing devices thus creating a new type of (bio)molecular sensor. The development is supported by analytical studies based on NMR and by theoretical and simulation studies.

Keywords: nanopores, biomolecular sensing, nanopore gating

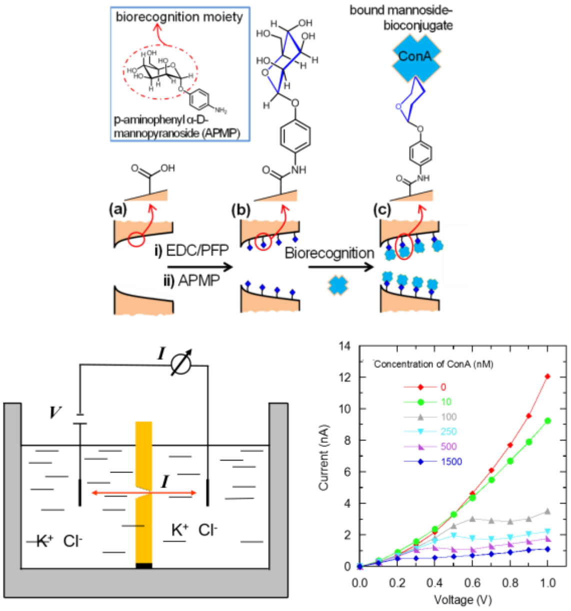

Figure 1: Top: Schematic presentation of (a) (b) immobilization of mannose at the nanopore walls (in cross section), (c) specific reaction with protein Concanavalin A (shown as blue cross) with mannose. Bottom: Electrochemical cell; the electrolyte current through the nanopore is shown in red. Electrochemical measurement of ionic current through the nanopore. The nanopore current is a direct function of the ConA concentration.

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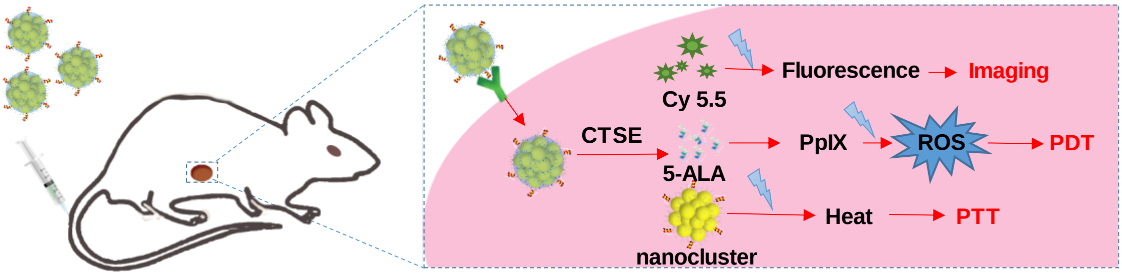
Confocal Laser Endomicroscopy Guided Photothermal/Photodynamic Therapy of Pancreatic Cancer

Hui Li, Kai Yang, and Yingsheng Cheng*

Abstract:

Pancreatic cancer is one of the most devastating malignancies in patients and there is great need for an effective method for treatment.In this work, we successfully developed a novel gold nanocluster-based platform for confocal laser endomicroscopy guided photothermal /photodynamic therapy of pancreatic cancer. Due to the strong coupling amongcross-linked AuNPs, the surface plasmon resonancepeak of nanoclusters shifted to NIR region,which makes the nanocluster useful for effective photothermaltherapy.*In vitro* and *in vivo* therapeutic studies showed the combination of active targeting tumor tissue, enzyme triggered release of 5-ALA and Cy5.5 and endomicroscopy guided photothermal /photodynamic therapy achieved optimal therapeutic efficacy while minimizing the side effects.Therefore, the delicate gold nanocluster concept demonstrated herein provides a promising strategy to enhance pancreatic cancer therapy efficiency.

Keywords: Gold nanoclusters, Fluorescent bioimaging, Pancreatic ductal adenocarcinoma, Enzyme-triggered release,Photothermal and photodynamictherapy



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Dual Metallofluorescent Nanoparticles for live cells assays

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Abstract:

Polystyrene nanoparticles have been proved to be one the most promising “smart” nanomaterials in nanomedicine, due to their absence of toxicity, being high valuable as diagnosis tools and as drug nanocarriers for therapeutic agents, expanding the field of theranostics.[1] In this contex, compatible multimodal particles play an important role as a connection point within different techniques in the diagnosis field. Herein we report the development of non-toxic metallofluorescent polystyrene-based particles, carrying simultaneosusly a fluorophore and a metal ion, that are easily nanofected[2] into living cells, providing effective bioorthogonal fingerprints for multimodal fluorescence imaging, fluorescence-based and mass spectrometry-based flow cytometry experiments.[3] These metallofluorescent nanoparticles provide the same nanofection profile in Flow Activated Cell Sorted (FACS) and Mass Cytometry (CyTOF) when nanofected into living cells, representing a extremely high valuable approach for the integration of one of the most stablished techniques in bio laboratories (FACS) and one of the most attracting and prominent techniques (CyTOF). Mass Cytometry tackles and overcomes the limitation of the number of fluorophores that can be simultaneously used in Flow Cytometry, expanding the capability for multiplexing assays. Mass Cytometry is a flow cytometry based ICP-TOF MS[4] that allows the simultaneous detection and quantification of dozens of markers within single particles,[5] providing multiplexing capabilities for single-cell experiments. This technique uses rare earth elements as tags, providing **bioorthogonal fingerprint signals** as they are not naturally presented in cells, thereby avoiding cellular background signals and being highly sensitive and specific. As a consequence, our metallofluorescent particles can be used as probes for cell barcoding. Moreover, these particles might be used as cytosolic organometallic catalysts nanoparticles within living cells[6]

Keywords: Nanoparticles; Biomaterials; Bioorthogonal; Flow Cytometry; Mass Cytometry; Fluorescence; Biology; Chemical Biology, CyTOF.

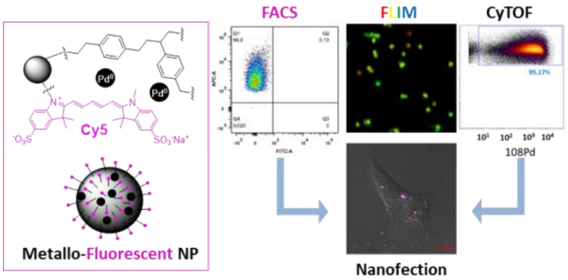

Figure 1: Figure illustrates the multimodal applications of the metallofluorescent nanoparticles.

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Design of Polyelectrolyte Microcapsules Encoded with Excitonic Nanoparticles and Prospects of their Applications as Novel Bio-imaging and Theranostic Tools

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Abstract:

The use of polyelectrolyte microcapsules is proved to be a promising approach to development of bioimaging and theranostic tools that can carry drugs and other compounds, including proteins, DNA, RNA, fluorescent dyes and specific diagnostic bioconjugates [1,2].

Compared to classical organic dyes, excitonic nanoparticles, e.g., semiconductor nanocrystals "quantum dots" (QDs) possess a high photostability and extraordinary optical properties, such as wide absorption and narrow size-dependent fluorescence spectra. Embedding QDs between the polyelectrolyte layers yields optically encoded highly fluorescent polyelectrolyte microcapsules whose interaction with live cells both *in vitro* and *in vivo* can be monitored.

Here, we are describing development and functional characterization of the next-generation theranostic agents based on polyelectrolyte microcapsules encoded with semiconductor nanocrystals. The ultrabright CdSe/ZnS QDs with the quantum yield approaching 100% have been synthesized, made soluble and stable using multifunctional PEG-based organic layer and employed to encode hollow polymeric microcapsules using a template-based synthesis [3]. The dynamic light scattering, electrophoresis and electron and confocal microscopies have been shown that developed QD-encoded microcapsules have an optimal size distribution and fluorescence properties for live cell imaging and tracking their cell uptake and transmembrane transport *in vitro* (Figure 1). The obtained results pave the way to novel applications of QD-encoded microcapsules not only for drug and diagnostic tools delivery but also for tracking and advanced bioimaging of these processes [3].

Keywords: excitonic nanoparticles, microencapsulation, polyelectrolyte microcapsules, theranostics, live cell imaging.

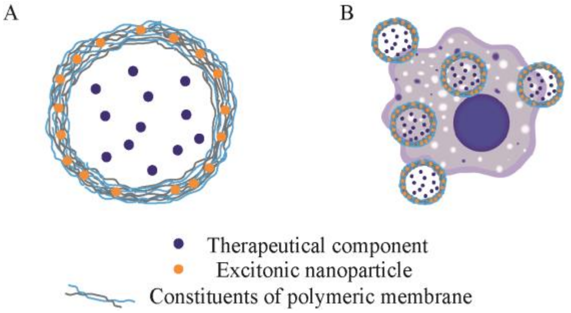

Figure 1: The schematic structure of the bio-imaging and theranostic tool based on polyelectrolyte microcapsule encoded with excitonic nanoparticles (A), and cell uptake of these microcapsules used for cell imaging (B).

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Acknowledgments:

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Development of new theranostic platforms based on carbon dots

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Abstract:

The recent discovery of carbon dots (CDs) and their very interesting physico-chemical properties (chemical stability, water solubility, low toxicity, biocompatibility, photoluminescence and resistance to photobleaching) make these carbon nanoparticles a powerfull platform for biomedical imaging and drugs delivery. The influence of various processing parameters to manufacture these nanoparticles using a bottom-up approach (activation condition, carbon source, passivation reagents, stoichiometry of reagents) has been investigated to optimize their properties in terms of transfection efficiency and photoluminescence (Figure 1). In order to produce efficient theranostic platforms, two strategies have been carried out (Figure 2). The first one refers to a "protocell" model in which the nucleic acid-CD complex is encapsulated in a functionalized lipid bilayer (pathway A) to 1-produce stealth particles and 2-possibly target specific receptors on tumor cells. Besides, the lipid bilayer also allows the doping with a "conventional" hydrophobic drug (e.g. paclitaxel) for combined therapies. The second strategy involves the establishment of a bifunctional layer (imparting both furtivity and targeting properties) around the nanoparticles through covalent bonds (pathway B). Furthermore, the incorporation of a hydrophobic intron should allow co-delivery of a hydrophobic drug for combined therapies. Our work to produce various NIR-fluorescent CDs for *in vivo* fluorescence imaging and nucleic acid and antitumor drug co-delivery will be presented. Finally, the synthesis of Gd-doped CDs for dual mode imaging (fluorescence and magnetic resonance imaging) will be discussed.

Keywords: carbon dots, nucleic acids delivery, photoluminescence, theranostic platform, magnetic resonance imaging.

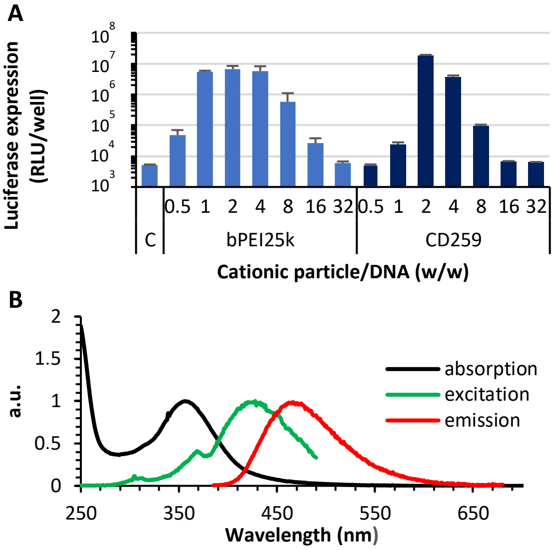

Figure 1: Optimization of CDs properties in terms of nucleic acids vectorization and photoluminescence. Comparison of transfection efficiency between bPEI25k (a standard transfection reagent) and CD259 (A). Absorption, excitation and emission spectra of CD259 (B).

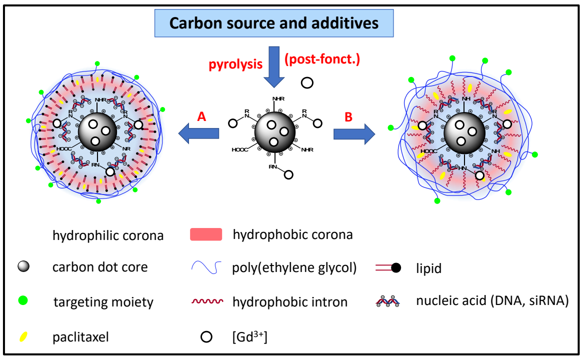

Figure 2: Strategies employed in the synthesis of theranostic nanoparticles for combined therapy purposes.

Reduction of methemoglobin to oxyhemoglobin under influence of nanoparticles of perfluorocarbon emulsion and cytoflavin.

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Abstract:

Normally in human blood, methemoglobin (MetHb) is about 1-2%.The influence of various pharm chemicals and ionizing radiation in blood can lead to damage of the redox balance in the blood, which in turn can trigger increased level of methemoglobin. Hemoglobin with Fe^{3+} (methemoglobin) can not transfer oxygen to tissues. We used ultraviolet (UV) irradiation in order to yield methemoglobin. In some experiments, this can be achieved by added $NaNO_2$. Optical density of solutions was measured with digital spectrophotometer Unico 2800 (USA) in wavelength range 500–700 nm with 1 nm step. When the suspension of perfluorocarbon (PFC) emulsion was added, methemoglobin is converted to oxyhemoglobin. This emulsion has nanoparticles of diameter 50–100 nm. Curve Fitting method was used to calculate the percentage of different hemoglobin forms. The experiments shown, as methemoglobin interacted with PFC nanoparticles the spectrum of hemoglobin significantly was changed and the component of oxyhemoglobin was increased. The color of RBC suspension changed from dark brown to red. We obtained that with an initial concentration of methemoglobin in average 85% the addition of nanoparticles of PFC decreases its concentration to control value.

In our work, we have also shown that cytoflavin reduces the level of methemoglobin (Figure 1). Incubation of RBC with cytoflavin after UV irradiation preserves the forms of erythrocytes almost at control level. Atomic force microscope (AFM) NTEGRA Prima, (NT-MDT, Russian Federation) was used to obtain the cell images.

Keywords: ultraviolet radiation, perfluorocarbon, cytoflavin, oxyhemoglobin, methemoglobin, red blood cells, morphology, spectrophotometry, atomic force microscopy.

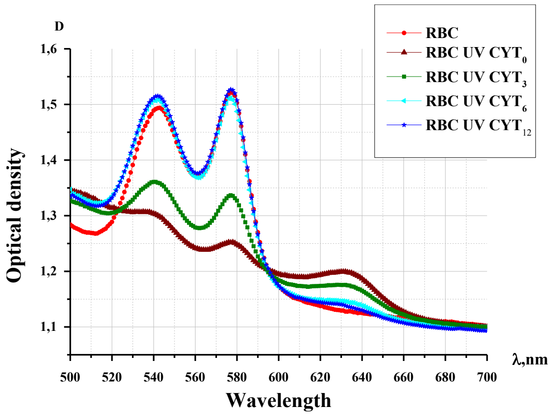

Figure 1: Figure illustrating absorption spectra of RBC suspension with cytoflavin after 24 hour of UV radiation. Incubation RBC suspension with cytoflavin allow to decrease the MetHb level more significantly.

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Nanostructure as biomarkers for the diagnosis of donor blood during long-term storage.

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Abstract:

Packed red blood cells (PRBC) were stored for 30 days under 4^0C in hermetic blood bags with CPD anticoagulant-preservative solution (according to WHO guidelines) for blood transfusion. By atomic force microscopy it was experimentally established that during storage topological nanodefects occurred on PRBC membranes by 9 - 14 days (fig.1a,b). They appeared as domains with grain-like structures sized up to 200 nm, height up to 20 nm. Later these domains merged and formed large defects on cells. The formation of domains with "grains" is onset process leading eventually to destruction of PRBC. By day 30 PRBC transformed into irreversible echinocytes and spheroechinocytes (fig 1a). Possible mechanisms of transformation of PRBC and their membrane are related to the alterations of spectrin cytoskeleton (fig.1b). Study of topological defects of membranes nanosurface may form the basis of assessing the quality of the stored PRBC. This method may allow to work out the best recommendations for blood transfusion.

Keywords: Atomic force microscopy Packed red blood cells Membranes Storage Defects of nanosurface Domains with grain-like structures.

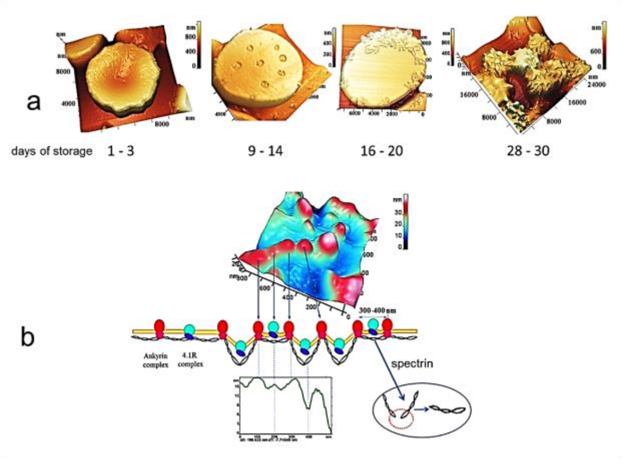

Figure 1: (a) changes in cell morphology during the 30 days of storage. (b) membrane nanostructure on 9- 14 days of storage – the formation of domains with grain-like structures and the violation of spectrin matrix.

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Novel Approach to Flow Label-Free Multiplex Biosensing via Photonic Crystal Surface Wave Detection Technique

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Abstract:

Circulating cancer markers are metabolic products, mostly proteins or peptides, specific for a certain type of malignant tumors. They are found in body fluids (such as blood or urine) of cancer patients. Cancer marker detection plays a key role in cancer diagnosis, treatment and monitoring. The growing need for early cancer diagnosis requires a quick and sensitive analytical approaches to detection of even minor quantities of cancer markers.The approach based on the Photonic Crystal Surface Wave Detection (PCSWD) was developed as a label-free high-precision biosensing technique [1,2]. This approach allows real-time monitoring of molecular and cellular interactions using independent recording of the total internal reflection angle and the excitation angle of the photonic crystal surface wave. Unlike in the widespread surface plasmon resonance (SPR) technique, the sensitivity of PCSWD approach does not depend on the variation of the temperature or composition of the medium.

Here, using the PCSWD technique (Figure 1), we developed a protocol for simultaneous detection of ovary cancer - associated marker CA125 and two breast cancer - associated markers HER2 and CA15-3. A newly developed assay is based on the real-time flow detection of affine interaction between the antigens and capture specific antibodies coupled with the photonic crystal surface of different channels of a PCSWD chip (Figure 1). It is worth mentioning that the possibility of multichannel recording with the same chip allowed multiplexed detection of several cancer markers in a single PCSWD experiment. As compared to most existing techniques, our label-free multiplexed approach not only greatly reduces the time but also the labor and material cost of analysis.

Keywords: biosensors, cancer markers, photonic crystal surface wave, capture antibodies, label-free techniques.

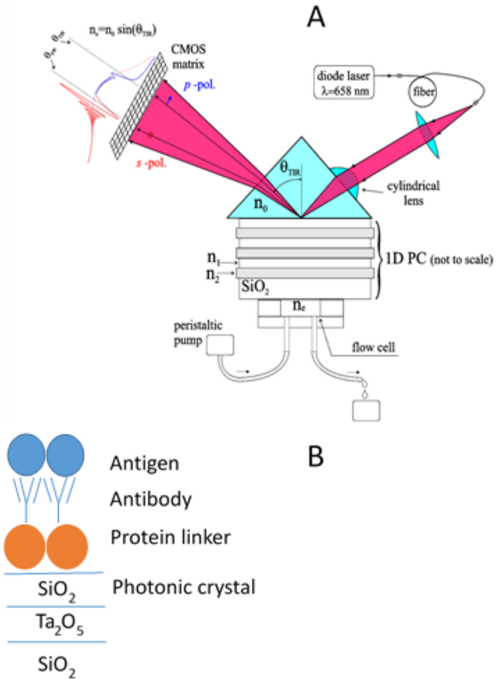

Figure 1: Principal scheme of the PCSWD approach, based on angle interrogation of a photonic crystal surface wave (Panel A).
The typical reflection profile is shown near the CMOS matrix. Panel is adapted from Ref.1.

Panel B shows schematic diagram of the cancer markers detection setup. Outer surface of the multilayer PCSWD chip is functionalized with capture antibodies (Abs) against cancer markers, and affine bindings of the cancer markers (antigens) with the Abs immobilized on the surface of PCSWD chip are detected.

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Feasibility of magnetic nanoparticles encapsulated inside carbon nanotubes for hyperthermia

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Abstract:

Nanomaterials have a tremendous impact as an effective therapeutic tool against cancer. Magnetic nanoparticles (MNPs) are of particular interest; they have the potential to heat up when they are subjected to an external (AC) magnetic field. This lead to their use as candidates for hyperthermia [1-3]. However, due to the potential toxicity resulted from the interaction with the biological environments and risk of agglomeration, MNPs should be well dispersed, chemically stable and have functionalizable surface. Carbon nanotubes (CNTs) can serve as nano-carriers for the filled MNPs, which improves the chemical stability, chemical functionality and biocompatibility.

In this work, different intermetallic alloys have been filled inside CNTs via wet chemistry. The potentiality of the resultant nanocomposites as candidates for hyperthermia has been tested by measuring their heating response upon the application of AC magnetic field. The potential toxicity of pristine and filled CNTs have also been tested via viability assay.

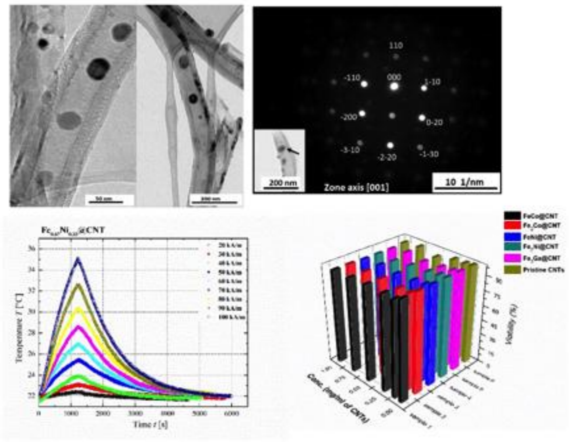

Figure 1: $Fe_{50}Ni_{50}$ nanoparticles encapsulated inside CNTs (*upper left*). Nanodiffraction pattern for selected MNP of the type $Fe_{67}Ni_{33}$@CNT (*upper right*). Temperature profile for $Fe_{67}Ni_{33}$@CNT upon the application of AC magnetic field (*lower left*). Viability assay for different CNTs-nanocomposites (*lower right*).

Keywords: Magnetic fluid hyperthermia, Magnetic nanoparticles, Carbon nanotubes, AC-magnetic field, viability assay.

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Magnetic Nanozyme-Linked Immunosorbent Assay for Ultrasensitive Influenza A Virus Detection

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Abstract:

Rapid and sensitive detection of influenza virus is of soaring importance to prevent further spread of infections and adequate clinical treatment. Herein, an ultrasensitive colorimetric assay called magnetic nano(e)zyme-linked immunosorbent assay (MagLISA) is suggested, in which silica-shelled magnetic nanobeads (MagNBs) and gold nanoparticles are combined to monitor influenza A virus up to femtogram per milliliter concentration. Two essential strategies for ultrasensitive sensing are designed, i.e., facile target separation by MagNBs and signal amplification by the enzymelike activity of gold nanozymes (AuNZs). The enzymelike activity was experimentally and computationally evaluated, where the catalyticity of AuNZ was tremendously stronger than that of normal biological enzymes. In the spiked test, a straightforward linearity was presented in the range of 5.0 × 10–15–5.0 × 10–6g·mL–1 in detecting the influenza virus A (New Caledonia/20/1999) (H1N1). The detection limit is up to 5.0 × 10–12 g·mL–1 only by human eyes, as well as up to 44.2 × 10–15 g·mL–1 by a microplate reader, which is the lowest record to monitor influenza virus using enzyme-linked immunosorbent assay-based technology as far as we know. Clinically isolated human serum samples were successfully observed at the detection limit of 2.6 PFU·mL–1. This novel MagLISA demonstrates, therefore, a robust sensing platform possessing the advances of fathomable sample separation, enrichment, ultrasensitive readout, and anti-interference ability may reduce the spread of influenza virus and provide immediate clinical treatment

Keywords: influenza virus; magnetic force-induced enrichment; magnetic nano(e)zyme-linked immunosorbent assay (MagLISA); nanozyme; point-of-care testing (POCT); three-dimensional immunoassay

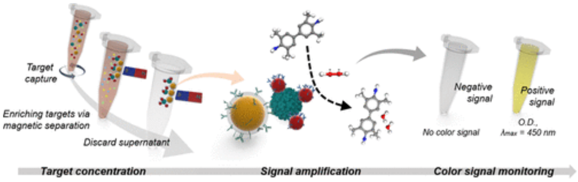

Figure 1: Procedure for the preparation of the MagLISA nanoprobes. Working principle for the quantification of influenza viruses using MagLISAbased colorimetric diagnostics kit.

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Targeting and Killing of Leukemic Cells with Magnetic Nanowires

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Abstract:

In the field of nanomedicine, there is a strong interest for the development of smart nanoparticles that target specific cells, due to their therapeutic potential and biomedical applications. Iron nanowires (NWs) are biocompatible nanoparticles that can be manipulated wirelessly like nano-robots, and they can be coated with various biological agents. Studies suggest that these NWs can induce death in cancer cells by a magnetomechanical effect, where the nanowires are vibrated inside of the cells by a magnetic field. The aim of this study is to functionalize iron NWs with anti-CD44 antibodies, a cell surface marker that is highly expressed in Leukemic cells compared to normal blood cells, in order to target leukemic cells and develop new approaches for their treatment.

Iron NWs with an average diameter of 35 nm and a length 3 µm were fabricated by electrochemical deposition into nanoporous alumina templates. They were coated with (3-Aminopropyl) triethoxysilane (APTES) in order to conjugate them with anti-CD44 antibodies via a covalent bond between the carboxilic group (COO^-) on the antibodies and the amine group of the APTES using a commercial cross linking component, as presented in Figure 1. To confirm the CD44 antibody maintained antigenicity after binding to the NWs, enzyme-linked immunosorbent assay (ELISA), immunoprecipitation and Western blot were used. In addition, the cytotoxicity effects and the transcriptomic changes of both functionalized NWs (i.e. CD44-NWs) and bare iron NWs in the presence and absence of a magnetic field (10 Hz, 100 mT) were studied, by using a colorimetric assay.

The iron NWs functionalized with CD44 antibodies showed a high level of biocompatibility in the absence of a magnetic field. CD44-NWs showed an increase in the targeting efficiency compared to bare NWs, based on the Western blot assay. Cell death can be induced by applying a magnetic field to the cells incubated with CD44-NWs, for just 10 mins. The presence of the magnetic field significantly affected the gene expression, where 360 genes were up-regulated. These results indicate the potential of the functinalized iron nanowires for new approaches to the treatment of Leukemic cells.

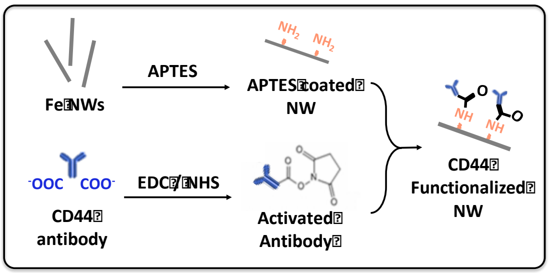

Figure 2: Schematic of the functionalization process of iron NWs. The NWs were coated with APTES, and by activating the (COO-) groups on the antibodies with (1-Ethyl-3-3-dimethylaminopropyl-carbodiimide (EDC) and N-Hydroxysuccinimide coupling) (NHS) they were able to bind to the free amine group on the NWs.

Keywords: Iron - Nanowires - APTES - CD44 antibody - functionalization - XTT assays

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Bare Magnetic Nanoparticles for Protein Recognition

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Abstract:

Biomolecule recognition plays an important role in nature as well as for modern industrial applications. Therefore the development of new ways of biomolecule recognition and design of affinity binding tags is of great importance in protein science. Magnetic iron oxide nanoparticles are an interesting counterpart for peptide tags as their properties facilitate an easy handling and manipulation. Furthermore, these particles can be synthesized with a low-cost co-precipitation route.

The key to the design of high-affinity peptide tags lies in an in-depth understanding of surface-peptide recognition patterns. We combine a model and an experimental approach. The Explicit Implicit Solvation Model (EISM) which has already been used for the design of affinity binding to gold surfaces is parameterized by data from peptide arrays incubated with iron oxide nanoparticles (Figure 1). EISM is an example of an implicit model of the surface with a computational protocol based on the Simulation of Molecular and Nanoscale Systems (SIMONA) engine, performing Monte Carlo calculations, supported by metadynamics, using force field methods as a system description. The EISM model has been parameterized for several surfaces, using empirical data as a basis for defining the affinity of amino acids to inorganic surfaces in certain experimental conditions.

Peptide arrays are used to develop new affinity tags for metals and metal oxides and therefore used for the parameterization of the computational model. This technique is particularly well suited, since iron oxide MNP stain distinctively, leaving dark spots when bound to peptides on a white cellulose membrane.

The goal of our investigation is to extrapolate specific peptide-surface interactions to rationally design iron oxide binding tags which can be used for various applications. Our main issue is therefore to identify different peptide sequences specifically binding bare magnetite nanoparticles in order to provide a computer-based platform of tag which can be genetically engineered and fused to proteins like existing affinity tag systems.

Keywords: bio-nano interactions, magnetic nanoparticles, affinity tags, molecular recognition, binding patterns, iron oxides, proteins, explicit implicit surface model.

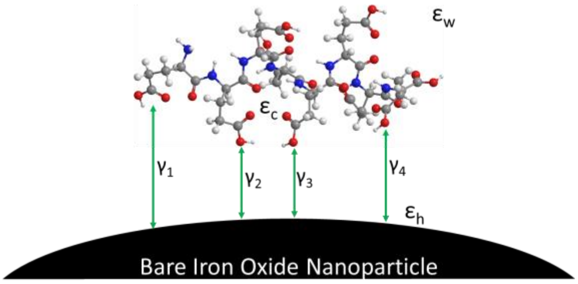

Figure 1: Atomistic Model for Electrostatic, van der Waals, Solvent Exposed Surface. Here a peptide octamer with 8 glutamic acid subunits is chosen, an aqueous solvent and an iron oxide nanoparticle surface.

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Focused Session on Nanotechnology for Drug and Gene Delivery

Magnetic Iron Oxide Nanoparticles Grafted by a Thermosensitive Peptide Brush: Uptake by Tumor Cells and Cytotoxicity by Magnetic Hyperthermia

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[2] IMOTION, Univ Bordeaux, Bordeaux, France.
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Abstract:

This communication reports the grafting onto iron oxide nanoparticles (IONPs) of recombinant polypeptides made of di-block elastin-like peptide (ELP_{40-60}) and cell-penetrating peptide (Tat) sequence.[1] The ELP_{40} block is thermosensitive and undergoes a water de-swelling transition at a critical temperature around 42 °C in solution, the ELP_{60} block is hydrophilic and provides colloidal stability to the resulting γ-Fe_2O_3@ELP_{40-60}-Tat core-shell IONPs. Magnetic IONPs were synthesized by a polyol pathway with either monocore (nanospheres) or multi-core (nanoflowers) morphology, size-dispersity and suitable heating efficiency under an alternating magnetic field (AMF).[2] The bio-functionalization of these IONPs with the di-block ELP_{40-60}-Tat was achieved by a convergent strategy through strong coordination bonding of a phosphonate group introduced near the N-terminus of the polypeptide. To the best of our knowledge, this is the first report on a thermosensitive ELP_{m-n} polypeptide brush grafting onto magnetic IONPs. Large temperature variations of the sample (up to 30 °C) could be obtained in a few minutes by applying an AMF. Fast size changes of the magnetic core-thermosensitive shell nanoparticles were measured by *in situ* dynamic light-scattering (DLS) while the AMF was on. Variations of the hydrodynamic size were compared to the classical polymer brush model revised for the highly curved surface of nanoparticles. Cellular internalization and toxicity assays were performed on a glioblastoma (U87) human cancer cell line in view of applications for drug delivery activated magnetically. Superior cellular uptake was observed for multicore IONPs compared to monocore IONPs (for the same PEG coating),[3] and for IONPs@ELP_{40-60}-Tat peptide-grafted nanoparticles compared to IONPs@PEG controls prepared from the same (spherical) cores. The internalization pathway in lysosomes was monitored by electron microscopy on microtomes and confocal optical microscopy on live cells. Cellular toxicity after AMF application with these core-shell IONPs was ascribed to lysosomal membrane rupture and leakage into the cytosol. The intra-cellular fate of such IONPs, from their internalization to the effect of an AMF application, validates the use of thermosensitive peptide brushes on IONPs as drug delivery systems, addressing lysosomal compartments and triggering leakage of their content by external AMF application. Preliminary in vivo experiments evidenced the positive effect of the Tat peptide end-sequence compared to the PEG brush control on the bio-distribution, with similar contents in the liver and in U87 model tumor in mice. Long term fate (after 48 h) is discussed in view of the cell division with equal sharing of the magnetically loaded lysosomes among daughter cells, possibly envisioning the successive application of magnetic hyperthermia on time scales superior to the cellular life cycle.

Keywords: magnetic nanoparticles, magnetic hyperthermia, cellular uptake, polypeptides, biomedical applications.

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Nano-Delivery
Overcoming the major challenges in Drug and Gene delivey

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[2] Co-Director Oxford Martin Institute of Nanomedicine

Abstract:

Although some progress has been made in developing targeted cancer therapies, surgery and systemic chemo-and radiation therapy remain the chief methods for cancer treatment. These methods are highly invasive, damage healthy tissues and cells and are accompanied by severe side effects. Also, these methods cannot control metastasis, formation of secondary tumours and cancer recurrence. The emerging filed of Nanotechnology has already made a big step on cancer research. In vivo tracking surface-functionalise nanoparticles had brought a therapy that combines diagnosis and real-time monitoring of cancer progression. Currently, in order to increase the stabilisation of chemotherapeutic agents, different nanostructures are being use as transport systems. It has been reported, the use of polyamines and nanoliposomes as transport for epipodophyllotoxin and topotecan drugs to target DNA topoisomerases and showing a promising antitumor activity. However, problems on damaging of healthy tissues and lack of an active multimodal treatment and still remain.

In my group we develop a new therapeutic agents delivery system based on desing of DNA-topological linked to nanoparticles that selectively target cancer cells. We have designed novel nanostructures that can be functionalised with therapeutic agents and studied cell targeting and uptake. This project named "NanoBioSystem" exploits the physical properties of circular double stranded (ds) DNA that make it possible to 'wrap' Nanostructures such SWCNTs and Gold NPs with DNA using non-covalent interactions. These dsDNA-NPs hybrids are soluble, do not degrade in water or serum, are stable over a temperature range of 20-80°C and, importantly, can be sorted by size. dsDNA-NPs can be designed to carry a large payload of therapeutic agents, by attachment of the therapeutic moiety to the outer surface of the nanoparticle. The interaction is reversible with the result that release of cargo occurs intracellularly. Thus dsDNA-NPs represent a possible new nano-delivery system, with possible applications in biomedicine and other areas of biosciences.

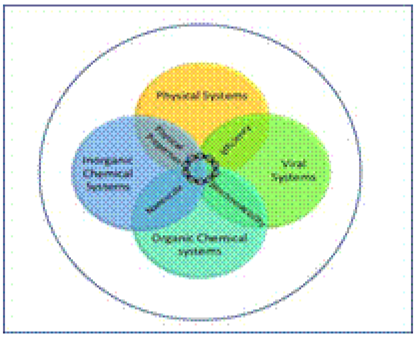

Figure 1: Future novel nano delivery systems properties are, standing at the functional intersection of physical, inorganic, organic chemical, and viral systems taking the essential properties of all of them.

Keywords: cell delivery, nanobiomedicine, biomaterials, AFM, biomedical applications.

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Mesoporous silica, periodic mesoporous organosilica, and mesoporous silicon nanoparticles for drug delivery and two-photon Photodynamic Therapy

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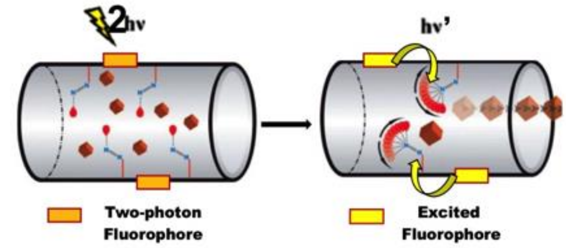
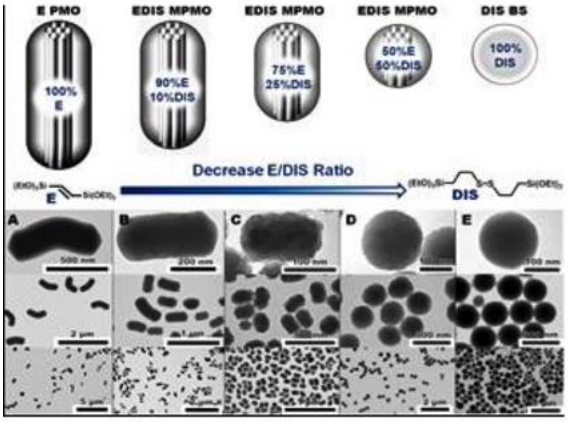
Abstract:

Mesoporous silica nanoparticles (MSN) have attracted much attention the last decade for nanomedicine applications due to their biocompatibility, flexible functionalisation, tunable pore size and diameter. We describe here MSN engineered for two-photon triggered drug delivery or photodynamic therapy, in MCF-7 breast cancer cells. The two-photon triggered drug delivery system was based on a FRET mechanism from a two-photon dye in the walls of the MSN to an azobenzene moiety in the pores of the MSN which kicks the anti-cancer drug molecules out of the pores by isomerisation, (nanoimpellers, scheme 1). Concerning photodynamic therapy, a two-photon photosensitizer was encapsulated in the walls of the MSN. Two-photon photodynamic therapy was performed in vitro and in vivo on mice bearing colon xenografted tumors. Targeting of colon cancer was performed with mannose whereas mannose-6-phosphate analogue was used for prostate cancer. We also studied the use of porous silicon nanoparticles (pSiNP) functionalized with both a photosensitizer and a targeting agent. Porous silicon is a biocompatible and biodegradable material which can generate $^1O_2$ when excited by visible light due to quantum-confinement effect. pSiNP had been shown to be degraded into non-toxic silicic acid byproducts *in vivo*. The multi-functionalized pSiNP studied here were able to target, image and kill cancer cells *in vitro* by photodynamic therapy mechanisms both with 1-photon and 2-photon excitation. Alternatively, the synthesis of disulfide-based biodegradable Periodic Mesoporous Organosilica Nanoparticles (nanoPMOs) was performed (scheme 2) and the nanoparticles were efficient in delivering doxorubicin in cancer cells.



Scheme 1: two-photon nanoimpeller.



Scheme 2: biodegradable nanoPMOs

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Two-Photon Excitation of Porphyrin-Functionalized Porous Silicon Nanoparticles for Photodynamic Therapy
Emilie Secret , Marie Maynadier , Audrey Gallud , Arnaud Chaix , Elise Bouffard , Magali Gary-Bobo , Nathalie Marcotte , Olivier Mongin , Khaled El Cheikh ,Vincent Hugues , Mélanie Auffan , Céline Frochot , Alain Morère , Philippe Maillard , Mireille Blanchard-Desce , Michael J. Sailor , Marcel Garcia , Jean-Olivier Durand , Frédérique Cunin **Advanced Materials, 2014**, 26, 7643–7648

Biodegradable Ethylene-Bis(Propyl) Disulfide-Based Periodic Mesoporous Organosilica Nanorods and Nanospheres for Efficient In-Vitro Drug Delivery
Croissant Jonas, Cattoen Xavier, Wong Chi Man Michel;, Gallud Audrey, Raehm Laurence, Trens Philippe, Maynadier Marie, Durand Jean-Olivier. **Advanced Materials 2014**, 26, 6174-6180

Two-Photon-Triggered Drug Delivery in Cancer Cells Using Nanoimpellers
Croissant Jonas, Maynadier Marie, Gallud Audrey, Peindy N'Dongo Harmel, Nyalosaso Jeff L., Derrien Gaelle, Charnay Clarence, Durand Jean-Olivier, Raehm Laurence, Serein-Spirau Francoise, Cheminet Nathalie, Jarrosson Thibaut, Mongin Olivier, Blanchard-Desce Mireille, Gary-Bobo Magali, Garcia Marcel, Lu Jie, Tamanoi Fuyuhiko, Tarn Derrick, Guardado-Alvarez Tania,M., Zink Jeffrey I. **Angew. Chem. Int. Ed.** , **2013**, 52, 13813-13817

Nanotherapeutics for Targeted Elastic Matrix Regenerative Repair in Vascular Disorders

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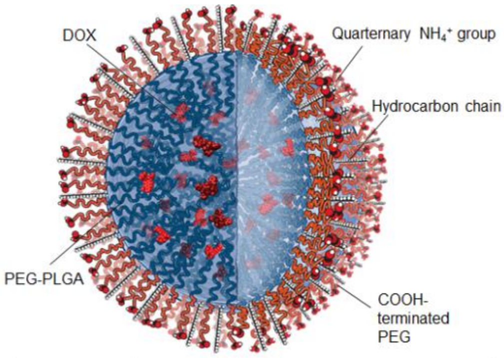
Abstract:

Abdominal aortic aneurysms (AAAs) are localized aortal wall expansions resulting from matrix-metalloproteinase (MMP)-mediated disruption and loss of elastic fibers in the AAA wall. Elastic fibers do not naturally regenerate/repair which prevents AAA arrest/regression [1]. We have shown that low µg/ml doses of doxycycline (DOX) stimulate elastic matrix neoassembly and crosslinking by cultured aneurysmal smooth muscle cells (SMCs) by upregulating TGF-β1 upon inhibition of the regulatory protein c-Jun-N-terminal kinase 2 (JNK 2). Using JNK 2 inhibition as a metric for pro-regenerative matrix effects of DOX, we presently demonstrate that sustained, steady-state release of DOX at the useful dose, from poly(ethylene glycol)-poly(lactic glycolic acid) nanoparticles (NPs) (**Figure 1**), provides pro-elastogenic and anti-proteolytic effects more efficacious than exogenous DOX alone, an outcome attributed to previously determined functional properties of cationic amphiphile-functionalized polymer nanocarriers [2]. Released DOX inhibited expression and phosphorylation of JNK which increased expression of TGF-β1 and increased elastogenesis and lysyl oxidase-mediated crosslinking of the elastic matrix. Independent of DOX-release, the surface-functionalized cationic amphiphile reduced expression and activity of MMP-2. Elastic fiber deposition was significantly enhanced in cell layers cocultured with the DOX-NPs versus cells cocultured with blank NPs and NP-treated cultures. Our results suggest that JNK inhibition is a useful metric to assess pro-elastic matrix regenerative effects and point to the combinatorial regenerative benefits provided by our multi-functional DOX-encapsulated NPs.

Keywords: Regenerative nanotherapeutics, elastic matrix, vascular disorders, tissue engineering, tissue repair



Component	Role
	Repels elastases Inactivates MMPs Attracts negatively charged LOX to increase crosslinking Facilitates vascular NP uptake
	Hydrophobically associates with elastin substrates Engages active site of MMPs to inactivate
	DOX provides both anti-MMP and pro-elastogenic effects
	Biodegradable and porous polylactic co-glycolic acid (PLGA) matrix for encapsulation and slow release of DOX
	PEG; Provides stealth properties, improves circulation time, prevents protein fouling

Figure 1: Schematic of matrix regenerative DOX-NPs formulated using a PEG-PLGA copolymer. Shown are key NP components and their functional roles.

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Challenges on the development of nanotherapeutics: biophysical studies to guide formulation development

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Abstract:
Nanotechnology has been a successful ally of medicine and pharmaceutical development; however many concerns persist regarding the efficacy and safety of nanotherapies (NTs). One of the challenges with NTs is that these nanosystems present increased surfaces and consequently are able to establish greater interactions in our body. *In vitro* assays may be interesting solutions in response to this challenge, since they allow to clarify and understand NTs' properties at the molecular level. Furthermore, under controlled conditions, the use of nanosystems as mimetic models of biological interfaces can help to rationalize and predict NT behaviours and their interactions in vivo.

This work aims to present some assays established within our research [1] based in spectroscopic biophysical methods (steady-state and time-resolved fluorescence; UV-Vis spectroscopy and fluorescence lifetime imaging microscopy (FLIM). The assays presented constitute a helpful set of tools (Figure 1) for developers offering the possibility to study different interactions between therapeutic compounds and nanocarriers, as well as, accessing the interactions of the NTs developed with biointerfaces (membranes and proteins), as this of utmost importance in anticipating NTs therapeutic and *off target* effects.

Keywords: Drug delivery, nanotherapeutics, lipid nanosystems, steady-state and lifetime fluorescence, derivative spectrophotometry, FLIM.

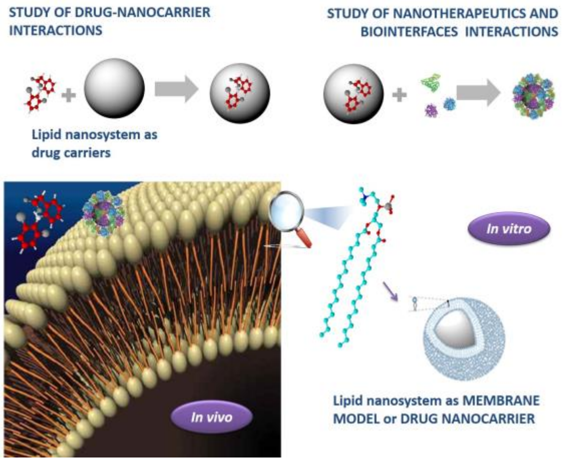

Figure 1: Figure illustrating the use of lipid nanosystems as membrane models or drug nacarriers for nanotherapeutics characterization

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Biophysical characterization based on biomimetic nanosystems/drug interactions: a new strategy for a rational drug design process

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Abstract:

Scientists involved in drug development carry out various *in vivo* and *in vitro* tests that often have contradictory results. This scenario involves an investment of time and money in many compounds that will never reach the market. The rationalization of drug development process is currently a requirement and the emerging tools that support decisions about changes in the chemical structure of the drug to improve its properties can be a solution.

To be effective, it is not enough that the drug has proven activity at target level. The drug must be able to reach the target site in sufficient concentration and time to achieve the required pharmacological effect and thus be eliminated without producing a toxic effect.[1] One of the greatest limitation for drug therapy is the wide variety of membrane barriers present in the body. Biological membrane mimetic nanosystems provide an alternative nanotech platform, allowing the study of drug-membrane interactions under very well defined and controlled conditions.[2] Thus, using several biophysical techniques (derivative spectroscopy; quenching of steady-state and time-resolved fluorescence; quenching of intrinsic fluorescence; synchronous fluorescence; dynamic and electrophoretic light scattering; differential scanning calorimetry and small and wide angle x-ray diffraction) and combining different nanosystems in a high-throughput screening approach it is possible to predict ADMET profiling (absorption, distribution, excretion and toxicity at the membrane level) of newly synthesized drugs. [3] All the gathered information obtained is intended to give researchers who develop new drugs some tools to understand how to improve some parameter of drug profiling.

Keywords: lipid based nanosystems, biomimetic membrane models, drug profiling, derivative spectroscopy, high-troughtput drug screening

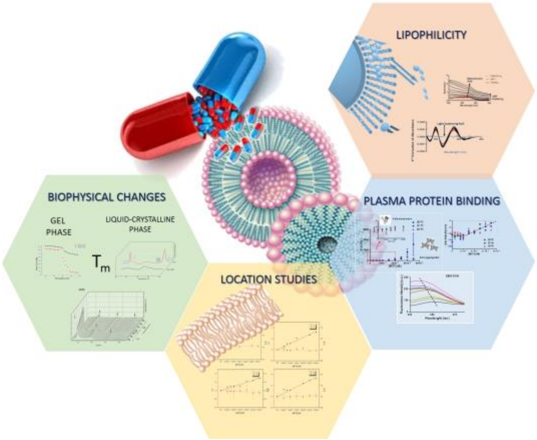

Figure 1: Figure illustrating the several parameters predicted using different biomimetic nanosystems as models.

Aknowledgements: The authors thank ELETTRA, Trieste, Italy, for beam time and support through the project 20155321

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Diclofenac interaction with lipid nanosystems as membrane models: a biophysical assessment of *in vitro* profiling

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Abstract:
Diclofenac (DCF) is a non-steroidal anti-inflammatory drug (NSAID) frequently prescribed to treat acute and chronic inflammatory diseases, e.g. osteoarthritis, rheumatoid arthritis and myalgia. [1] Unfortunately, due to gastrointestinal toxicity its use is limited. Furthermore, DCF is known to interfere with mitochondrial physiology and to cause idiosyncratic hepatotoxicity. [2] DCF needs to cross several cell membranes, composed by lipid and proteins, in order to reach the target site in a concentration able to promote biological activity. By crossing these membranes DCF affects their biophysical properties, inducing on one side the expect anti-inflammatory action and on the other side toxicity.

Accordingly, in this study, we attempted to characterize DCF effects on membrane biophysical properties using membrane mimicking lipid models in order to study: partition coefficient (Kp), membrane location and the effect of this drug in membrane lipid phase transition and order. The membrane model systems used contained the main phospholipid classes of cell membranes: phosphatidylcholine (PC) and the main phospholipid classes of the inner mitochondrial membrane: phosphatidylcholine (PC), phosphatidylethanolamine (PE) and cardiolipin (CL). The partition coefficient (Kp) of DCF was evaluated by derivative spectroscopy to relate the interaction of the drug with liposome/water system, since this is a more realistic description of the drug distribution between the aqueous and membrane phases and is also able to characterize the extent of drug penetration into the membrane and/or interactions with phospholipids or other membrane components. Hydrophobic fluorophores (DPH and TMA-DPH) were used as membrane probes and steady-state, as well as, time-resolved fluorescence measurements have proved useful in monitoring the preferential location of DCF in membranes. Furthermore, the effects in symmetry and in the long and short-range organization of bilayers; in the molecular packing of the bilayers as well as in the chain conformation of the molecules upon the interaction of the bilayers with DCF have been investigated by small and wide angle X-ray scattering (SAXS and WAXS).

Quenching of the fluorescent probes DPH and TMA-DPH revealed a peripheral insertion of DCF in the simple PC model systems, while in the lipid composition of the inner mitochondrial membrane, DCF has a deeper location in the hydrophobic portion of the bilayer. Overall, the present study reinforces that DCF is a membrane-active compound capable of interfering with membrane structure and dynamics, hence influencing membrane-mediated physiological processes. The relevance of these findings will be discussed in terms of the reported DCF interference with lipid gastric lining and on mitochondria toxicity.

Keywords: Dicoflenac, mimetic nanomodels, derivative spetroscopy, steady-state fluorescence, time-resoved fluorescence, small and wide angle X-ray scattering, fluorescence quenching

Acknowledgements: The authors thank ELETTRA, Trieste, Italy, for beam time and support through the project 20155321.

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Novel oxide nanomaterials for drug delivery through the blood-brain-barrier

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Abstract:

Nanoparticles (NPs) and other nanomaterials are thoroughly researched due to their wide range of qualities and consequent applications. One of those qualities is the ability to pass through physiological barriers like blood-brain barrier (BBB). Wide band-gap oxides nanoparticles doped with rare-earth metals have been proven to pass through most barriers including BBB. In this study we began the evaluation of wide band-gap NP's doped with rare-earth metals ability to transport bioactive substances through blood-brain barrier.

Mice received suspension of Y2O3:Tb:Lectin NPs (10mg/ml; 0.3ml/mouse) via gastric gavage (IG) and were sacrificed after 24h, 48h and 1 week. Control group received equivalent suspension of pure lectin. All protocols were conducted according to EU guidelines and approved by LEC agreement No 44/2012. . Following the sacrifice, brain tissue was collected for the analyses under confocal microscope and scanning cytometry. Lectins were chosen as a perfect model substance for the use of NPs as carriers, due to the fact that physiologically they are not absorbed from the gastrointestinal tract.

Signal level for lectin in control group did not exceed background noise. In the research group, signal for lectin coincided with NPs red fluorescence in the brain as soon as 24h after IG. Following 48h, the convergence lowered and after 1 week only free lectin were observed in the brain tissue.

In conclusion, oxide NPs proved to be able to transport bioactive compounds through the blood-brain barrier. After entering brain tissue complexes of nanoparticles and lectin dissolved and free lectin was deposited in the tissue.

Keywords: oxide nanoparticles, lectin, drug carriers, blood-brain-barrier

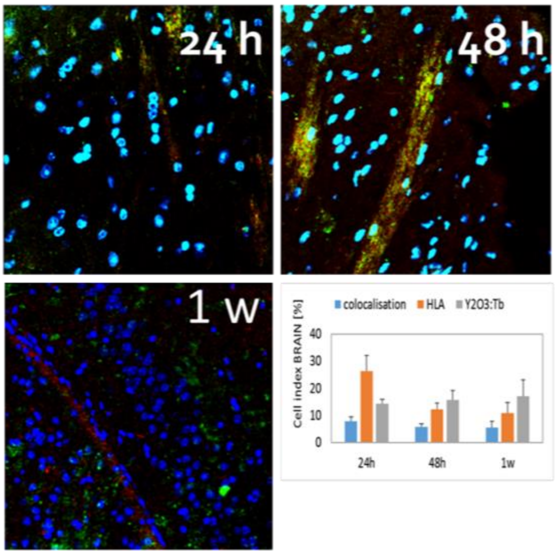

Figure 1: Y_2O_3:Eu:lectins a model nanoparticle capable of the bioactive compounds delivery through the blood-brain-barrier. Y_2O_3:Eu – red fluorescence, lectin (HLA) – green fluorescence, nuclei counterstained with HOECHST 33342, time indicates hours/weeks after oral administration.

Acknowledgments:

The research was partially supported by the National Centre for Research grants "Maestro" 2012/06/A/ST7/00398 and "Sonata-Bis" UMO 2012/05/E/NZ4/02994 supported by the grant from 05-1/KNOW2/2015 "Healthy Animal-Safe Food".

SiO_2 nanoparticles as a vehicle for delivery of nucleoside triphosphate analogues into cells

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Abstract:
Nucleoside analogues represent the cornerstone of any antiviral regiments and are widely used in cancer chemotherapy. The therapeutic efficiency of nucleoside analogues strongly depends on their intracellular accumulation and conversion into 5'-triphosphate (dNTP). The low conversion results in the development of drug resistance and high toxicity, ultimately compromising the effectiveness of this therapy. A plausible strategy to avoid resistance can be the use of a pre-phosphorylated nucleoside as a drug to bypass intracellular phosphorylation. However, nucleoside triphosphates are very poorly internalized by cells.

Recent advances in nanotechnology have provided a number of nanomaterials for cellular delivery of nucleotides. Because active dNTPs cannot be directly administrated into cell, we present here strategy for their efficient delivery using SiO_2 nanoparticles as a vehicle [1-4]. A simple and versatile method has been developed for the preparation of SiO_2-dNTP conjugates via click chemistry between SiO_2 nanoparticles containing alkyl azide groups and dNTPs bearing alkynylated γ-phosphate group (Fig. 1). Conjugates of SiO_2 nanoparticles and phosphorylated dideoxynucleoside antivirals zalcitabine, AZT, lamivudine and ddU (the latter entirely inactive against HIV in its nucleoside form) have been obtained. The conjugates exhibit similar cytotoxicity and cell cycle perturbations in vitro and faster cell accumulation at much lower dose compared with parental drugs, illustrating their therapeutic potential. The results suggest that SiO_2 nanoparticles could be an efficient transport system for delivering phosphorylated nucleosides into cells to increase their potency as antiviral or anticancer drugs.

Keywords: SiO_2 nanoparticles, copper(I)-catalyzed azide-alkyne cycloaddition, phosphorylated dideoxynucleoside analogues, HIV-1, colon cancer cells, cytotoxicity, silica-based biomaterials.

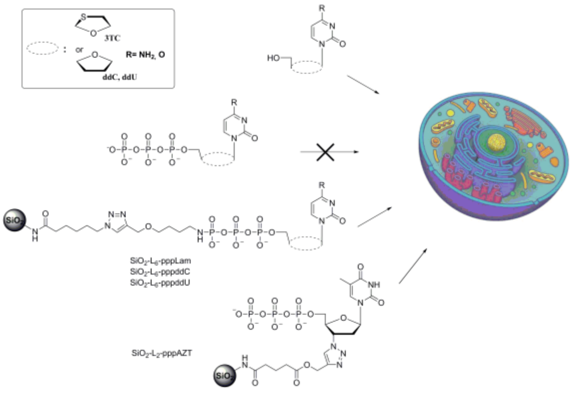

Figure 1: SiO_2 nanoparticles as a vehicle for delivery of nucleoside triphosphate analogues into cells.

Acknowledgment: This work has been funded by Russian Science Foundation (grant № 17-44-07003) in the study of the antiviral properties of nanocomposites. The synthesis of modified nanoparticles was supported partially by RFBR (grant No. 18-515-05007).

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Synthesis of PHA nanoparticles for drug delivery: optimizing the size distribution *via* the effect of the surfactant

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Abstract:

Biopolymer materials as carriers for drug delivery have been extensively studied as they exhibit a low toxicity and can easily be tuned in relation with the nature of the active pharmaceutical ingredients (API), the administration way and the target. Amongst them, the class of polyhydroxyalkanoates (PHAs) presents the advantage of being biocompatible, biodegradable and non-toxic, and includes a large variety of monomeric units in terms of functionality and length of the side chain[1].

In the context of drug delivery, it is particularly relevant to prepare carriers with a well-defined size, which is often specific to the application, as the particles may have to cross boundaries, e.g., the cell membrane, the brain-blood barrier or cell tissues. Besides the size, the chemistry, density and porosity of the carrier affect also greatly the drug release during its delivery and at the target. It is therefore essential to control these characteristics carefully to obtain particles with low distribution of the pharmacokinetic parameters. It is also of importance that they are low in endotoxins, a typical contaminant originating from the bacterial cell wall and in residual compounds from particles synthesis.

Diverse methodologies have been employed for the synthesis of PHA nanoparticles[2], however, the results remain scattered. Moreover, they are often based on toxic surfactants, required both for the preparation of the nanoparticles and for their stable dispersion in solution.

In the present report, the effect of the nature of the surfactants in the emulsion-diffusion method will be thoroughly discussed as it is of importance for the determination of the size, size distribution, density and stability of the particles in solution. Poly(3-hydroxybutyrate) (PHB) was used as polymer and diverse surfactants were tested and compared to standard surfactants such as cetyltrimethylammonium bromide (CTAB). Scanning electron microscopy, dynamic light scattering and zeta potential measurements were conducted in order to characterize the particles size and polydispersity index and get an insight on their surface charge. The latter parameter can be related to the dispersion stability of the nanoparticles in various media.

The final goal is to establish a robust and reliable protocole for the synthesis of PHB nanoparticles in order to obtain a narrow size distribution of dispersion stable nanoparticles, so that they can be further used for testing their biocompatibility and/or behavior *in vitro*. An API can also be encapsulated in the future. This project takes place within the frame of the GoNanoBioMat project (Grant PNIII-P3-285 Polymeric NanoBioMaterials for drug delivery: developing and implementation of safe-by-design concept enabling safe healthcare solutions)

Keywords: biopolymers, polyhydroxyalkanoates, PHB, nanoparticles synthesis, drug delivery, emulsion, surfactants, size distribution

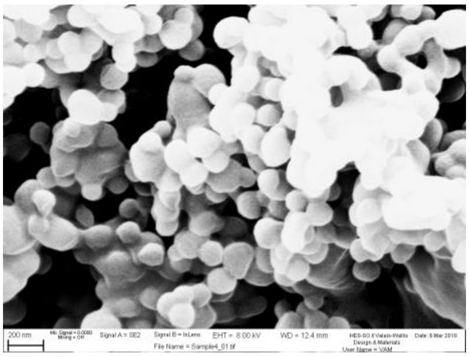

Figure 1: P3HB nanoparticles with CTAB as surfactant.

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A report on synthesis of NIR light responsive nanoparticles-in-microparticles by a double emulsion method: Photothermal and drug delivery use in future

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Abstract

Near-Infra-Red (NIR) light responsive polymeric nanoparticles and liposomes widely are used for drug delivery and photothermal ablation of cancer cells. However, there is an increased chance of nanoparticles getting escape from the target site due to diffusion. Previous studies used for the treatment mainly involve nanoparticles-in-microparticles composite system to find purpose as drug delivery and biosensor applications. Therefore, herein we report the use of novel NIR responsive gold coated PLGA nanoparticles (Au-PLGA) loaded on polycaprolactone (PCL) microparticles (NIM) to serve the purpose. The particles are prepared using double emulsion solvent evaporation method with the average size 100nm. The PCL microparticles were prepared by single solvent evaporation with average size 50µm. The PCL microparticles were characterized with environmental scanning electron microscopy (ESEM) and found in spherical shape with smooth surface morphology. To confirm the loading of Au-PLGA nanoparticles in PCL microparticles first we loaded the fluorescent rhodamine dye in Au-PLGA nanoparticles and later incorporated into PCL microparticles, which was confirmed using bright field microscopy. Further, these NIM composite systems were characterized using different techniques such as Scanning Electron Microscopy (SEM), FEG-TEM (Field Emission Gun-Transmission Electron Microscopy), and EDS (Elemental diffraction pattern. Our intention is to apply the formulation for localized photothermal therapy of cancer and light responsive drug delivery in future.

Keywords; Near-Infra-Red, Polymeric Nanoparticles, Photothermal therapy, Cancer, Nanoparticles-in-microparticles

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Focused session on Nano magnetism - Part I

Spin electronics based sensors for nanoparticle detection.

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Abstract:

Spin electronics based magnetic sensors, GMR and TMR, are regularly improved and can now reach picoTesla range detectivity at room temperature[1]. Due to their small size, they allow single nanoparticle detection.

In a first part, We will present recent improvements on magnetic sensing including routes to reduce the low frequency noise of this kind of sensors.

One important application is the detection of biological objects through specific labeling. Two different approaches will be described.

The first one is a dynamic approach for cell recognition. The principle is to incorporate magnetic particles functionalized with the proper specific antibody in a solution containing the biological fluid and biological objects of interest and to inject the mixture in a microfluidic channel with sensitive magnetic sensors placed underneath. A perpendicular magnetic field polarizes the magnetic particles and their stray dipolar field is detected.

The second one is a static approach aiming at replacing optical evaluation of lateral flow immunoassay to give a more accurate and quantitative evaluation of specific proteins. For that application large arrays of GMR or TMR sensors are used to provide a magnetic imaging of the test strip.

Keywords: Nanoparticle detection, spin electronics sensors.

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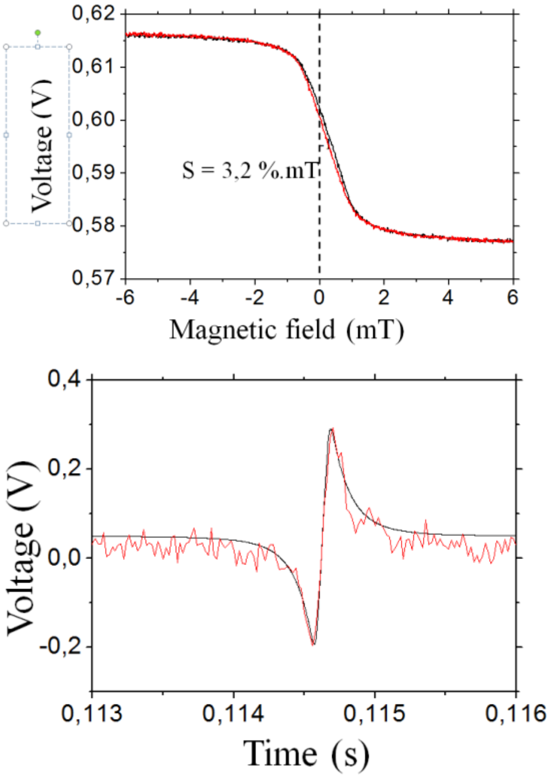

Figure 1 : response of a GMR sensor 3µm wide incorporated in a microfluidic channel (top). Example of a signal created by a cell labelled with nanoparticles (bottom)

The magnetic skyrmions: newcomers in spintronics

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Abstract:

Magnetic skyrmions are topological spin textures [1] that can be found in magnetic materials which break bulk or interface inversion symmetry, in which the skyrmions are stabilized by the Dzyaloshinskii-Moriya interaction (DMI) [2]. Due to their reduced size (as small as a few atomic lattices) and expected low depinning threshold for current-induced motion, magnetic skyrmions are expected to allow for improved scalability and be suitable for "abacus"-type applications in information and communication technologies [3].

Up to the last years, magnetic skyrmions were observed mostly at low temperature and under large magnetic fields in a few bulk non-centrosymmetric compounds and magnetic monolayers. In this talk, I will present experimental results at RT on small skyrmions (30-80 nm) in several types of multilayers associating magnetic layers of Co and nonmagnetic layers of heavy metals (Pt, Ir, Ru etc…) [4]. Then I will illustrate the wealth of skyrmions and will describe i) the creation of skyrmions by current pulses and its mechanism [5], ii) the detection of skyrmions (one by one) by Anomalous Hall Effect measurements [6], iii) the current-induced motion of skyrmions, the influence of defects on velocity and Skyrmion Hall Angle [5]. Finally, I will present results on shaping skyrmion profile and chirality in 3D [7] by a control of the relative values of DMI and dipole interactions for a given number of layers (experimentally determined by x-ray magnetic scattering, XRMS) and its impact on spin torque induced dynamics [8].

These advances made in technologically relevant materials opens the way for the development of several concepts of skyrmion based devices going from race-track memory type to MRAM, from still highly silicon-compatible memories, such as multi-level MRAM or skyrmion racetrack memories to disruptive "beyond CMOS" technologies such as neuro-inspired architectures.

Keywords: Nanomagnetism; spintronics; chiral spin textures;

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d-zero Magnetism in Nanostructures

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Abstract:

A challenging question is whether spontaneous ferromagnetic order is possible at ambient temperature in materials with no *d*-electrons. There are numerous reports in the literature of a ferromagnetic-like response at room temperature to an applied magnetic field for bulk, thin film or nanocrystalline samples of oxides and other materials without any magnetic cation doping. Typical values of the saturation magnetization are tiny, only 1/1000 of that of Fe, Co or Ni, (0.1 - 1 kAm^{-1}), and the magnetization curves show little sign of any coercivity or temperature-dependnce. Once contamination and artefacts are painstakingly discounted, The effect appears to be related to lattice defects, but it is a puzzle to understand how electrons associated with the defects could order ferromagnetically at room temperature and above. The phenomenon depends critically on the sample nanostructure. It will be illustrated by data on three oxide systems: i) $SrTiO_3$ surfaces[1] ii) nanoporous alumina membranes[2] and iii) CeO_2 nanoparticles[3]. Straightforward defect effects are considered, and models based on conventional ferromagnetic superexchange or double exchange will be discussed, as well as exchange splitting of a defect-related impurity band. A key issue is the fraction (if any) of the sample volume that is spontaneously ferromagnetic. A remarkable obsevation — so far restricted to CeO_2 nanoparticles — is that there is a characteristic cluster length scale of ~100 nm below which the magnetism disappears.

Analysis of the magnetic properties suggests that the conventional explanations of the magnetism may be untenable. Results are compared with a new model of athermal *giant orbital paramagnetism* that involves no spontaneous ferromagnetic order. The nonlinear magnetic response is associared with mesoscopic coherent electron states forming in response to the zero-point fluctuations of the vacuum electromagnetic field[4], a magnetic analog of strong-coupling effects discovered in chemistry[5].

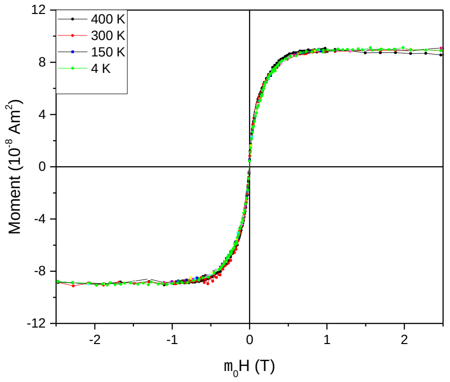

Figure 1. *d^0* magnetism of a mild-anodized nanoporous alumina membrane. The magnetizaton curves are anhysteretic, and superrpose, regardless of temperature from 4 – 400 K. From reference 2.

Keywords: magnetic oxides, nanoparticles, *d*-zero magnetism, quantum fludtuations

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Coherence in electron spin chain: A potentential new kind of qubits.

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Abstract:

Coherence of electron spin has attracted a great interest for the last decade due to its potential application as quantum bits i.e. elementary piece of a quantum computer. Usually, electron spin qubits are made of paramagnetic impurities[1]–[3], which loose they coherence because of the environment interactions (spin bath, phonon bath…) .

Hereby we will present a completely new concept: in strongly correlated Heisenberg spin chain, the isotropic exchange protects the loss of quantum memory. A non magnetic defect polarize the surrounding spins and create a quantum soliton of total spin S=1/2. Since the soliton belongs to the chain it is protected from the environment by the exchange interaction.

Moreover it has been proved theoretically that two qubits belonging to the same spin chain are by nature entangled (necessary condition for quantum communication). However up to now no observation of quantum coherence in such a system has been reported.

We will show the first observation of quantum coherence in electron spin solitons in the organic chain $(TMTTF)_2PF_6$[4]. This result paves the way for the implementation of a different type of quantum computer.

Keywords: electron paramagnetic resonance, qubit, quantum information, strongly correlated magnets, defects.

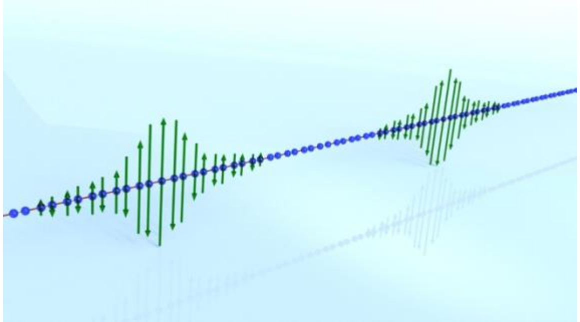

Figure 1: Scematic representation of two sol-qubits connected by the spin chain.

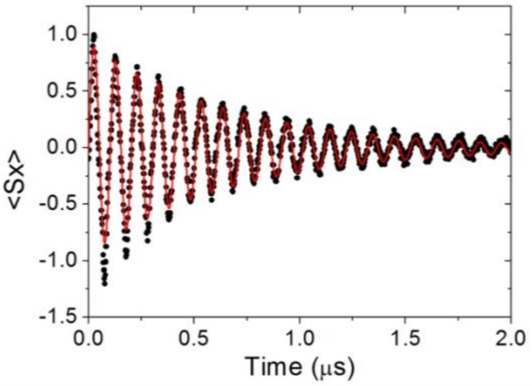

Figure 2: Rabi oscillations of a sol-qubit in $(TMTTF)_2PF_6$

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Magnon-based computing on the nano-scale

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Abstract:

Magnons, the quanta of spin waves, are the collective excitations in magnetic solids. These waves are a promising candidate for data carriers in a solid-state wave-based logic to complement standard CMOS. Proof-of-concept devices in lab-scale experiments like the demonstration of magnonic majority gates [1] have illustrated the advantages of a logic based on wave interference where information can be encoded in the amplitude and phase of spin waves, enabling complex logic functionality with a simple device design. The prospect to create advanced wave-based logic elements and circuits, where information can be encoded in the amplitude and phase of spin waves, has stimulated large research efforts condensing in the research fields of magnonics. In parallel, large attention is paid to the interface of magnonics with standard electron-based spintronics and standard CMOS via spintronic effects, a research direction referred to as magnon spintronics [2]. In my talk, I will give a brief introduction into magnon dynamics. I will provide an overview of prototype magnonics devices and highlight some of the key features of magnons like low power consumption, tunability, nonlinearity and good scalability in the microwave frequency range, which render them such an excellent data carrier. Finally, I will address a selection of our recent efforts to downscale magnonics devices to the nano-scale as well as to increase their functionality.

Keywords: magnetism, spintronics, magnonics, spin waves, wave computing, nanostructuring, logic devices, beyond CMOS.

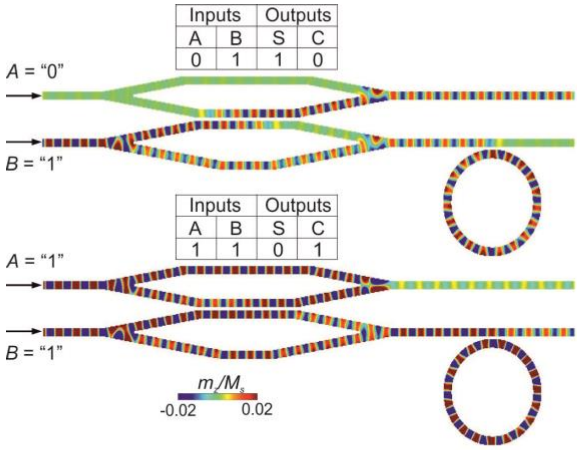

Figure 1: Snapshots from a micromagnetic simulation showing the realization of a magnonic half-adder. If only one input is present, a signal is only dected at the output 'S', whereas a stimulus at both inputs leads to an output only in channel 'C'.

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Ultrafast Lorentz Microscopy: A tool to study laser- and current-driven magnetization dynamics

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Abstract:

Lorentz microscopy is a widely applied technique for the nanoscale mapping of magnetization structures. Its adaptation to time-resolved imaging offers fascinating prospects for studying ultrafast magnetization dynamics [1,2].

The Göttingen Ultrafast Transmission Electron Microscope (UTEM) is a newly developed instrument [1], which allows for studies of ultrafast magnetization and demagnetization dynamics induced by radio-frequency currents or optical pulses [3]. This is facilitated with an electron source which can either deliver a continuous electron beam or electron pulses with a duration down to 200 fs at a 0.6 eV spectral width and a sub-nm focal spot size [1]. In this contribution, we investigate the gyrotropic motion of a magnetic vortex confined within a 20nm thick 2µm x 2µm permalloy nanoisland [5]. Exciting the magnetic vortex with an in-plane spin current near the resonance frequency of 101MHz, we follow the trajectory of the vortex core with a localization precision of better than 3 nm r.m.s. Furthermore, we investigate the response of the vortex to non-periodic excitations. Using a sinusoidal current pulse which only lasts for a few cycles, we can trace the build-up and relaxation of the vortex gyration, which yields the damping and the spectral characteristics of our sample system.

Keywords: Ultrafast Transmission Electron Microscopy, magnetization dynamics, ultrafast demagnetization, time-resolved magnetic imaging, Lorentz Microscopy

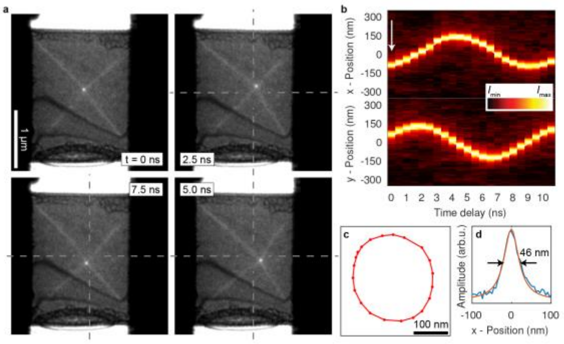

Figure 1: (a) Time-resolved Lorentz micrographs of the gyrotropic motion of the vortex. (b) Line profiles along x- and y-direction as a function of time delay. (c) Positions of the vortex core during a single cycle. (d) X-profile of the vortex core t=0 ns with a full-width half max of 46 nm.

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Focused session on Nano Magnetism - Part II

Magnetic Oxides-based Hetero-Nanostructured Ceramics: From Nanomaterial Engineering to Exchange-bias Coupling

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Abstract:

In the last few decades, the increasing world needs for more and more efficient and cheap electronic devices put in evidence the necessity to rely the technological development of advanced functional materials. Most of these consumer goods contain magnetic materials. These materials are essential components for energy, telecommunication, transportation, medicine applications, among others. The characteristics of the employed magnetic material play a fundamental role on the design of a specific application. For example, smaller size devices, operating at lower electronic power, are required. Moreover, the possibility to integrate magnetically contrasted composite materials, in such devices, open up the possibility to design new systems with enhanced electromagnetic properties. These properties of course derived from all the single constituents but also from their mutual coupling. For instance, coupling a ferromagnetic (F) phase to an antiferromagnetic (AF) one gives rise to exchange interactions, called exchange bias (EB), that may impact in different ways the final properties. It usually enhancee the magnetic thermal stability of the small F structures, overcoming their superparamagnetic limit [1]. It is thus considered to increase the storage capacity of magnetic recording media [2]. It is also pursued to stabilize the magnetization of the soft F reference layer in giant magnetoresistance (GMR) based computer read heads [3,4]. Similarly, it is employed in commercial magnetic random access memories (MRAM) circuits Freescale [5]. As it is investigated as a physical basis for the development of rare-earth free magnets [6].

The origin of EB can be described by an alignment of the AF spins at the F–AF interface parallel to the F spins occurring during the field-cooling procedure. The coupling between the AF and F spins exerts an additional torque on the F spins, which the external field has to overcome. As a consequence, EB induces a shift and/or a broadening of the hysteresis loop, [7]. Currently, the most studied E-biased systems are thin films and nanopowders [8]. Very few works exist on consolidates. This deficiency is mainly due to the fact that sintering involves heating at high temperature inducing grain growth, reducing significantly the surface/volume atomic fraction and therefore EB effect. Nevertheless, the emergence of Spark Plasma Sintering (SPS) technique has propelled a renewed interest in consolidated hetero-nanostructures exhibiting EB. Indeed, SPS operates operates at moderate temperatures for short times, favoring ultrafine microstructure and high density [9]. It is also a powerful solid-state chemical route for the preparation of single [10] and multi-phases [11]. In this context, we propose to prepare highly dense, fine-grained magnetically contrasted solids using SPS, strating from E-biased nanopowders or mixtures of preformed F and AF ones, to investigate EB feature. We also propose to focus on magnetic oxide materials, namely F spinel ferrite and AF rock-salt transition metal monoxide phases, as models. We describe and discuss then our main results in terms of material processing optimization, microstructure analysis and magnetic behavior characterization, underlining the advantageous and/or disadvantageous of SPS in the design of multifunctional ceramics.

Keywords: Exchange Bias, Nanoparticles, SPS, Nanoceramics, High Resolution Transmission Electron Microscopy (HRTEM), Magnetometry.

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Strain-mediated all-magnetoelectric memory cell

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Abstract:

One of the most prospective principle of random access memory that ensures high energy efficiency is based on strain-mediated magnetoelectric interaction in magnetic-piezoelectric heterostructures. The principle allows ~~for~~ writing information in the magnetic subsystem as well as detecting the magnetic states by means of electric field pulses[1]. The Design of the magnetoelectric memory (MELRAM) requires a detailed study of the strain-mediated interaction in nanoscale devices. Here, we report the results of simulation of strain distribution in the MELRAM nano cell and its expected dynamic parameters. As a basic magnetic component of the cell we considered giant magnetostrictive intermetallic multilayer *N*($TbCo_2$ /FeCo) (50x50x400nm^3) elastically coupled to a ferroelectric nano-pillar PMN-PT <011> (200x75x500nm^3) (Figure 1). The magnetic multilayer acts also as a top electrode.The pillar is a part of the ferroelectric substrate. The bottom electrode is located on the substrate around the pile. At nanoscale the elastic and electrodynamic boundary conditions affect essentially the parameters of devices. The shape of the cell presented on Figure 1 is chosen to reduce as much as possible the inhomogeneity of the strain distribution in the magnetic subsystem. The dynamic parameters of the cell were calculated by the same approach as in ref.[2] but taking into account the strain and electric field inhomogeneity. The magnetoelectric energy density responsible for the magnetization ***M*** switching between *x* and *y* directions is defined as:

$$F_{ME} = \frac{1}{2} a_{ME} V_c(t) B \left(M_x^2 - M_y^2 \right) / M^2$$

where $V_c(t)$ is the electric voltage applied to the electrodes, *B* is the magnetostrictive constant. The magnetoelectric coupling factor was found equal to α_{ME}=-1.47 10^{-3} 1/V. The capacitance of the cell and the readout voltage were found equal to *C*=1.57 fF and V_{ME}=4.7 mV, respectively. For effective anisotropy field including technologically induced and shape anisotropy H_A =300 Oe and control voltage V_c=0.2V the energy consumption is found to be *E*=60 aJ/bit and switching time t_S=0.5 ns.

Keywords: magnetoelectric memory, magnetostriction, ferroelectricity, inhomogeneous strain, dynamic parameters, energy efficiency.

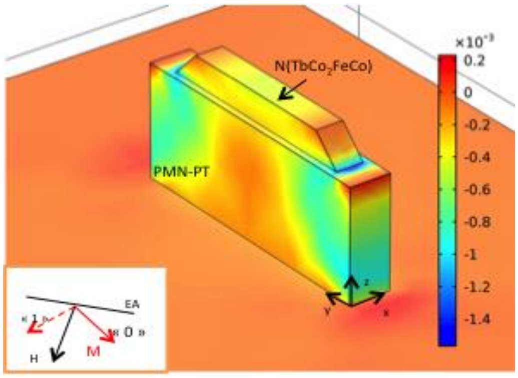

Figure 1: Figure illustrating inhomogeneous strain distribution in the components of the MELRAM cell under a control voltage V_c=0.2V applied between intermetallic magnetostrictive layer *N*($TbCo_2$/FeCo) and bottom electrode surrounding the ferroelectric PMN-PT pillar. The average anisotropic deformation in the layer <u_{xx}-u_{yy} >= -2.95 10^{-4}.

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Acknowledgment:

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Probing Nanoscale Magnetic Properties Using a Pt-based Hall Device

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Abstract:
It is generally known that interface (or surface) aspects play an important role in the magnetic and structural properties of magnetic thin film systems. A thorough and detailed structural and magnetic characterization with interface specificity is required. However, challenges for understanding and probing nanoscale magnetism at interface (or surface) structure still remain. A recently discovered spin Hall magnetoresistance (SMR) phenomenon promises to provide new insight into nano-magnetism. SMR in bilayer structures consisting of a heavy metal (HM) and a ferromagnetic (FM) insulator (or metal) has been proposed as a tool for probing interface magnetism which is difficult to obtain with any standard magnetometer [1, 2].

In this work, the interface roughness effect on the SMR for Pt-based heterostructures such as Pt/Fe_3O_4 and Pt/Mn is systematically investigated. We report the interplay between surface morphology and the magnetic properties of FM Fe_3O_4 and antiferromagnetic (AF) Mn films. Our results reveal that the electrical properties of the Pt Hall bar strongly depend on the interface geometry of Pt/Fe_3O_4 and Pt/Mn. As the interface roughness increases, we observed strong enhancement of spin-mixing conductance that is extracted from the SMR effect measured at low temperature (at 77 K). Moreover, the temperature dependence of the resistivity of Hall bars cooled under application of an external magnetic field provides important information for understanding interface magnetic properties of Fe_3O_4 and Mn. The resistivity versus temperature curves measured under a magnetic field applied along different crystal directions exhibit a clear difference between the zero-field-cooled (ZFC) and field-cooled (FC) traces, from which the direction of the magnetic easy-axis can be determined. The morphological evolution of the magnetic films (Fe_3O_4 and Mn) was monitored as a function of film thickness ranging from 2 nm to 10 nm by Atomic force microscopy (AFM). Our results highlight that SMR effect plays an important role in the development and study of new emergent phenomena at interfaces.

Supplementary Figure S4. Temperature dependence of the resi
film as a function of temperature.

Keywords: spin Hall magnetoresistance, spin trnasport, interface effect, surface effect, magnetic properties

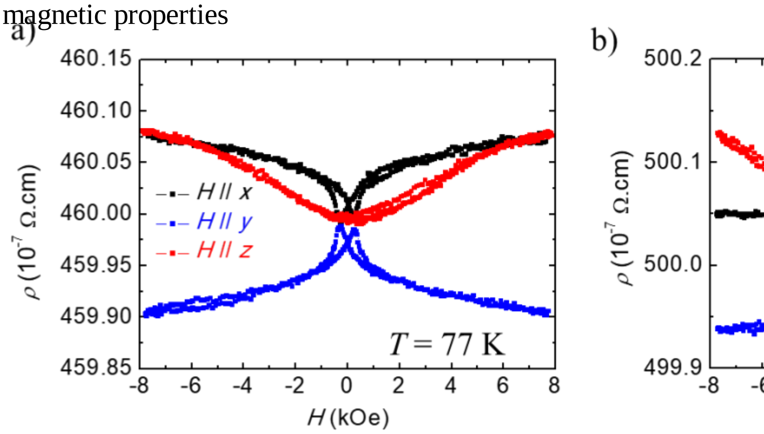

Figure 1: Magnetic filed dependence of the resistivity of a thin Pt Hall bar grwon on Fe_3O_4/MgO(001).

Supplementary Figure S5: (a) Magnetic field dependence of the re
sample B1 at T = 77 K, for an external magnetic field applied along th

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Best of Two Worlds: Combination of Magnetic and Semiconducting Properties in (Ga,Mn)(Bi,As) Nanostructured Thin Films

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Abstract:

In a highly-demanding time of the Information Age requirements for new ideas to push the classical limits of the electronics are very high. Combining miniaturization, search of new/enhanced materials with improved characteristics and state of the art development of alternative concepts [1], we're working on spintronic nanostructures made from quaternary alloy of (Ga,Mn)(Bi,As) thin ferromagnetic semiconductor [2].

In order to provide an overall description of the material, a quick overview of the III-V ferromagnetic semiconductors theory will be given, ensured by samples structure and magnetization characterization check: superconducting quantum interference device (SQUID) and highly polarized muons spectroscopy measurements (LT-µSR) combined with general layers quality description by X-ray diffraction (HR-XRD). Furthermore, we'll show cross-like (Fig. 1) and ring-shape geometries of nanostructures, tailored using electron-beam lithography patterning and chemical etching from 10-nm thick (Ga,Mn)(Bi,As) epitaxial layers with 6% Mn and 1% Bi contents.

An interplay between original magnetic in-plane anisotropy of the material and patterned-induced anisotropy, introduced via the lithography process, creates well-defined magnetic defects (domains). As a result, we achieve resistance difference between contacts pairs, that can be driven by an applied low magnetic field or a spin-polarized current and increased as a result of enhanced spin-orbit coupling by bismuth incorporation. Series of thorough magneto-transport and magnetic measurements on similar structured thin layers of (Ga,Mn)(Bi,As) / GaAs and earlier concepts [3] based on well-known (Ga,Mn)As / GaAs semiconductor proves stability and utility of such a magnetic memory unit.

Keywords: dilute magnetic semiconductors, spintronics, SQUID, LT-µSR, HR-XRD, spin-orbit coupling.

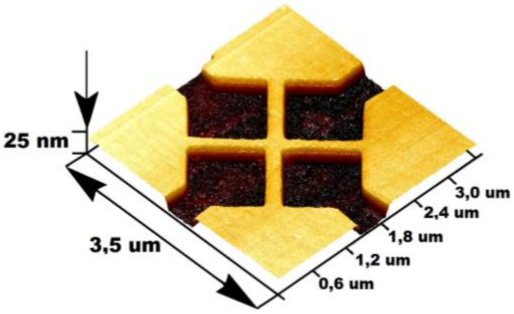

Figure 1: Atomic force microscopy (AFM) image for the cross-shaped nanostructure of (Ga,Mn)(Bi,As) thin epitaxial layer grown on semi-insulating GaAs. The darker contrast corresponds to non-conducting areas etched to the substrate.

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NanoMatEn 2018 / Session II.C: Nanomaterials for Energy / NanoElectronics

Layered and 2D materials: electronic properties and structural instabilities from first principles

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Abstract:
We will present some of our recent work [1-5] on the understanding of the electronic properties of layered materials and their 2D relatives by means of first principles electronic structure calculations. In particular, the presentation will focus on the correlation between the crystal structure and the electronic properties, with special emphasis on the structural instabilities which have an electronic origin. This will be done in connection with recent experimental studies that have been able to demonstrate the presence of charge density waves (CDW) in several 2D single-layer materials like $NbSe_2$ and $TiSe_2$ and $TiTe_2$. For $NbSe_2$, we have focused on the nature and atomic displacements associated with the CDW. The evolution of the CDW with external electrostatic doping, which has been achieved experimentally using field effect transistor setups, will be analysed for the case of $TiSe_2$ [4]. For the case of $TiTe_2$, we focus on the recently observed CDW in the single layer, which is not present in the bulk material [5].

Keywords: 2D Materials; Transition Metal Dichalcogendes; Charge Density Waves; Density Functional Theory; Electronic Structure; Electronic Instabilities.

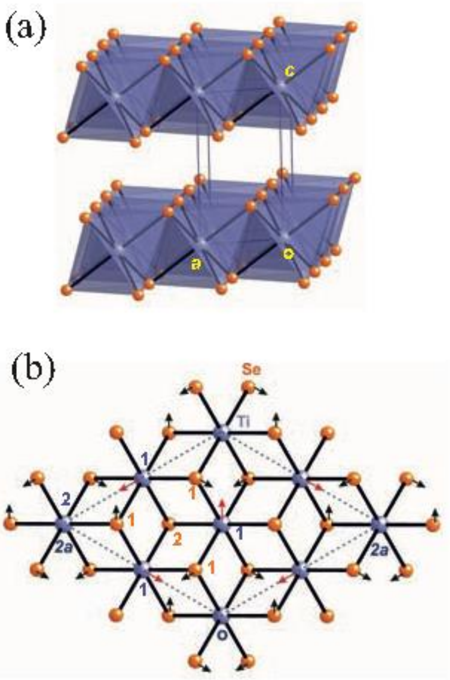

Figure 1: (a) Crystal structure of $TiSe_2$. (b) Schematic representation of the displacements occurring in a single-layer of the 2x2 CDW structure of $TiSe_2$.

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Development of nanogenerators for mechanical energy harvesting and self-powrered electronics

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Abstract:

Development of renewable energies is crucial for meeting future energy needs. Solar, mechanical and kinetics energies can provide sufficient electricity needed in daily life. Mechanical energy harvesting approaches, such as electromagnetic, piezoelectric, triboelectric and electrostatic effects, have been utilized for energy conversion. Generally, piezoelectric generator (PEG) is based on piezoelectric polarization effect, while triboelectric generator (TEG) is based on the coupling of triboelectric and electrostatic induction effects. In particular, TEG has attracted attention due to its simple working mechanism and fabrication process, high power output and efficient energy conversion. Flexible hybrid generators based on silicon rubber (PDMS) composite films embedded with functional materials combining piezoelectric and triboelectric properties are fabricated. Meanwhile, single effect generators are also fabricated in order to analyze the contribution of each effect in the hybrid output and to understand the transduction mechanism of each effect and the impact of each material on the piezoelectricity or triboelectricity during the power generation process. To improve the output power density and energy conversion efficiency, nanostructures of zinc oxide are grwon on the surface of the composite films for enhancing the effective contact area. The ratio between triboelectric and piezoelectric effects (T:P ratio) in composite generators is then introduced and analyzed. In addition to composite films, the investigation shows the triboelectric charge density can be boosted by embedding gold nanoparticles in bulk materials for enhancing the energy generation potential. Fabrication of flexible and lightweight mechanical energy harvester is a promising approach for wearable electronics. In this pursuit, textile based generators are developed using a facile fabrication process. The surface properties of textiles play significant roles in the output performance. Demonstration of a cashmere based harvester as a power source shows potential application in self-powered wearable electronics. By growing ZnO nanostructures on the textile surfaces, piezoelectric properties can be incorporated and utilized as pressure sensors. While solid-solid based TEG have proved to produce higher voltage in dry conditions, contact electrification charges are also generated at liquid-solid interfaces. Among renewable energy sources, water energy, being one of the most abundant source covering 70% of the earth's area, has great potential as power source toward sustainable development. The impacts of contact over a broad frequency range and output characteristics under resistive and capacitive load for different liquid types are investigated using a PTFE based TEG. Optimum contact frequency and load conditions for maximizing the power density and energy conversion efficiency are also presented. Toward designing effective structures and power management as well as for future simulation of a range of single and hybrid generators, a comprehensive theoretical and experimental study conditions was conducted on the impacts of a wide range of design parameters on the output properties and load characteristics under resistive and capacitive load.

Keywords: mechanical energy harvesting, water wave energy, wearable electronics, triboelectric effect, piezoelectric effect, pressure sensor.

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Self-Powered Flexible Inorganic Electronic Systems

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Abstract:
This seminar introduces three recent progresses that can extend the application of self-powered flexible inorganic electronics. The first part will introduce self-powered flexible piezoelectric energy harvesting technology. Energy harvesting technologies converting external sources (such as vibration and bio-mechanical energy) into electrical energy is recently a highly demanding issue. The high performance flexible thin film nanogenerator was fabricated by transferring the perovskite thin film from bulk substrates for self-powered biomedical devices such as pacemaker and brain stimulation. The second part will introduce flexible electronics including large scale integration (LSI) and high density memory. Flexible memory is an essential part of electronics for data processing, storage, and radio frequency (RF) communication. To fabricate flexible large scale integration and fully functional memory, we integrated flexible single crystal silicon transistors with 0.18 CMOS process and memristor devices. The third part will discuss the flexible GaN/GaAs LED for implantable biomedical applications. Inorganic III-V light emitting diodes (LEDs) have superior characteristics, such as long-term stability, high efficiency, and strong brightness. Our flexible GaN/GaAs thin film LED enable the dramatic extension of not only consumer electronic applications but also the biomedical devices such as biosensor or optogenetics. Finally, we will discuss laser material interaction for flexible and nanomaterial applications. Laser technology is extremely important for future flexible electronics since it can adopt high temperature process on plastics, which is essential for high performance electronics, due to ultra-short pulse duration. (e.g. LTPS process over 1000 °C) We will explore our new exciting results of this field from both material and device perspective.

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Circularly Polarized Luminescent Polymer Film Fabricated with Chiral Nano-fibrils

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Abstract:

This paper demonstrates a new strategic approach to create chiroptically active and luminescent polymer film, which can be achieved by compositing with chirally assembled nanofibrils. This approach is based on the fact that the glutamide (***g***) derivative as a low-molecular organogelator, which is characterized by introduction of a functional head group and double alkyl chains to glutamic acid through amide bonds, forms one-dimensional chiral stacking states both in organic solutions and polymers (Figure 1). The dispersion behaviors of the ***g*** derivatives are quite unique: for example, when 1 mM of the enantiomeric ***g*** derivative having an anionic head group was dissolved in cyclohexane and allow to stand at room temperature, a transparent and colorless gel was formed. TEM and SEM observations indicated that the gel formation was through three-dimensional network formation with nano-fibrillar aggregates (Figure 1). When a cationic and non-chiral fluorophore such as a cyanine dye was mixed with the gel, CD spectroscopy exhibited strong exciton couplings around the absorption band of the non-chiral dye, which indicated induced chirality toward the dye from the ***g***-aggregates. On the basis of these observation, we succeeded to detect extremely strong circularly polarized luminescence (CPL), which has attracted attention as a next-generation light source because of its distinct advantages over normal light, such as extensive optical information and a lack of angular dependence. No similar result was observed in the absence of the ***g***-derivative but also in the condition when the ***g***-molecule dispersed as a disordered state. In this paper, we describe that the intensity enhancement of induced chirality and CPL can be enhanced by a small amount of aditive but also a CPL-exhibiting polymer film can be fabricated by simple mixing the dye-***g*** binary system with polymer.

Keywords: Glulutamide, organogel, self-assembly, nano-fibril, secondary chirality, circularly polarized luminescence, transparent optical film.

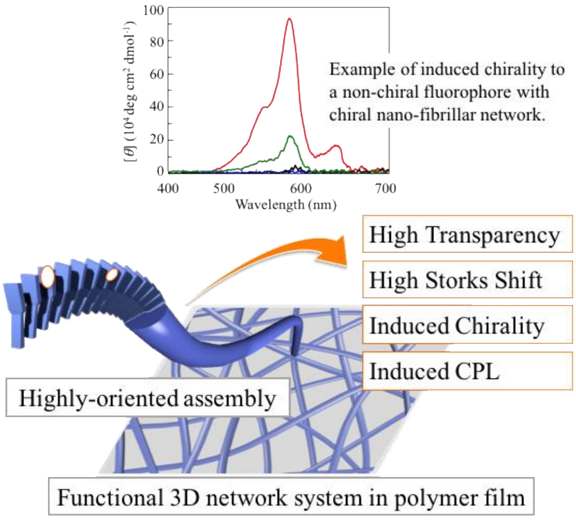

Figure 1: Schematic illustration on luminescent polymer film functionalized with chiral nano-fibrillar webs. The CD spectra indicate a temperature-dependent chirality change on cyanine dye in the presence of *g* assembly with trimethyl-amine: (red line) at 25 ˚C; (blue line) at 50 ˚C.

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Nanomaterials for High Temperature Photonics

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Abstract

Recent research results will be presented on nanomaterials as selective emitters and for near field radiative transfer for thermophotovoltaics and on tailored photonic glasses as non-iridescent structural colors.

Emission of thermal radiation is a fundamental physical process defined by the dielectric properties of the thermally excited materials. Radiation into far field is described by Planck's law and is limited by the blackbody emission. In near field, additional thermal energy transfer can be achieved due to evanescent fields, which are orders of magnitude larger than in far field. In the far field, emission, e.g. of long wavelengths below the energy of a semiconductor receiver band gap, can be suppressed in band edge emitters from nanostructured hyperbolic optical metamaterials as well as with resonantly coupled dielectric particle layers on top of plasmonic substrates. We demonstrate selective band edge emitters for thermophotovoltaic devices stable up to >1200°C based on W-HfO_2 refractive metamaterials as well as ZrO_2 based ceramic particles on tungsten. We further report on ceramic photonic structures as high-temperature stable structural colors. A careful choice of the interplay between lattice and motif parameters of the photonic glass allows for structural colors with strong color saturation.

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Metal Selenides as Efficient Cathodes for Dye-Sensitized Solar Cells

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Abstract:

Solar energy is the most abundant renewable energy available to the earth and can meet the energy need of mankind, but efficient conversion of solar energy to electricity is an urgent issue of scientific research. As the third-generation photovoltaic technology, dye-sensitized solar cells (DSSCs) have gained great attention since the landmark efficiency of ~7% reported by O'Regan and Grätzel. As one of the key materials in DSSCs, the counter electrode (CE) plays a crucial role in completing the electric circuit by catalyzing the reduction of the oxidation state to the reduction state for a redox couple (e.g. I_3^-/I^-) in the electrolyte at the CE/electrolyte interface. To lower the cost caused by the typically used Pt CE, which restricts the large-scale application due to its low reserves and high price, great effort has been made on developing new CE materials alternative to Pt. A lot of Pt-free electrocatalysts, such as carbon materials, inorganic compounds, conductive polymers, and their composites with good electrocatalytic activity, have been applied as the CEs of DSSCs in the past years. Metal selenides have been widely used as the electrocatalysts of oxygen reduction reaction and the light-harvesting materials for solar cells. Our group first expanded their applications to the DSSC field by using *in situ* growth $Co_{0.85}Se$ nanosheet and $Ni_{0.85}Se$ nanoparticle films as the CEs.[1] This finding has inspired extensive studies on developing new metal selenides in order to seek more efficient CE materials for low-cost DSSCs, and a lot of meaningful results have been achieved in the past years. In this presentation, we summarize recent advances in binary and mutinary metal selenides applied in DSSCs as the CEs.[2] Metal selenide CEs can be prepared *via* several methods, among which the *in situ* growth strategy is superior to other methods, because it offers more homogeneous dispersion on the substrate, stronger adhesion to the substrate, and more effective catalytic sites. The effects of morphology and stoichiometric ratio on the electocatalytic and photovoltaic performance are discussed in this paper. It is found that metal selenides demonstrate excellent catalytic activity with low-cost and good stability, and they will become strong competitors as CE materials for large-scale applications.

Keywords: dye-sensitized solar cell, metal selenide, electrocatalyst.

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Back-Contact Perovskite Solar Cells

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Abstract:

Back-contact concepts are well established in the field of silicon solar cells, where their implementation has resulted in significant efficiency gains, compared to conventional sandwich architectures. Charge collection in these devices is typically facilitated by a set of two interdigitated finger electrode arrays, co-located on the backside of the silicon wafer. Here we describe the fabrication and study of back-contact methylammonium lead iodide perovskite solar cells (bc-PSCs). The main advantage of back-contact concepts is that optical transmission losses can be avoided, arising from the top charge collection electrode, which for PSCs typically is a thin conducting oxide (TCO) layer. We present a number of novel back-contact electrode architectures which are more defect tolerant than the conventional interdigitated finger design[1]. We demonstrate that these novel microelectrode designs can be fabricated with low-cost mask-less lithography techniques. Furthermore we report a novel photovoltaic device concept based on a gold-perovskite-gold Schottky-junction bc-PSCs in which the work-function of the gold electrodes is controlled by the presence of self-assembled molecular monolayers (SAM)[2]. We provide evidence of the successful workfunction tuning by means of Kelvin probe microscopy while also presenting the photovoltaic performance date of these devices. We show that the presence of these SAMs can produce photovoltages of up to 600 mV and photocurrents in excess of 12 mA/cm^2 under simulated sunlight, despite a large center-to-center electrode spacing of 6.5 µm.

Keywords: Nano and microtechnology for energy applications, perovskite solar cells, solution-processable, back-contact.

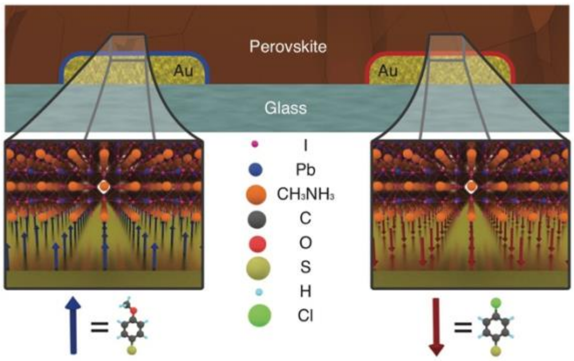

Figure 1: Cross-sectional diagram of a gold-perovskite-gold heterojunction solar cell modified with 2 self-assembled monolayers with different dipole properties.

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Efficient and Stable Flexible Perovskite Solar Cells with Nano-Engineered Solution-Processed NiO Hole-Transporting Layers

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Abstract:

Organic/inorganic hybrid perovskite solar cells (PSCs) are a promising type of solar cell devices owing to their high efficiency and ability to be fabricated with solution-based processes. Replacing the commonly used organic hole-transporting layer (HTL) of PSCs with a NiO one has been shown to significantly enhance their efficiency and stability, but the solution-based processes of a NiO HTL require high processing temperatures, which limit the NiO HTL's compatibility with organic active materials and flexible polymer substrates. This study presented a novel method for fabricating high-quality solution-processed NiO HTL at much reduced temperatures, with which highly efficient and stable flexible PSCs based on polymer substrates were demonstrated. The method involved embedding NiO sol-gel precursors with a nanostructured metal phase, whose catalytic functions enabled the percursors to completely react and crystallize into high-purity and crystalline NiO films at temperatures considerably lower than those without the nano metal phase. Extensive morphological and compositional analyses were conducted to elucidate the mechanism of the reduction in processing temperature. Utilizing the low-temperature-processed NiO HTLs, flexible and rigid PSCs achieved high power conversion efficiencies of up to 15.9 and 19.0 %, respectively, while showing excellent stability under accelerated aging condition. Several sol-gel metal oxides besides NiO were also demonstrated to exhibit similar processing-temperature reductions when subjected to the method of metal-nanostructures embedded. Our findings provide a practical route for low-temperature fabrication of high-quality oxide functional films from solution-based sol-gel processes, which will be valuable to a wide variety of applications in addition to thin film solar cells.

Keywords: organic/inorganic hybrid perovskite, photovoltaics, metal nanostructures, flexible electronics.

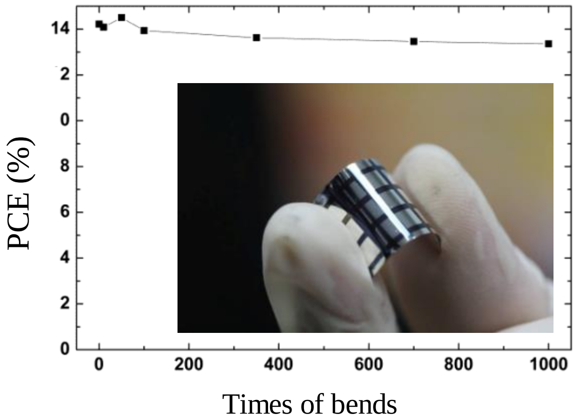

Figure 1: Power conversion efficiency (PCE) of a flexible PSC device with a low-temperature-sintered Ni_xO HTL as a function of the number of bends at 1.35 cm radius of curvature, with an inset showing a photo image of the bent device.

Control of Structural Ordering of InGaAs/AlGaAs Quantum Dots in MBE and Application to Intermediate Band Photovoltaics

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Abstract:

Application of quantum nanostructures such as quantum dots (QDs) for high-efficiency intermediate band solar cells (IBSCs) has recently attracted much interest. In IBSCs reported to date, observed two-step photon absorption/current generation via IB states becomes significantly small at room temperature [1]. In order to both increase the photocurrent generation and the operating temperature, we have investigated two issues: (1) To control both the in-plane and vertical structural ordering of stacked InGaAs QDs on GaAs (311)B substrate [2] for improved solar photon absorption, and (2) To embed QDs in a wide bandgap host material in order to suppress thermal escape of photo-carriers out of QDs [3]. In particular, the relationship between the photon absorption in QDs and optical cross-sectional area is not well understood. For this purpose, we have systematically investigated the vertical ordering and photovoltaic characteristics of InGaAs/AlGaAs IBSCs grown on GaAs (311)B substrate.

The InGaAs/AlGaAs QDs were grown on GaAs (311)B substrate by solid source molecular beam epitaxy (MBE). First, thermal cleaning was performed at 590°C for 20 minutes to remove the surface oxide layer, and then a 250 nm-thick GaAs buffer layer was grown at 560°C. Next, 10 layers of InGaAs QDs were grown at 480°C with In composition of 35%. The deposition amount of InGaAs was 8.6 monolayers, and growth interruption of 40s was introduced after InGaAs growth to promote surface migration for final formation of QDs. The spacer layer used was $Al_{0.2}Ga_{0.8}As$, and different thickness (d_{SL}) of 20, 30, and 40 nm were used. Figure 1 shows the cross-sectional images viewed along [-233] by scanning transmission electron microscope (STEM). The vertical alignment of QDs is clearly evident, and as d_{SL} increases the inclination angle of vertical alignment of QDs gradually increases from 3°, 5° to 15°. The difference in the strain on the surface of the QDs with different d_{SL} of AlGaAs spacer layer is thought to affect the inclination angle of QDs. For 10-layer stacked InGaAs/AlGaAs QDSCs fabricated on GaAs (311)B substrate, though not shown, resulted in a higher QD absorption compared to reference QDSCs grown on GaAs (100) substrate. A more detailed mechanism for the in-plane and vertical structural ordering of stacked InGaAs QDs on GaAs (311)B substrate as well as their effect on solar cell characteristics will be the topics of focus at the conference.

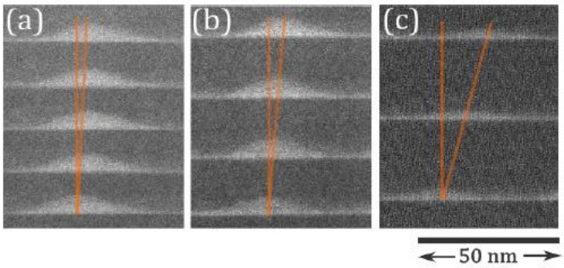

Figure 1: Cross-sectional STEM images of vertically aligned InGaAs/AlGaAs QDs on GaAs (311)B sub. viewed along [-233]. d_{SL} = (a) 20 nm, (b) 30 nm, (c) 40 nm, respectively.

Keywords: self-organized quantum dots (QDs), molecular beam epitaxy (MBE), QD solar cells, high-efficiency photovoltaics application

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Photochemical deposition of ZnS buffer layers for $Cu(In,Ga)Se_2$ thin films solar cells via reusable solutions

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Abstract:
In order to achieve high-efficiency $Cu(In,Ga)Se_2$ – based solar cells, the use of Cadmium sulfide (CdS) buffer layer is needed. However, because of its high toxicity and due to the limitation of opto-electronic performance, many Cd-free materials have been studied. Among them, the Chemical Bath Deposited Zn(S,O) is one of the most promising alternative for replacing CBD-CdS in $Cu(In,Ga)Se_2$ solar cells as the world record efficiencies have been achieved using such material [1]. Even if the ZnSO CBD uses low deposition temperatures and (<80 °C) and non-toxic reactants, one of the biggest drawbacks are the relatively high consumption of precursors and the large amount of waste-water produced for each deposition due to the non-reusability of the deposition baths. In this work, a new bath composition which is highly decreasing the material consumption is developed. Moreover, this new formulation allows the reusability of chemical baths for several times. The main advantage of this new bath are that reactants concentration can be reduced down to 10 times compared to classical CBD, no complexing agents such as ammonia are necessary and depositions are carried out at room temperature using light to photo-induce the film deposition. Since CIGSe is a p-type semi-conductor, the irradiation of this substrate with light leads to the creation of an electron-hole pairs at the semi-conductor-electrolyte interface. These carriers are possibly collected by chemical species at the surface leading to the formation of ZnSO based films. This leads to the formation of a 10-20 nm thick layer whose properties such as thickness, homogeneity and oxygen content directly influence the opto-electronic performance of the solar cells. In this work, the effect of two parameters, namely the deposition time and the reusability of the solutions is studied. This is carried out using both material characterization such as SEM and XPS and opto-electronic characterization of complete devices.

Keywords: cadmium free materials, photochemistry, $Cu(In,Ga)Se_2$ solar cells, thin films, XPS characterization , optoelectronic characterization

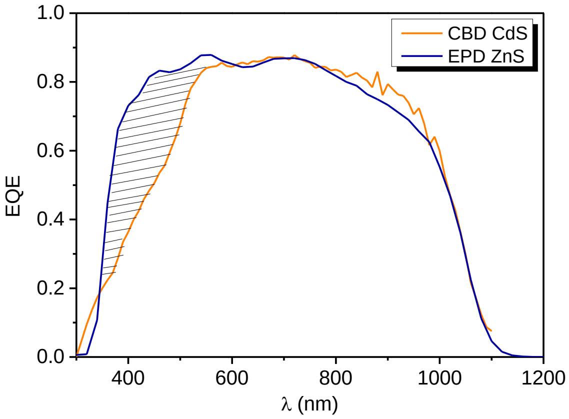

Figure 1: Gain in optical performance of CIGSe solar cells with a ZnS buffer layer compared to CdS-based ones. The gain in sun light absorption takes place in the UV-zone of the solar spectrum.

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Optical up-conversion erbium-doped nanoparticles as coaters for solar cells efficiency improvement

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Abstract:
Optical up-conversion process using tri-valent lanthanide elements hosted by low-phonon environment is helpful in wide variety of biomedical, sensing, and optical-energy harvesting applications. In up-conversion process of erbium-based nanoparticles, infra-red photons have been absorbed and converted into visible light through two-photon absorption mechanism. In this work, erbium-doped ceria and Fluoride nanoparticles, of mean diameter around 10nm, are synthesized and optically-characterized through up-conversion process. Cerium oxide (ceria) and sodium-ytterium fluoride are selected as a host due to their relatively-low-phonon medium in addition to their conductive properties. The main optical core centers, erbium atoms, are responsible for optical conversion process of the range of ~520nm emission under 780nm excitation. Then, the synthesized nanoparticles are coated on the edges of frontside of silicon solar cell in addition to the backside. The optical efficiency improvement within the up-conversion process is expected due to better spectrum utilization. The backside coating is helpful to offer a conductive medium for the generated photoelectrons to be easier moved to the electrodes. The efficiency of solar cell is found to be improved due to the coated nanoparticles to 15.20% compared to the uncoated solar cell of 15%, with a clear increase in the value of short-circuit current.

Keywords: solar cells, up-conversion, erbium-doping, ceria nanoparticles.

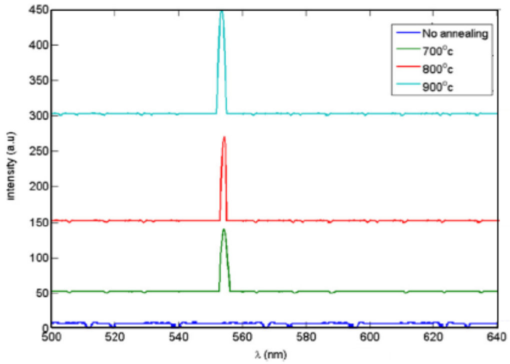

Figure 1: Up-conversion emission of erbium-doped-ceria nanopaticles at different annealing temperature.

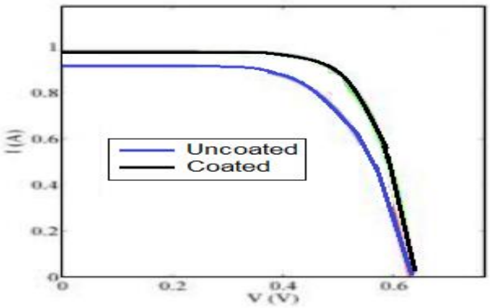

Figure 2: I-V characteristics of both uncoated and coated Si-solar cell with erbium-doped-ceria nanoparticles

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Ionic liquids confined in carbon nanotubes membranes: a route for a better electrolyte?

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Abstract:

The goal of this work is the development of new sustainable and safe systems for the energy storage. Due to their electrochemical and physical/chemical stability, we have focused our efforts on a particular class of electrolytes: Ionic Liquids (ILs)[1]. The competition between electrostatic and van der Waals interactions of the charged and a-polar alkyl side-chain(s) moieties of their cations drive a specificity of IL: a nanometric structuration[2-3]. We propose the nanometric confinement as a solution to frustrate the self-organization and hence turn the IL to a homogeneous liquid (with no density fluctuation) showing improved transport properties. We have confined imidazolium-based ILs in carbon nanotube (CNTs) membranes. These systems show a macroscopic orientation of their cylindrical pores network, which can be exploited to orient the ionic dynamics towards a preferential direction.

We study the self-organization effects on the ionic dynamics at different time and length scale in the case of bulk ILs. For this purpose we probe the nanometer/nanosecond dynamics of bulk OMIM-BF_4 by Quasi-Elastic Neutron Scattering (QENS) and Neutron Spin-Echo (NSE). We also probe the same IL on the microscopic (µm and ms) scale by Pulsed Field Gradient NMR[4]. In order to interpret the neutron data, we introduce a new physical model to account for the dynamics of the side-chains and for the diffusion of the whole molecule, which is able to describe the observables over the whole and unprecedented investigated Q ([0.15 -2.5] $Å^{-1}$) and time ([0.5 - 2000] ps) ranges.

When the OMIM-BF_4 is confined in CNT membranes (tubes' diameter ≈ 2 nm), we observe a remarkable enhancement of factor 3 of the electrolyte's transport properties at the microscopic (by Pulsed Field Gradient NMR) and macroscopic scale (by Impedance Spectroscopy), due to the severe confinement conditions[5]. A patent has been filed[6] on the use of CNT membranes as a possible solution to boost the transport properties and hence the specific power of lithium batteries.

Keywords: Ionic liquid, nanometric confinement, porous, carbon nanotube, electrolyte.

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Design of Different Polymer Electrolytes for LithiumBattery Application

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Abstract:
In the present work, composite nanofibers based on hBN/polyacrylonitrile were synthesized by means of electrospinning method and after loading with electrolyte, they applied to lithium ion battery. Different composite nanofibers with various hBN contents were produced and their characterizations were done by FT-IR, TGA, XRD, SEM instruments. Systematically, porosity, fiber diameter, liquid electrolyte absorptions were studied with respect to (hBN) and polymer (PAN) ratios. Electrospun hBN/PAN was loaded with 1M $LiPF_6$ in EC/EMC a liquid solution and then ionic conductivity and cyclic voltammetry (CV) measurements were done. The nanofiber/electrolyte system yielded a maximum lithium conductivity of 10^{-3} S cm^{-1}. The materials have a promising electrochemical stability which showed 4.7 V vs Li^+/Li. A capacity retention of %92.4 and discharge capacity of 144 $mAhg^{-1}$ was obtained and from the constructed cell Li//10wt% hBN/PAN//$LiCO_2$. In addition to this study, blend electrolytes based on single ion conducting lithium polyacrylic acid oxalate borate (LiPAAOB), polyvinyl alcohol oxalate borate (Li(PVAOB)) with poly(ethyleneglycol) methacrylate (PEGMA) were prepared. Their production and characterization results will be communicated.

Keywords: Polymer Electrolyte, single-ion conductor, Li battery

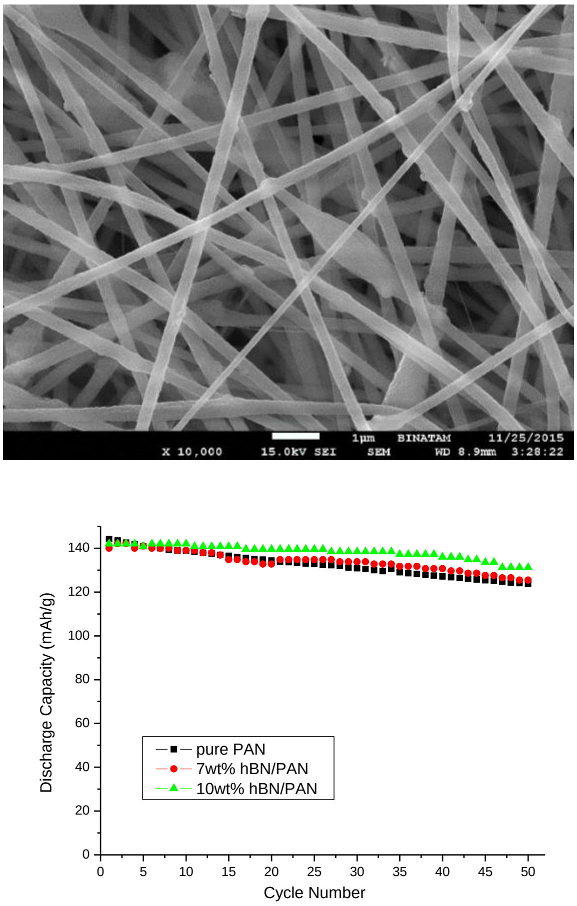

Figure 1: PAN/BN Nanofiber and Performance of cell.

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Size-dependent charge storage of graphene flakes

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Abstract:

The electrochemical property of a material is directly dependant on its morphology and size. In the case of graphene where most of the electrochemical active sites are found at the flake edges, it is crucial to study the size-dependent charge storage of different graphene flake sizes. Thus, this work focuses on the charge storage properties of reduced graphene oxide (rGO) in different flake sizes. Sonication is used to exfoliate rGO into different flake sizes, as confirmed by the spectroscopy and microscopy techniques. The oxygen-related functionalities on rGO samples are quantified by Fourier transform infrared spectroscopy and reveal that higher amount of unreduced oxygen functionalities can be found on rGO with smaller flake size. The charge storage properties of rGO in different flake sizes are studied by cyclic voltammetry, galvanostatic charge discharge and electrochemical impedance spectroscopy. The findings demonstrate that the rGO with smaller flake size possesses higher charge storage capability (238 F g^{-1}), as compared to that of rGO with larger flake size (147 F g^{-1}). Apart from larger surface area contribution, the unreduced oxygen functionalities in rGO with smaller flake size also plays an important role in contributing pseudocapacitance effect to the rGO. The current findings add substantial understanding of rGO flake size effect towards electrochemical properties.

Keywords: graphene, supercapacitor, flake size, electrochemistry, oxygen functinalities

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On the mechanism of dehydrogenation of MgH_2

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Abstract:
It is widely known that dehydrogenation of magnesium hydride (MgH_2) involves incubation period. This is characterized by the extremely sluggish kinetics of dehydrogenation process (low α: converted metal fraction and $d\alpha/dt$). The mechanism of dehydrogenation during incubation period and the reasons for the latter at 320, 350 and 400 °C are investigated in nanocrystalline MgH_2. Dyhydrogenation of MgH_2 comprises of nucleation of Mg crystallites and their eventual growth. Pre-existing Mg crystallites can enhance Mg nucleation during incubation period as suggested by the very low estimated activation energy for nucleation (12±2 kJ/mol H). The released H-atoms enter MgH_2 lattice as interstitials. This is indicated by MgH_2 unit cell contraction, increased equatorial Mg-H bond length, negative charge density distribution in the interstitial region from charge density maps, and decreased H-H distance in {001} plane up to midway of incubation period. Eventually, hydrogen vacancies are created as indicated by red shift in E_g and A_{1g} peaks in Raman spectra. The estimated activation energy for Mg growth is high (209±8 kJ/mol H). This high activation energy for growth of Mg vis-à-vis that for its nucleation renders its growth very difficult. This explains the reason for incubation period.

Keywords: MgH_2, dehydrogenation, incubation, interstitial, vacancy, red shift, charge density distribution

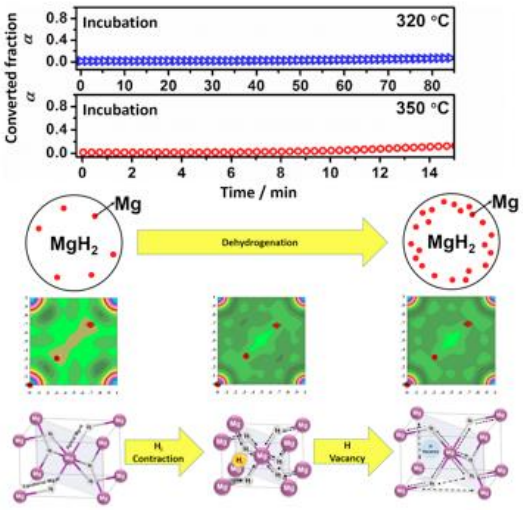

Figure 1: The mechanism of dehydrogenation during dehydrogen of nanocrystalline MgH_2 to form Mg is illustrated. Dehydrogenation exhibits incubation period characterized by very low converted fraction with time. During dehydrogenation, hydrogen interstitials exist in MgH_2 lattice. The eventual removal of hydrogen results in their vacancies. The presence of the hydrogen interstices and vacancy destorts the MgH_2 unit cell and retards the dehydrogenation process.

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Tunnel Barrier Optimization for Room Temperature Operation of Single Electron Transistor

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Abstract:
Room temperature operation of Single Electron Transistors (SET) and its CMOS process compatibility open up a new window of hybrid SET-MOS circuits for ultra-low power and/or high-performance applications. For successful operation of SET at room temperature, Coulomb Blockade (CB) and Quantum Mechanical Tunneling (QMT) must be witnessed. As CB and QMT depend profoundly on tunnel barriers, there has to be strategic barrier optimization. This paper proposes barrier engineering of a grounded gate SET. It employs aluminum island in UTB SOI device with poly source and drain. SiO_2 tunnel barrier is optimized between 1 nm to 4 nm to obtain room temperature operation and enhance current driving capability of the SET. Mathematical analysis for all SET structures is carried out using orthodox theory of CB and QMT while Sentarus TCAD is used for process simulation and device charcterization. CMOS compatible processes have been used for process simulation of SET for all tunnel barrier thicknesses. Schenk direct tunneling model, doping dependent mobility model and default drift diffusion model are incorporated for device operation. CB and QMT have been analyzed at room temperature using current-voltage (I-V) and charge-voltage (Q-V) characteristics. This analysis is further extended to compare the CB voltage (V_{CB}) and change in electrostatic charging energy (ΔE) with simulated results. Tunnel barriers of 3 nm and 4 nm thicknesses unveil notable CB of 23.44 mV and 40.80 mV with tunneling current of 72 nA, and 7.15 nA respectively, at room temperature. The results manifest that the devcice can be implemented for low power hybrid SET-MOS circuits.

Keywords: Coulomb-blockade, quantum-mechanical-tunneling, room-temperature-operation, Single-Electron-Transistor, TCAD tunnel-barrier-optimization

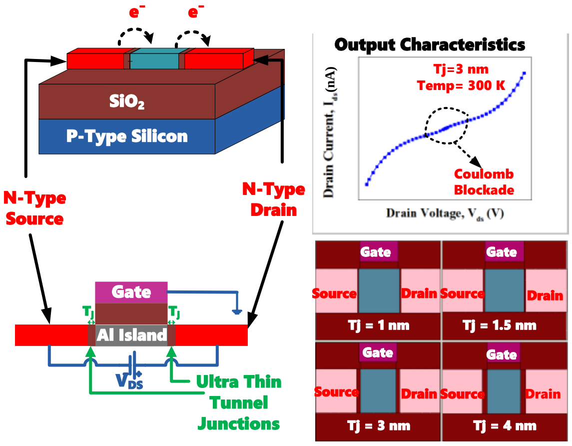

Figure 1: Room Temperature operation of SET with enhance current driving capability using tunnel barrier optimization approach.

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Storage Memory and Selector Functions in Silicon nitride Memristor

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Abstract:

DRAM and NAND Flash, which are currently commercialized charge-based memories, have faced scaling issues. Therefore, there is a growing interest in the development and research of next generation memory based on resistance change. Typically, these two terminal devices, such as phase-change random access memory (PRAM) and resistive-switching RAM (RRAM), require a selector that suppresses the current at low voltages in order to increase the array size as well as the memory function with non-volatile properties.[1] RRAM exhibits various resistive switching characteristics depending on the material. Silicon nitride (Si_3N_4) has traditionally been used in passivation layers in the CMOS process. Recently, NAND flash has not only a charge trap layer but also excellent RRAM characteristics due to its abundant traps.[2,3] In this work, we fabricated Ag/SiN/p^+Si device and characterize the threshold switching as well as memory switching. 5-nm thick SiN_x layer which shows non-stoichiometric properties was deposited by low-pressure chemical vapor deposition (LPCVD) ay 785 °C. Figure 1(a) and 1(b) shows the threshold switching. For threshold switching, a low compliance current limit (< 100 μA) is needed. Ag conducting bridge in SiN_x is formed and decomposed voluntarily, which is attributed to the unstable Ag conducting path. On the other hand, bipolar memory switching is observed when higher compliance current limit (500 μA) is applied to the devices. Duality attributes with simple compliance in this device provide flexibility in device design.

Keywords: Memristor, RRAM, Memory, Selector, Silicon nitride, conducting bridge, compliance current.

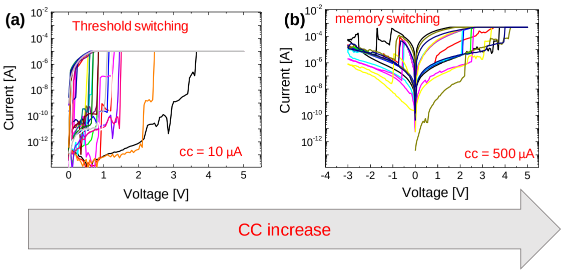

Figure 1: Figure illustrating (a) threshold switching and (b) bipolar resistive switching for selector and memory, respectively.

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Reduced Thermal Conductivity of Nanotwin Random Layer Structures: Effect of twin boundary for phonon localization

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Abstract:

Nanotwinning was demonstrated as an effective mechanism for improving physical and mechanical properties of materials such as thermal stability[1], hardness[1,2], fracture toughness[2] etc. However, the impact of twin boundary on the phonon transport process is still not well understood. The atomistic study of Porter et al[3] on bulk Si and Si NWs intrinsic interface scattering was identified when the twin period is higher than 22.6 nm, having constant value to interface conductance (6.8 GW/m^{2}K) irrespective to the heat flux. Moreover, the Kapitza thermal boundary resistance was seen to be reduced with decreasing twin period after 22.6nm indicating the existence of superlattice phonons (coherent phonons)[3]. This study was motivated by the realization of coherent phonons at nanotwin superlattices[3,4], which may be subject to localization in case of random arrangement of twin boundaries[5]. Nanotwin structures with low thermal conductivity as efficient thermoelectric materials would be a promising future direction due to their other superior physical and mechanical properties.

In this study, non-equilibrium molecular dynamic simulations are conducted using LAMMPS to investigate the phonon localization of Si nanotwin random layer structures (NTRL) where layer thicknesses are varied randomly contrary to the regular layer thicknesses of nanotwin superlattices (NTSL)[3]. Figure 1 illustrates the comparison of thermal conductivity of NTRL and NTSL structures of total length 90nm. It is interesting to see that ~23% reduction in thermal conductivity is achieved by NTRL structure of lowest mean layer thickness over corresponding. The study is extended for Si/Ge nanotwin hetero-random layer structures where random arrangement of Si/Ge material interfaces are combined with the random arrangement of twin boundaries to attain even lower thermal insulating performance. Moreover, these two random distributions are optimized to evaluate the possibility of breaking the corresponding random-alloy thermal conductivity limit.

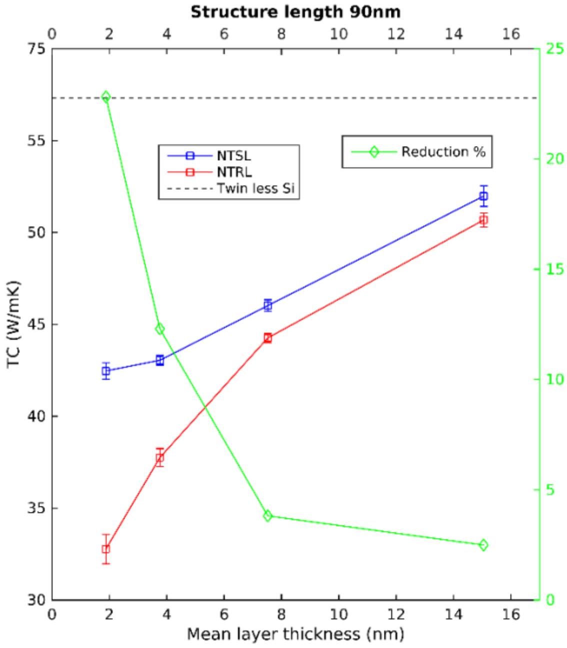

Figure 1: Thermal conductivity of NTSL and NTRL structures of length 90nm.

Keywords: twin boundary, random layers structures, phonon localization, thermal transport, thermoelectric materials

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Piezo-phototronic effect in III-Nitrides semiconductors and applications

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Abstract:

As the third-generation semiconductors, III-Nitrides exhibits great potentials in the solid-state lighting, display, power device, photovoltaics and so on. The piezoelectric property is the great difference between III-Nitrides and previous semiconductors (Silicon, Germanium, etc.). Prof. Wang pointed it out that the piezo-potential can be used as a gate to tune/control the carrier generation, transport, separation and/or recombination via external strain, and thus tuning the device performances.

This report focuses on piezo-phototronic effects in III-nitrides. Firstly, in the framework of the quantum perturbation theory and constitutive equations, we proposed a self-consistent model to study the piezo-phototronic effects in quantum structure[1]. This model matches well with the optical excitation in InGaN/GaN quantum well under the various external stress field. Furthermore, we studied the carrier dynamic process in piezo-phototronic effects with the transit piezo-phototronic model and the time-resolved photoluminescence for the first time. The piezoelectric field was partly “canceled”, which increased the overlap of wavefunctions to decrease the carrier decay time. Thus, the maximum speed of a single chip was increased from 54 MHz up to 117 MHz in a blue LED chip under 0.14% compressive strain. Finally, the piezo-phototronic effect was used to effectively improve the conversion efficiency of InGaN/GaN quantum well and compensated the thermal degradation in high power InGaN/GaN micro-strip LED arrays [2].

These researches deepen our understanding on carrier’s excitation and transportation under external strain filed, and exhibits important applications in communication, lighting and energy collections.

Keywords: Piezo-phototronic effect, III-Nitrides, optoelectronic device

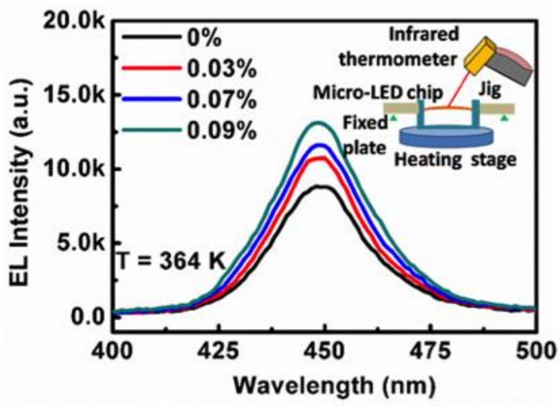

Figure 1: Figure illustrating the enhanced EL intensity of microstripe InGaN/GaN LED under stress.

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Piezopotential Modulated Graphene Semiconductor Devices

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Abstract:

Piezopotentials created in a non-central symmetry crystal under an external strain offer a low-energy-consumption solution for powering electronic devices. Diverse electronic systems that rely on piezopotential power have been prepared and have inspired rapid progress in broad applications ranging from external stimuli sensation to environmental monitoring. The feasibility of integrating these devices into in-vivo biomedical devices that harvest biochemical energy and biomechanical energy has been explored. Furthermore, piezopotential inputs created by external stimuli can enable the incorporation of diverse functions into electronic systems to achieve active digital signal/data processing capabilities, such as high-resolution dynamic pressure sensor arrays, active and adaptive matrices for tactile imaging, and interactions between machines and humans or the environment.

With the advantages of chemical inertness, low fabrication temperatures, photo-stability and compatibility with polymer semiconducting materials, piezoelectric polymers have been intensively studied for energy harvesting and piezotronic applications. This presentation will mainly discuss about the piezopotential produced by piezoelectric polymer and its application for modulation of the charge transport behaviors in the channel of field effect transistors for strain sensor, programming in a memory device through a MIS structure and modulation of Schottky barrier height in grahene/semiconductor heterostructures. The modulation of various semiconductor devices through external interaction offers good opportunities to piezoelectric polymer for micro-sensational electronics, human-robot interface and transducers in the Internet of Things (IoTs).

Keywords: protein folding, nanoporous sol-gel glasses, silica-based biomaterials, circular dichroism spectroscopy, surface hydration, crowding effects, micropatterning, biomedical applications.

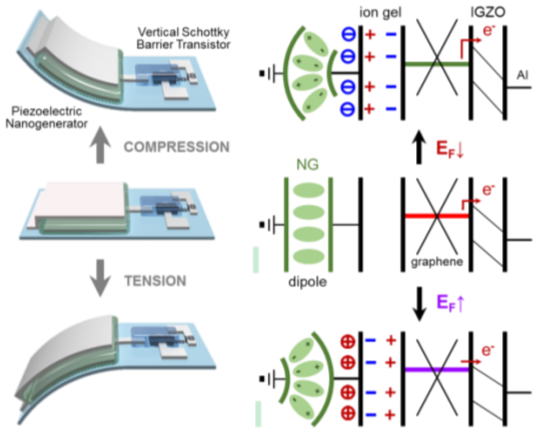

Figure 1: Band diagrams of piezopotential modulated vertical graphene-IGZO heterostructure through ion gel.

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Environmental Impact Assessment of Triboelectric Nanogenerator Materials for Energy Harvesting

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Abstract:
Triboelectric materials are widely been utilized to produce electricity, harvesting ambient mechanical energy through movement for sectors and products, from sensors, to biomedical devices, to small portable electronics. Polyethylene terephthalate (PET) and Polymethyl methacrylate (PMMA) lead the market among hundreds of triboelectric polymers to create an autonomous energy supply. Recently emphasis has been given to research on both polymers due to their increasing popularity in triboelectric nanogenerator applications to build self-powered electronics replacing conventional batteries. The production steps of both materials from raw resources are hazardous to the atmosphere in terms of toxicity and human-health effects. However, no quantification of the possible environmental impacts for the manufacturing of PET and PMMA exists. This research paper addresses their comparative environmental effects, in terms of pollutant emissions during manufacturing from raw materials. A comprehensive Life Cycle Inventory (LCI) model is developed for step-by-step systematic evaluation of their environmental impacts. Life Cycle Assessment (LCA) has been carried out by the ReCipe 2016 Endpoint, Raw material flows, Ecopoints 97, and CML 2 baseline methods, using the ecoinvent database and SimaPro software. The impacts are considered in 21 categories such as global warming, acidification, eutrophication, terrestrial ecotoxicity, human toxicity, human carcinogenic toxicity, and fine particulate matter formation, marine ecotoxicity etc. The results reveal that there is a more significant environmental impact caused by PET than with PMMA polymer during the manufacturing process. The reason behind these impacts is the amount of toxic chemical elements present as constituents of the PET raw material and its production steps. It can be recommended that a superior environmental performance can be obtained through optimization, especially by carefully selecting substitute elements and machines, taking consideration of the toxicity aspects, and by reducing the impacts associated with designs, production methods and practice.

Keywords: nanogenerator, polyethylene terephthalate, polymethyl methacrylate, life-cycle assessment, environmental impact, energy harvesting.

Piezophototronic Based Sensors and Applications

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Abstract:

Multifunctional micro/nano devices and systems are of important applications in smart electronics for health care, human-machine interfacing, infrastructure monitoring and security. In recent years, piezophototronic effect is developed fast since it offers a new method to improve/tune the optoelectronic properties dramatically. The key characteristic of the piezo-phototronic effect is that the carrier generation, transport, separation and/or recombination at the heterojunction/ interface can be tuned by modulating the piezopotential which created and further tuned by externally applied strain. Therefore, one method to enhance piezo-phototronic effect is increasing piezoelectric charge at the interface. Another method to improve piezo-phototronic effect is reducing charge carrier recombination probability, the design of semiconductor composites heterojunction/interface should take into account their band positions and band gap. By interface engineering the p-n junction, piezo-phototronic effect can be improved.

Piezophototronic effect can enhance the sensitivity of photodetector dramatically. Here, we show a self-powered GaN flexible film-based metal-semiconductor-metal (MSM) UV photoswitch. The asymmetric MSM structure was designed to suppress carrier recombination and enhance carrier transport. At self-powered condition (no external bias voltage), its UV on/off ratio reaches up to $4.67*10^5$ with high reliability of on/off switching response. Also its UV detection shows an excellent sensitivity ($1.78*10^{12}$ $cmHz^{0.5}W^{-1}$). In particular, strain modulation can improve the UV on/off ratio (~154%) by piezo-phototronic effect.

Besides photoelectric conversion and electroluminescence, photoluminescence can be tuned by piezoelectric charge as well. Here have developed a new method of pressure sensing by using pressure/strain induced piezoelectric charge to tune PL intensity of InGaN/GaN MQW under small strain (0~0.15 %). Such modulation effect is distinct, linear and ultrafast. Based upon it, an all optical pressure sensor array by the piezo-phototronics effect has been developed to measure dynamic pressure distribution without the need of electricity. Beyond the limitations of electrical connection, our all-optical device offers a novel and suitable way for large-area, high-uniform, high resolution, ultrahigh speed pressure/strain distribution sensing.

Keywords: piezophototronics, sensors, semiconductor, multi-field coupling

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NanoMetrology France 2018 / Focused Session: Metrology of NanoParticles (NP) in Complex Media

Detection and quantification of engineered and natural nanoparticles in small sub-watersheds of Seine River

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Abstract:
Engineered nanoparticles (ENPs) are intensively used [1] owing to their remarkable properties related with their size on the nanoscale and their large ratio of surface area to volume. Their exponential production leads to their release and accumulation in the environment raising several concerns about their possible effects and risks. Their detection, quantification, and characterization is thus inevitable. However, most studies on ENPs are performed at high concentrations or in simple artificial matrices [2]. These conditions are far from those found in natural environments, where the concentrations are very low and transformations can occur due to the presence of salts and natural colloids.

The recent technique single particle ICPMS (sp-ICPMS) can answer to the analytical limitations due to its sensibility and selectivity to the ENPs when dispersed in complex matrices. To understand the origin, the fate and fluxes of engineered and natural NPs under different land use, ENPs concentrations and sizes are measured by using sp-ICPMS in river water samples. The campaign is conducted monthly during one year, in three Seine river sub-watersheds with different land use, ca. forest, agriculture and urban. Here, we present the evaluation of detected Ag, which results mostly from the anthropogenic activity, and TiO2 NPs having both natural and manufactured origins.

The results of one-year sampling show that Ag NPs and TiO2 NPs are present in the sub-watersheds of Seine river at the concentration of 105 to 106 particles/mL, consistent with predicted values by modelling [3]. Moreover, their concentrations vary as function of sampling site and sampling period. For instance, we observed a higher Ag NPs concentration in summer than in winter for forest and agriculture sites, while it seems stable in the case of urban river. Besides, the presence of these NPs is confirmed by microscopy analysis (SEM).

Asymmetrical flow field flow fractionation (AF4) coupled with ICPMS has also been used, in order to study the size distribution of NPs and compare this with result obtained by using sp-ICPMS. on the porous glass surface that we have enlightened with potential optical applications.

Keywords: nanoparticles, environmental matrix, sp-ICPMS, AF4

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Following nanoparticles in complex turbid media

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Abstract:

Nanoparticles (NPs) have become an indispensable component of food, cosmetics, medicines and health-care products. The necessity to combine specific properties with stability usually leads to complex formulations and the particles can be included into systems containing surfactant micelles, oil droplets, protein globules, gel network etc. Interactions are possible both between these components and NPs and between the particles themselves. This fact together with the turbidity of the final systems makes it difficult to follow the internal dynamical processes which control the product stability. We have used the turbid nature of the samples as an advantage and used the signal from their multiple scattering to characterize the NP evolution[1]. Diffusing wave spectroscopy (DWS) is used to determine the size and volume fraction of NPs within a foam taken as an example of a turbid media. The presence of two types of scatterers – dispersed NPs and liquid/gas interfaces – leads to two-fold dynamics in the system (Figure 1). Two characteristic decays of the temporal autocorrelation function are observed, their position and amplitude are dependent on particle concentration and foam age. Since only those NPs which are performing Brownian motion decorrelate the signal, one can follow the dynamics of particles' trapping in the foam matrix during the evolution of the system. This technique is a direct and noninvasive way to detect NPs in turbid media[2].

Keywords: multiple scattering, diffusing wave spectroscopy (DWS), Brownian motion, evolution dynamics, *in situ* nanoparticle characterization

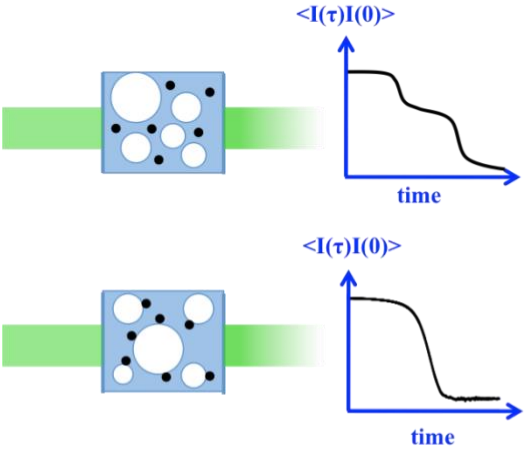

Figure 1: Autocorrelation function of the scattered light intensity fluctuation: two-fold dynamics of the foam doped with NPs and its modification under the particles' trapping.

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Investigations of the hazard assessment of selected nano-objects used as additives for EVA-matrix nanocomposites

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Abstract:
Waste management is a challenge for any developed country, especially since economic development and technical progress causes a general increase in waste volume and complexity. The main purpose of waste management systems is to reduce and control the effect of waste on the environment. This can be done in numerous ways, but the three most common waste management processes are recycling, incineration and landfilling. Products containing nanomaterials are generally not labelled specifically, so there is no easy way to identify nanomaterials in waste treatment processes. Hence, many nanomaterials may end their life cycles in waste treatment facility.

Information and literature about the end-of-life of nanocomposites often remains partial and does not address the overall fate and transformations of nanoparticles that may affect biological responses.

This presentation underlines that the physico-chemical features of nanoparticles can be modified by the incineration process and the available toxicological data on pristine nanofillers might not be relevant to assess the modified nanoparticles included in soot. Combustion tests have been performed at lab-scale using a cone calorimeter modified to collect fumes (particulate matter and gas phase) and have been characterized using various techniques.

Nanocomposites selected were Poly(ethylene vinylacetate) (EVA) containing nanoparticles, boehmites or alumina. Evaluations of cytotoxicity responses on pristine nanofillers, soot and residual ash, show that safe boehmite nanoparticles, become toxic due to a chemical modification after incineration process.

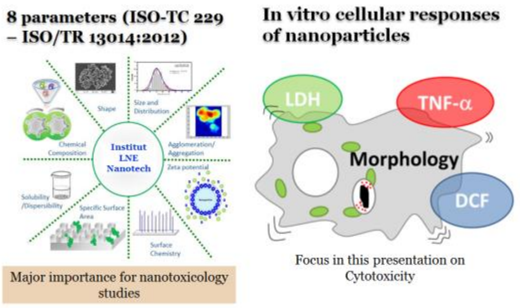

Figure 1: Characterization of nanoparticles and Cytotoxicity assessment

Keywords: Nanoparticles size, metrological characterization, boehmite, alumina, cytotoxicity, incineration, nanocomposite, aerosol and residues.

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Designing plasmonic hard shells to control the self-assembly of gold nanorods into supercrystals

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Abstract:

Plasmonic periodic structures have stimulated many research fields such as biosensors, nanophotonics, catalysis and light harvesting. Among the different types of nanoparticles, gold nanorods are a benchmark type of nanoparticles due to their outstanding optical properties and ease of synthesis. Under controlled conditions, supercrystalline structures of gold nanorods can be obtained with a hexagonal symmetry which have been demonstrated to be excellent candidates for ultrasensitive Surface Enhanced Raman Scattering (SERS) spectroscopy. The intriguing collective properties can be generated from directed self-assembly when nanoparticles are located at very short distances, increasing dramatically the electromagnetic fields at interparticles gaps so called hotspots. Tailoring the arrangement of the nanoparticles so as the hotspots is thus a great challenge for the predictive design of new materials. The colloidal fabrication of gold nanorods coated with silver (AuNR-Ag) have been shown whereby the rods adopt a cuboidal shape upon coating. The shape modification of the AuNR is at the origin of the tetragonal local organization in AuNR@Ag supercrystals. Importantly, this hierarchical organization led to a dramatic enhancement of the SERS sensing property. Inspired by this, we questioned ourselves on the possible existence of a silver thickness "threshold" above which we could observe the tetragonal configuration.

In this work we investigated AuNR-Ag supercrystal in which the silver shell thickness was systematically varied in order to not only control the distance between the gold core but also the symmetry of the lattice. Different AuNR-Ag have been synthesized and functionalized in order to yield supercrystals by droplet evaporation. The AuNR-Ag in colloidal suspension or in solid form are characterized by a combination of techniques in order to ensure a good description of the structures. In particular, Small Angle X-Ray Scattering (SAXS) is systematically used to characterize the large-scale organization of the gold nanorods with various shells thickness. We found a strong entanglement between hard shell thickness and the local organization of the rods. A better understanding of such effects is of great interest to ultimately study the collective optical properties and pave the way toward an optimized architecture design.

Keywords: hierarchical organization, gold nanorods, heterostructures, SAXS.

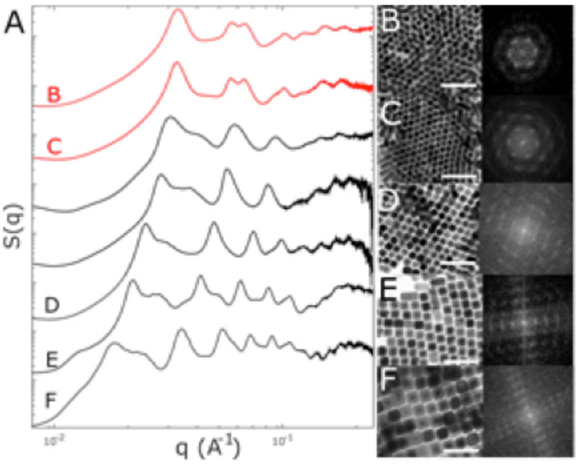

Figure 1: Determination of the critical silver thickness toggling in plane arrangement from hexagonal to square lattices. A) Representative SAXS spectra of AuNR-Ag supercrystals. The two spectra in red correspond to a hexagonal arrangement whereas the ones in black corresponds to a square lattice. B-F) Corresponding TEM images of AuNR-Ag monolayers. Insets are a FFT of the TEM regions. Scale bar on all images is 100 nm.

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Metrology of Nanoparticles with Small Angles X-Ray Scattering (SAXS): from simple cases to nanoparticles in complex media

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Abstract:

Small-Angles X-Ray Scattering (SAXS) has been established as a metrological method for the determination of nanoparticles size and size distribution. Modern SAXS Laboratory experiments, by involving synchrotron-based instrumentation at an affordable price and very stable X-ray source, are more and more used in nanomaterials metrology .

The CEA Paris-Saclay is well equipped with 4 laboratory SAXS instruments (homemade[1] and commercial setup) specially designed for nanomaterial studies, and particularly the mechanisms comprehension of nanoparticles synthesis.

In the frame of the EURAMET “Innanopart” project, we have developed a methodology and expertise for the size, size distribution and concentration determination of spherical nanoparticles. This protocol involves a precise sample preparation, a rigorous procedure for the data acquisition, and a set of homemade software tools for the data processing - from the acquisition, the absolute scaling, to the analysis.

The SAXS technique is very accurate for the characterization of simple cases using nanoparticles: monodisperses, spherical form, unique composition. But it is more complicated in the case of nanoparticles size mixtures and in case of nanoparticles in complex media.

Recent works in the laboratory showed it is possible to achieve precise measurement on mixtures of spherical nanoparticles and nanoparticles in complex media using different methodological approaches involving software development and coupling different techniques.

Keywords: Metrology, SAXS, Nanoparticles, Nanomaterials

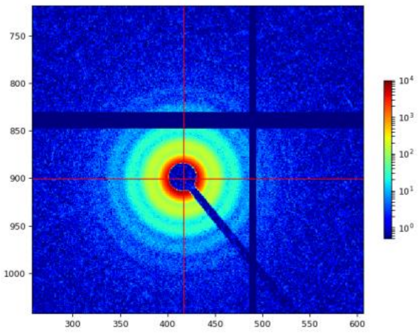

Figure 1: SAXS detector image

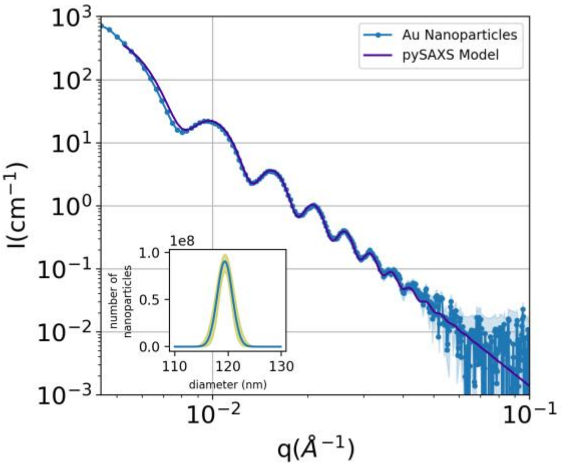

Figure 2: absolute scattered intensity diagram for gold spherical nanoparticle suspension, continuous purple line: sphere Gaussian distribution fitting

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Infrared nano-imaging for intra-cellular cancer research and analysis of drug delivery

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Abstract:
Mid-IR spectroscopy (λ ≈ 5 to 12µm) is widely used to identify chemicals. It exploits the fact that molecules absorb light at certain frequencies that are particular to their structure. Traditional methods have high spectral resolution, but are diffraction limited to large spatial resolutions of ~10µm, and so can only allow for the study of groups of cells, for example[1].

Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) offers a way of beating the diffraction limit. S-SNOM uses an extremely sharp (~10nm radius) AFM probe, close to a sample. The probe scatters the incident light in such a way that the information of the optical near-field is collected in a region only ~10nm in diameter. The tip is raster scanned across the specimen to produce an optical image with resolution of ~λ/1000 in the mid-IR. Until now this has only been used for controlled solid state systems.

Using a new range of widely-tuneable mid-IR Quantum Cascade Lasers (QCLs), it is now possible to map chemical composition of unaltered samples at unprecedented (nanometric) spatial resolution[2]. This talk will include examples of nanoscale mapping of the anti-cancer drug bortezomib within a single human myeloma cell, as well as infrared nano-imaging of sub-cellular organelles[3]. The possibility of live-cell nano-imaging will also be discussed.

Keywords: super-resolution, infrared spectroscopy, chemical mapping, biomedical applications, s-SNOM, intra-cellular imaging

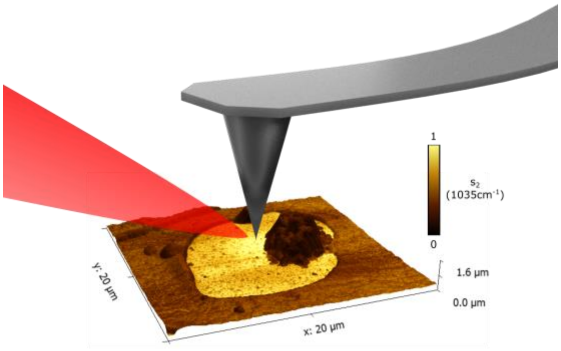

Figure 1: Infrared nano-imaging of a single bortezomib-dosed human myeloma cell.

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Probing lipid membrane nano-mechanics

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Abstract:
Cell membranes contain many inclusions (such as protein membranes) which deform the underlying lipid bilayer, by thinning or thickening it to match the thickness of the transmembrane domain of the protein. This deformation engenders between the included objects an interaction, which simple elastic theories predict to be attractive. Combined with the high concentration of inclusions, such an attraction should lead to their aggregation. However, a large majority of membrane proteins remain well dispersed.

To solve this long-standing puzzle, we use a complete elastic theory for the deformation [1] in order to determine the interaction potential between gramicidin channels in membranes by fitting small-angle X-ray scattering data recorded at varying channel concentration [2] (Figure 1). We show [3] that the essential ingredient is the preferred slope at contact, which induces a short-range repulsion. In phospholipid (DLPC) bilayers, the membrane thickness decreases with an angle of about 30° away from contact.

We confirm our results by predicting (with no adjustable parameters) numerical simulations for the interaction of gramicidin channels in other types of membranes as well as experimental conductivity data for the lifetime of the channels in DOPC, bringing together three completely different experimental techniques within one theoretical framework.

Keywords: membrane proteins, lipid bilayers, continuum elasticity, force measurement, SAXS, biomedical applications.

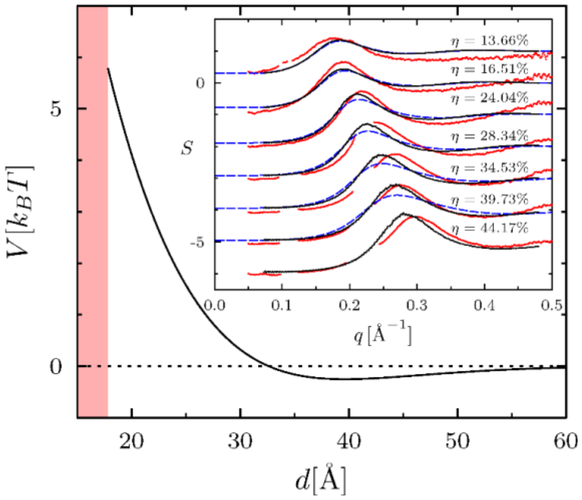

Figure 1: Interaction energy V between two gramicidin channels in a DLPC bilayer as a function of their center-to-center distance d. Inset: Structure factors S as a function of the scattering vector q for gramicidin channels in DLPC bilayers at different surface fractions η of inclusions: experimental data (red dots) and fits using the interaction energy V(d) (lines).

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Nanoparticle concentration measurement is essential and, fortunately, quite easy to achieve

Dr Camille Roesch
Izon Science

Abstract:

The ability to accurately measure nanoparticle concentration has been commercially available for around 8 years since the advent of TRPS, with the underlying theory established in the 1970s. Concurrent with this concentration measurement capability has been the ability to accurately measure particle size distribution and more recently, single particle charge and charge distribution. These capabilities have made older tools irrelevant.

Providing particle concentration as single number is still considered in some circles to be an adequate representation of the data. With highly polydisperse samples, the size range to which the concentration measurement applies needs to be stated as a minimum. The preferred approach is to display the particle measurement data as a 2-D histogram of size vs concentration. The concentration is a fundamental property that needs to be included in the size histogram. Note that any particles outside of the measurable range will not be measured but may nevertheless be present. An example is biological fluids like blood which contain particles from molecules through to cells.

TRPS routinely uses calibration particles which are traceable back to monodisperse standards. There is a general benefit in confidence from improving the traceability of concentration standards but unlikely that there will be any significant improvement in overall accuracy. Accuracy arises from choosing the correct method and correctly applying that method.

Comparison data from TRPS and a famous optical technique (NTA/PTA) will be shown. The data shows that TRPS can be made accurate for concentration to a few percent on a linear scale, even with complex mixtures, whereas NTA is at best accurate on a log scale. A methodology for testing the accuracy of both methods will be outlined to enable users to check this for themselves.

Two disadvantages of the TRPS method have been the minimum measureable particle size and the size range from a single measurement. Recent work has driven the practical measurable particle size down to sub 35nm. For fields like exosome analysis this will be a major improvement and expected to result in a rethink of prevailing dogma in that field, which has largely been created by incorrect measurement. Improvements to the measurable size range have also been made and are expected to continue over time.

An important project for the future is to develop reliable particle charge standards.

Physicochemical characterization of nanomedicines and metrology: Evaluation of size and zeta potential

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Abstract: Nanomaterials (NMs) offer promising possibilities to improve medical diagnosis and therapy of severe diseases. Among physico-chemical parameters commonly used to describe properties of NMs, size and surface properties i.e. zeta potential are key parameters as they may influence *in vivo* behaviour of NMs.

Here we will present methodological approaches proposed to validate protocols for the evaluation of these parameters.

The methodology was based on International Conference on Harmonisation guidelines Q2(R1) and the ISO standards (ISO 22412:2008(E) and ISO 13099-2:2012) to investigate robustness, precision and trueness of protocols to evaluate size measurement by dynamic light scattering and zeta potential by electrophoretic light scattering. Appropriate materials were used to perform the validation and methods using analysis of variance were used to interpret data. The applied approaches proposed in this work could demonstrate that protocols of size and zeta potential evaluation can be validated consistently with the ISO standards. Scopes of the validated protocols were investigated using various nanomaterials (inorganic nanoparticles, polymer nanoparticles, liposomes). Methodologies to achieve the analytical transfer of the previously validated protocols were suggested and applied to prove the ability of different laboratories to successfully perform protocols with equivalent performances.

Acknowledgements: This work was supported by BpI France (Project NICE).

Keywords: nanomaterials, nanomedecine, metrology, standardized protocol, size, dynamic light scattering, zeta potential, electrophoretic light scattering, validation, certified reference material, reference material, analysis of variance, transfer, scope.

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Assessing the interactions between a single dendrimer and (bio)surfaces using atomic force microscopy

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Abstract:
Quantifying the binding propensity of nanoparticles (NP) to (bio)surfaces is essential to understand biochemical processes potentially underlying NP toxicity. In this presentation, we will discuss how recent developments of atomic force microscopy (AFM) functionalities now make possible the evaluation and interpretation of complex interactions between single NP (of diameter below 10 nm) and abiotic or living cell surfaces. First, we will demonstrate that the sign of the electrostatic interaction acting on a soft zwitterionic NP (namely carboxylated-terminated PAMAM dendrimers) in the vicinity of an abiotic charged surface may be reversed by changing solely the concentration of monovalent electrolyte concentration in solution.[1] Then, using the same original strategy -where a single-NP is grafted at the apex of an AFM tip (Fig. 1)- we will show how the attachment of such dendrimers to living bacteria can be modulated by the presence of biomolecules (*e.g.* polysaccharides) at the cell surface.[2] It is anticipated that the methods presented here will be useful to control NPs binding to organisms upon proper modification of their nano-interphase features.

Keywords: dendrimers, interactions, AFM, single-NP force spectroscopy, electrostatic interactions, electrokinetics, bacteria.

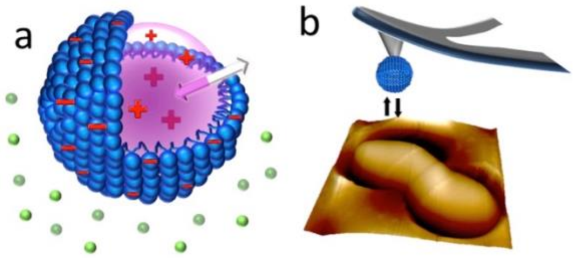

Figure 1: Schematics representing (a) a zwitterionic nanodendrimer composed of a positively-charged amine core and a negatively-charged carboxylic peripheral shell, (b) the AFM set-up adopted to probe the interactions between a single-NP attached to the AFM tip and a bacterial surface.

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NanoMatEn2018/ Session III.A: Nanotechnology for Environmental Application / Water Treatment

Free-standing nanostructures at atomic scale: from growth mechanisms to local properties at the nanoscale

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Abstract:

Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. Materials for spintronics, electronics, optoelectronics, sensing, energy applications and new generations of functionalized materials are taking advantage of the low dimensionality, improving their properties and opening a new range of applications. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique physical properties (optical and electronic) and relate them to the changes originated at the atomic scale, e.g.: linked to changes in (electronic) structure of the material.

In the present work, I will show how combining advanced electron microscopy imaging with related spectroscopies in an aberration corrected STEM will allow us to probe the elemental composition and electronic structure simultaneously with the optical properties in unprecedented spatial detail.

The talk will focus on several examples in advanced nanomaterials for optical, plasmonic and energy applications. In this way the latest results obtained by my group on direct Visualizing and modeling materials at atomic scale will help to understand their growth mechanisms (sometimes complex [1,2]) and also correlate their physical properties (electronic and photonic) at sub-nanometer with their atomic scale structure. The examples will cover a wide range of nanomaterials: quantum structures self-assembled in a nanowire: quantum wires (1D) [3] and quantum dots (0D) [4,5] and other complex nanowire-like morphologies for photonic and energy applications (LEDs, lasers, quantum computing, single photon emitters, water splitting cells, batteries) [7,8,9,10], nanomembranes and 2D sheets [8,11].

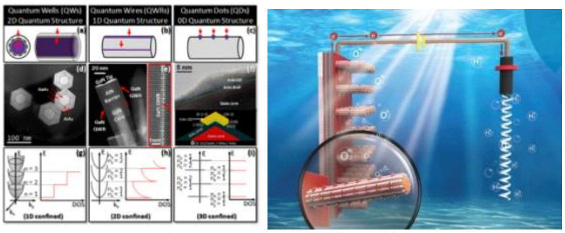

Figure 1. (left) Sketches of different quantum structures: (a) Quantum Wells or 2D structures (QWs); (b) Quantum Wires or 1D structures (QWRs); (c) Quantum Dots or 0D structures (QDs). (d-f) Experimental STEM and HRTEM images of the quantum structures [6,7]. (right) Enhanced Photoelectrochemical Water Splitting of Hematite Multilayer Nanowires Photoanodes [9].

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TreAting contamination through NanoremedIAtion: the TANIA project

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Abstract:

Huge areas are contaminated in Europe, the number of potentially contaminated sites in Europe is estimated around 2.5 millions. Site management costs ca 6.5 billions a year. Nanoremediation is an effective strategy for water and soil remediation. However, conventional techniques are often preferred because of issues concerning technology novelty and governance models. The objective of the TANIA project is to address these limitations, by using interregional exchanges (involving partners from Italy (coordinator), Finland, France, Greece, Hungary) and participation of stakeholders from environmental and innovation fields.

Nanoremediation involves not only nanosized materials but also nanostructured macro-sized ones, biocompatible nanocontainers able to carry and deliver substances.

The challenges that have been found are : 1) the need for a standardised methology to evaluate, monitor and control technologies, as well as an European regulatory framework, 2) pilot applications, 3) patents, 4) incentives for in situ use and 5) awareness.

The objective of this commununication is to present a state of the art of projects and pilot applications in Europe, dedicated to soil and groundwater nanoremediation. Examples will be given to illustrate the remediation of sites contaminated by chlorinated solvents by reductive dechlorination using zerovalent (or modified) iron nanoparticules (e.g. case study from Soleo Services company – France (Figure 1), Nanorem project).

The TANIA project is co-funded by the Interreg Europe programme, through ERDF Funding 2014-2020, https://www.interregeurope.eu/tania/. Contact details are available on this web page.

Keywords: water and soil remediation, nanosized and nanostructured materials, field test, pilot application, regulatory framework

Figure 1: Figure illustrating the field remediation of a site contaminated by chlorinated solvents, by injecting zerovalent iron nanoparticules into the soil and groundwater by soil mixing (© Soléo Services company).

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Physicochemical characterization of nanoparticles-containing spray coating generated by atomization process

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Abstract:
Nanomaterials are nowadays the great concern of scientists. They are are used in a wide range of industrial applications and incorporated into many common products (cosmetic, foods, consumer electronics, textiles, …). Paints and coatings are part of these products and nanoparticles (NPs) are increasingly been added to their formulations to improve mechanical, physicochemical and antimicrobial properties. Spray painting is known to cause harmful effects (workers exposure to small paint aerosol) due to the generation of nano-size particles during the spraying process. Inhalation is the major route for airborne NPs and their potential effects on the human heath (in particular on the deep lungs) remains unclear. In this work, we report the characterization of the non-volatile fraction of paint overspray created by air spray guns. Different techiniques were used as Centrifugal Liquid Sedimentation (CLS), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDX) and Electrical Low Pressure Impactor (ELPI). Paint containing TiO_2 NPs was studied and aerosols were produced by using IWATA 1,3 mm gun (flow rate: 20 g /min). TEM confirms the presence of two kind of droplets in the aerosol spray: microdroplets (1 µm to 10 µm) and nanodroplets (100 nm to 1 µm). NPs appear only in the form of agglomerates (average size: 460 nm), no individualized NPs are observed and they are preferentially located inside microdroplets. Characterizations show also that NPs seems strongly embedded into the polymer matrix, this means that interactions as hydrogens bonds, electrostatic and Van Der Waals interactions may take place between the NPs and the polymer. In parallel to this study, the acute potential toxicity of the paint aerosol in a whole-body exposure model is been evaluated. For this, hispathological examinations of mains organs, and evaluation of the biopersistence by using Particles Induced X-ray Emission (PIXE) are being performed.

Keywords: engineered nanoparticles, paints, coatings, spray can aerosol, spray painting process, airborne particles, automotive industry.

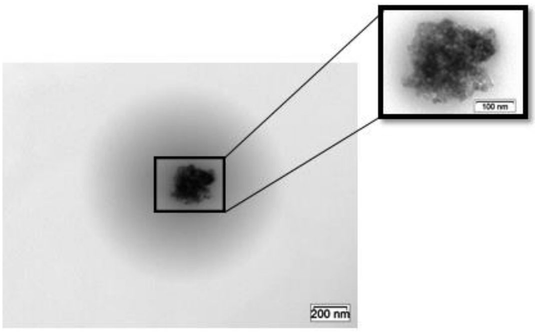

Figure 1: TEM image of a paint droplet containing TiO_2 nanoparticles. Sample was analysed with a Philips Tecnai 10 operating at 100 keV and in bright-field mode.

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Bridging homogeneous and heterogeneous catalysis through MOF support platforms and other efforts to obtain new class of highly active recyclable catalysts

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Abstract:

The talk will focus around developing recyclable catalysts and analytical methods to study them. We will start with the discussion with synthesis, analysis and catalytic properties of Metal-Organic Frameworks (MOFs) with immobilized bidentate nitrogen ligands. This will include discussion on preparation of a number of alkyne functionalized ligands and their immobilization on the MOF surface through azide-alkyne "click" reaction. We will then shift the discussion to nanoparticle solubilization in nonpolar media with terminally functionalized Polyisobutylene (PIB) oligomers and application of this method to analyze MOF particles with immobilized complexes.[1] We will show that MOF nanoparticles solubilized through this method can be interrogated through methods used for solution state analyses.

Keywords: Catalysis by Metal Organic Frameworks, nanoparticle solubilization.

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Carbide core-shell nanostructures for oxygen reduction reaction

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Abstract:

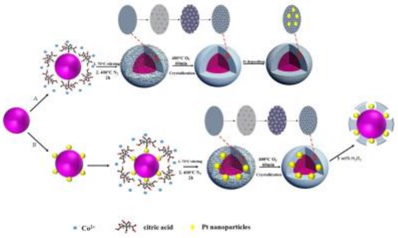
Carbides have attracted increasing attentions recently as novel nonprecious electrocatalysts for the oxygen reduction reaction (ORR) with high activity and stability. Early transition metal (groups 4-6) carbides (WC, TiC etc.) especially exhibit a fairly good ORR catalytic activity due to its platinum-like physico-chemical properties including chemisorption of hydrogen and oxygen[1] at a lower cost. Nevertheless, some carbides are less stable and easily oxidized at high potentials (>0.8V vs RHE for WC; >1.5V vs RHE for TiC).[1] A seducing approach to increase the carbide core electrochemical stability without compromising its performance is the core-shell structure.

Here, we reported the synthesis of two different electrocatytic nanomaterials. Both approaches include the deposition of a thin layer of cobalt (oxide) nanoparticles on the carbide core. The first method consists in depositing platinum after the cobalt layer whereas in the second method, Pt is deposited before the cobalt layer. In the 2nd method, hydrogen peroxide was used to burst the cobalt shell to expose platinum nanoparticles.

The results confirmed that the platinum nanoparticles are in contact with both the carbide core, cobalt shell and Nafion layer. These coated carbide nanomaterials have remarkable improved stabilities as supports compare to pristine carbides (ECSA changes after 4 weeks and chronoamperometry curves obtained at 0.6V vs RHE) without compromising their catalytic activities, which opens a new way for the synthesis of the next generation of commercial fuel cell catalysts.

The ORR catalytic activities and durabilities of the two catalysts made from above-mentioned two different methods have been compared in the alkaline condition.

Keywords: carbide, core-shell, crust, oxygen reduction reaction (ORR)



Scheme 1. Illustration of the process flow to prepare carbide core-shell structures.

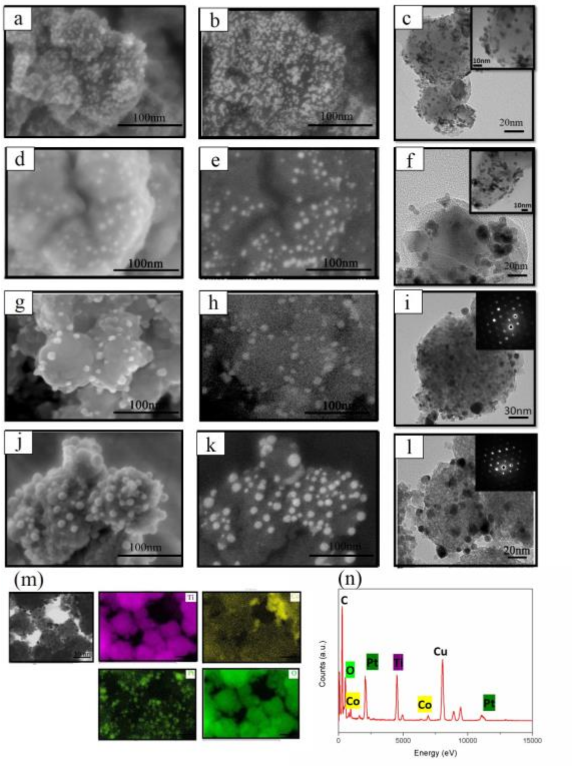


Figure 1. Structural evolution process of the catalyst for before (a-c) and after bursting cobalt shell (d-f) and its chemical compositions as the final product after bursting shell (g).

References:

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Case studies of different wastewater treatment processes by means of nanotechnologies

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Abstract:
In this work, some case studies of nanotechnology application for wastewater treatment purposes are presented.
The treatment of wastewater streams represent one of the mayor challenges in the next future. The available water suffers from a sensible decrease in quality due to intensified industrialization and use, leading to heavy pollution and the recen appearance of new, toxic pollutants in the environment.
To overcome these problms, the treatment processes requires to be more effcieint than the conventional ones. Nanotechnologies may provide solutions to specific needs, due to their enhanced properties in pollutant degradation at the molecular level. Moreover, the integration of nanotechnologies requires synergic and novel process design, that assit updated processes to reach the desired treatment targets. On the other hand, these processes requires to be cheap, since water has a low added value. Economic feasibility shoul therefore be pursiuted. This is not always an easy task to accomplish, since nanotechnology has high intrinsic costs.
For example, this applies well to a widerange of membrane processes: the use of specific nanomaterials provides a pre-treament of the wastewater to sensibly reduce membrane fouling issues. Moreover, novel process design provide higher life time to membrane modules. By adoptin this strategy, it is possible to operate membrane processes for the treatment of wastewater streams for many years, thus reaching economic sustainability.
During the discussion, some nanotechnology-based tecniques for wastewater treatment will be presented, such as membrane technologies and photocatalysis.

In detail, following case studies will be shown:

1. Olive mill wastewater treatment processes by photocatalysis (nano-magnetite cores coated with doped titania) and membranes
2. Tannery wastewater treatment by membranes with additional Cr recovery

Nanotubular and nanoporous titanium dioxide films for photocatalytic applications

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[2] ITC – CNR, Construction Technologies Institute, San Giuliano Milanese, Milan, Italy

Abstract:

Titanium dioxide is one of the most renowned photocatalysts for both water and air purification. It is generally used in the form of nanopowders, which unfortunately pose a hazard for the environment if released accidentally from the photocatalytic reactor, or from the material that contains them. Therefore, the use of immobilized photocatalysts is crucial in the purification of both polluted air and liquids wastewaters. Titanium dioxide films obtained by anodic oxidation would avoid release of nanoscale materials in the environment, since they are grown directly on the titanium substrate, ensuring optimal adhesion.

This work presents a study on anodizing process parameters, such as electrolyte and voltage, in order to identify the most efficient and robust technique for the production of TiO_2 layers with different morphologies with high photocatalytic activity in both gas and liquid phase. Nanoporous layers were first obtained by anodic spark deposition, a high voltage technique, then the process was optimized to produce titanium dioxide nanotubes, whose specific surface area is much larger than that of a nanoporous oxide, therefore allowing more active sites for photocatalytic reactions. Toluene was used as model reactant for gas phase photocatalytic depuration, while an organic dye, rhodamine B, was chosen as model for wastewater purification.

Keywords: Titanium dioxide; nanotubes; anodic oxidation; photocatalysis; gas phase; liquid phase

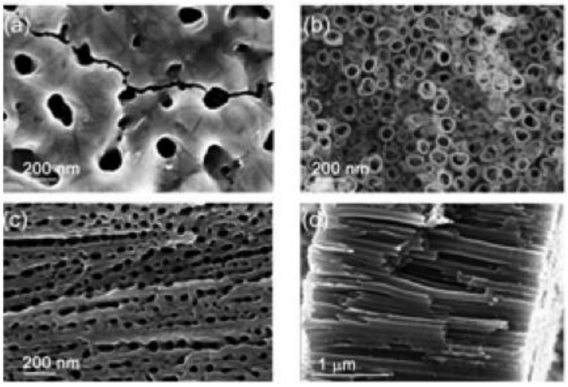

Figure 1: SEM images of (a,b,c) top morphology of oxides obtained in different electrolytes and (d) cross section of oxide (c).

References:

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Nanocomposites for the Removal of Radioactive Cesium from Water and their Applications

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Abstract:
The release of radionuclides, including fission products, from the long-term use of nuclear fuels and occasional nuclear disasters, such as at Chernobyl and the Fukushima Daiichi nuclear power plants, is an emerging issue. In particular, radioactive cesium (^{137}Cs), a fission product formed in nuclear reactors, is a problematic contaminant owing to its high radioactivity, relatively long half-life (30.2 years), and bioavailability. Radioactive cesium can cause a number of significant health problems, including carcinoma of the liver, kidney, bladder, renal functions, cardiovascular disease and gastrointestinal distress. A variety of materials has been investigated for the removal of ^{137}Cs, including polymers, zeolites, clay minerals, silica, and other nanomaterials.
In my talk, recent efforts in our research group, utilizing both organic and inorganic composites safe design and fabrication to aiming at removing radioactive cesium from water. And it will be introduced key issues to such novel nanocomposites based on recent advances for environmental applications.

Keywords: nanocomposites, radioactive cesium, nuclear energy, water, environment, health problem.

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Study of modified electrodes with silver and gold nanoparticles to determine heavy metals in polluted waters

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Abstract:

Recently, nanotechnology and, in particular, nanoparticles (NPs) such as Ag-NPs and Au-NPs are present in Analytical Chemistry due to their great potential to improve the performance of most sensors. In this work, Ag and Au nanoparticles have been synthesized using two methods. Seed mediated approach was used to sinthezise Ag-NPs and Au-NPs [1] [2]. A green route where grape stalk waste extract was also used as a reducing agent [3], in order to obtain the metal nanoparticles to customize the surface of comercial screen-printed electrodes (SCPE) from Dropsens®. In order to dope the SCPE surface, spin coating method was used with two cycles of 3000 rpm for 3 minutes. The resulting electrodes were used in a detection study of cadmium (Cd^{2+}) and lead (Pb^{2+}) by differential pulse anodic stripping voltammetry (DPASV). Electrodes modified with Ag-NPs or with Au-NPs presented the higher sensitivity and best performance than non-modified SCPE. The results showed that the best detection was obtained for the SCPE modified with AgNPs with the best response to low metal concentrations. Ag-NPs synthesized by the green route exhibited the best LOD which is lower than the most restrictive regulation. Additionally, the electrodes modified with green NPs showed even lower low detection limits (0.4 $\mu g \cdot dm^{-3}$ of Pb^{2+} and 0.1 $\mu g \cdot dm^{-3}$ of Cd^{2+}) compared with green Au-NPs (which is 20 $\mu g \cdot dm^{-3}$ of Pb^{2+} and 38 $\mu g \cdot dm^{-3}$ of Cd^{2+}).

Keywords: silver nanoparticles, gold nanoparticles, modified electrodes, spin coating, cadmium detection, lead detection.

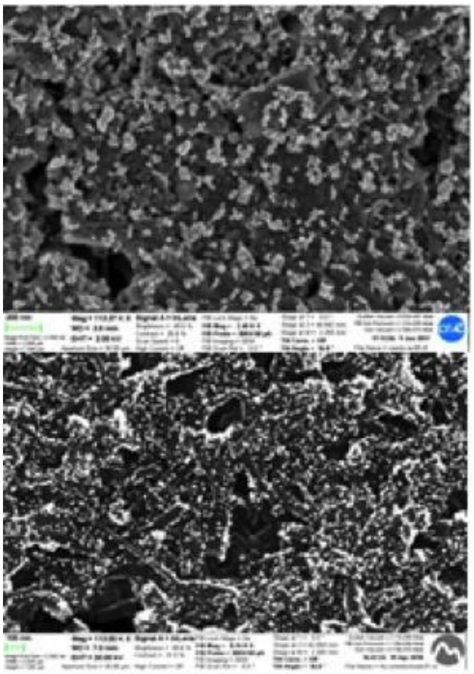

Figure 1: SEM image showing the modification of SCPE electrodes with (a) AgNPs and (b) AuNPs.

Acknowlegements:

This research has been supported by Ministerio de Economia y Competitividad and Fondo Europeo de Desarrollo Regional (FEDER), CTM2015-68859-C2-2-R. Authors also acknowledge Michelle Pérez Solis for helping in the experimental part of this work

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Zn-ferrite nanoparticles, potential photocatalysts for water depollution: Why do we still need detailled structural characterizations?

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M. Selmane[4], G. Wallez[5], J.M. Greneche[6] and R. Cole[7]

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Abstract:

Water depollution by photocatalysis (with the activated O-radicals formed by irradiation) is a very interesting and modern subject, with important societal consequences. This depollution remains a major challenge for students, researchers, laboratories and decision makers due to increasing complexity of human and water interactions. So far, it has been established that semi-conducting oxides can be useful, TiO_2 being the most represented. But titania large band gap implies the use of a UV irradiation. Since UV corresponds to less than 5% of the solar light, changing of solid to obtain a good activity in the visible is required. We have first tried to use iron oxides but amelioration procedures are complex because of strong photo-corrosion [1]. We have used Zn-ferrites [2] because their photocatalytic activity under visible light is demonstrated and because of their stability in water and band gap values are compatible with excitation by visible light. The exact amount in Zn(II) and Fe(III) ions in octahedral (Oh) sites has been evaluated with detailed X-ray studies and Mössbauer measurements. Zn-ferrite nanoparticles have been obtained by two techniques: precipitation in water starting from chlorides with added surfactants and replication inside the ordered pores of SBA-15 silica grains. The reactivity of the prepared solids for two practical applications under visible irradiation (with a halogen lamp) has been tested: on the one hand, for a dye elimination (methylene blue) and on the other hand, for the decomposition of bacterium staphylococcus epidermidis that can cause cutaneous and urinary diseases.

Our approach combine routine characterization techniques and specialized physico-chemical characterization facilities. This can lead to a better understanding of cleaning water-related issues and potentially sustainable trajectories.

Keywords: Ferrites, Depollution, Water, Visible irradiation

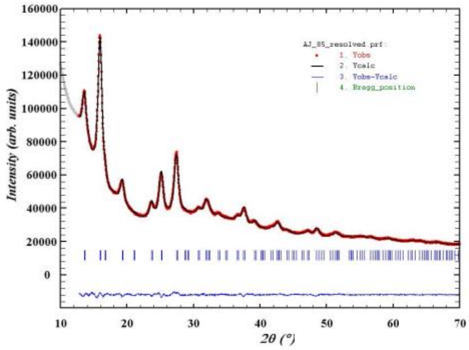

Figure 1. FullProf modelisation (Zn-ferrite obtained by precipitation) illustrating the fundamental question that we are tempting to solve experimentally: is a routine X-ray Diffraction measurement enough to understand and fully justify differences in photocatalytic activity of ferrites

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Synthesis of Polysulfone/Carbon Nanotubes-Polyamide Thin film Nano-composite Membranes for Forward Osmosis Applications

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Abstract:

Forward osmosis (FO) is gaining potential as a promising alternative to reverse osmosis (RO) in membrane-based water desalination applications. FO water flux, salt rejection and reverse solute flux are three critical parameters affecting membrane performance. In the current study, functinoalized multiwalled carbon nanotubes (F-MWCNTs)- polyamide (PA) thin film nano-composite (TFNC) membranes were synthesized on top of polysulfone (PSF) porous support layers by interfacial polymerization (IP) using m-phenylenediamine (MPD) in water and trimesoyl chloride (TMC) in hexane. The PSF support layer was synthesized by phase inversion in a water bath of a casting solution of PSF and polvinylpyrrolidone (PVP) dissolved in anhydrous dimethyl formamide (DMF). Multiwalled carbon nanotubes were functinoalized by oxidation, and then incorporated in the MPD aqueous solution during IP. The amount of F-MWCNTs was varied to study their effect on the membrane morphology and performance. The obtained membranes were characterized using Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Fourier Transform Infrared Spectrophotometry (FTIR) and Brunauer-Emmett-Teller surface analysis (BET). FO performance was investigated using deionized water as the feed solution and 2M NaCl as the draw solution. It was found that F-MWCNTs enhanced the membrane hydrophilicity and surface roughness (Figure 1) that led to increased FO water flux. The membrane with 0.01 wt/vol% F-MWCNTs showed the highest salt rejection (90.05%) with a FO water flux of 55.23 L/m^2 h and a reverse solute flux of 2.76 g/m^{2}h; thus outperforming thin film composite FO membranes reported in literature. Based on these results, it can be concluded that promising FO membranes with high salt rejection and FO water flux with low reverse solute flux can be synthesized by incorporation of F-MWCNTs in the polyamide rejection layer.

Keywords: Forward osmosis, polysulfone, polyamide, carbon nanotubes, phase inversion, interfacial polymerization.

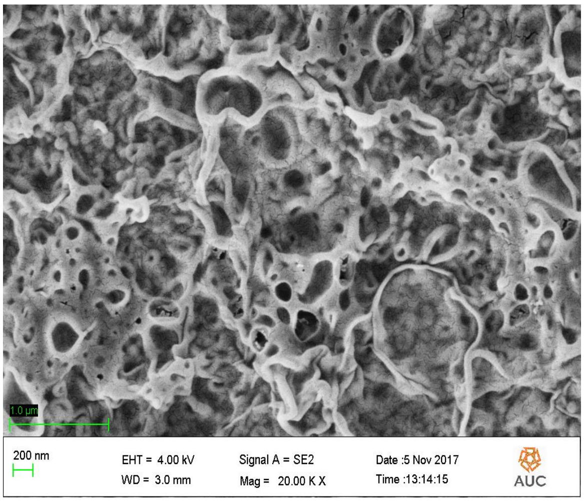

Figure 1: Surface mophlogy of F-MWCNTs polyamide-polysulfone thin film nano-composite membrane.

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NanoMatEn 2018 - Session III.B: Nanomaterials for Clean and Sustainable Technology

Porous carbon nanostructures for biological energy conversion and the utility of glucose biofuel cells.

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Abstract:

Due to the increasing interest in alternative and miniaturized energy generators with low environmental impact, new materials are under extensive investigations. Between others, carbon nanotubes (CNTs) are promising alternatives as building blocks in bioelectrochemical devices due to their unique electrical, mechanical properties, biocompatibility and high specific surface. In the past years, we focused the development of biofuel cells based on such carbon nanostructures . Our efforts in this domain aim the construction of nano-architecture at molecular scale associating different nano-objects via organic or organo-metallic connectors to immobilize and to wire redox enzymes . The possibility to generate electrical power out of fruit juice, soft drinks, or even body fluids focused biofuel cell research on the bioconversion of glucose since it is one of the two required compounds with oxygen which are both present in vegetal and living organisms. However, in spite of this promising evolution, there are still essential issues to be resolved before enzymatic glucose biofuel cells become competitive in practical applications. Two critical obstacles are short lifetime and poor power density, where both are related to enzyme stability, electron transfer rate, and enzyme loading. One of our designs of bioelectrodes for enzymatic biofuel cells is based on free standing carbon nanotube electrodes that allows high enzyme loading in a protective environment while allowing optimal flow of the “fuel” and oxygen containing solutions with satisfying stabilities [1]. Other carbon nanotube shapes like buckypapers were functionalized and tested for the energy conversion using glucose as fuel [2]. Some alternative approaches to optimize the electron transfer [3] and directed developments for alternative applications [4] are presented in the *“Nanomaterials for Clean and Sustainable Technology”* session.

Keywords: Carbon nanostructures, enzymes, Glucose biofuel cells, electrocatalysis, electron transfer, free standing bioelectrodes.

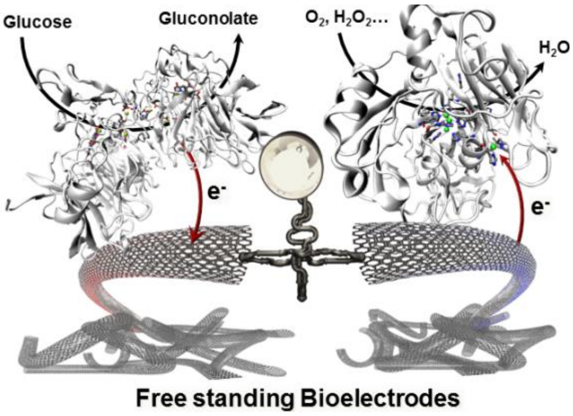

Figure 1: Figure illustrating the principle of biological energy conversion using enzymes as electrocatalysts wired to a CNT matrix, and glucose as fuel.

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Ultralow lattice thermal conductivity and high thermoelectric performance of polycrystalline SnSe

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Abstract:

20% – 50% of energy consumed in the industrial sector is lost by waste heat in the US. Substantial amounts of lost energy are generated by fossil fuels. Achieving economically viable means of recovering such a ubiquitous and a huge energy source should contribute to reducing energy consumption as well as fossil-fuel-related greenhouse emissions simultaneously. Thermoelectric power generation can directly convert heat into electricity, thereby a promising renewable energy harvesting technology for waste heat. The main interest of thermoelectric research has been discovering new materials and developing their thermoelectric figure of merit ZT. While most of the recent advances in the enhancement of the thermoelectric figure of merit (*ZT*) resulted from a decrease in lattice thermal conductivity by nanostructuring, there have been very few attempts to enhance electrical transport properties, namely, power factor. We employed nanochemistry to stabilize bulk Bi_2Te_3 that goes beyond phase equilibrium, i.e., phase-pure n-type $K_{0.06}Bi_2Te_{3.18}$. Incorporated potassium and tellurium in Bi_2Te_3 far exceeds their solubility limit, leading to simultaneous increase in the electrical conductivity and the Seebeck coefficient along with decrease in the thermal conductivity. Consequently, a high power factor of ~43 $\mu W\ cm^{-1}\ K^{-2}$ and a high $ZT > 1.1$ at 323 K are achieved. Our current synthetic method can be used to produce a new family of materials with novel physical and chemical characteristics for various applications.

Keywords: thermoelectric, renewable energy, waste heat, n-type Bi_2Te_3, power generation.

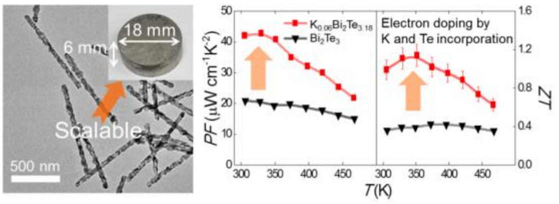

Figure 1: Excessive potassium and tellurium incorporated Bi_2Te_3 nanotubes and their thermoelectric properties.

References:

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Effect of the electrode polarization on the water properties in the system with and without glow discharge electrolysis

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Abstract:

Recently, the water treatment process using atmospheric-pressure plasma has attracted attention. This process uses the hydroxyl radical that is generated from water and moisture when high voltage is applied to a water electrode. Hydroxyl radical shows a high oxidation reduction potential (which is a measure of reducing power). Therefore, it is considered to be effective in the treatment of contaminated water that contains refractory organic compounds such as acetic acid that cannot be decomposed by hydrolysis. This is because hydroxyl radical decomposes the refractory organic compounds in water and can purify the contaminated water to be acidic water that is harmless to the environment.

We have also studied the water treatment process using the DC glow discharge, and the effects of the glow discharge, including the potential distribution in water and chemical reaction of water on acetic acid solution and tap water, were systematically investigated.

In this study, the effect of DC atmospheric pressure glow discharge on tap water quality and hydroxyl radical generation mechanisms were systematically investigated based on the charge transfer process, and the results were compared to the process without glow discharge (Figure 1, 4 conditions). In addition, the influence of current direction (the charge transfer process) on water properties was studied. To the best of our knowledge, this is the first study that compares the differences between these two processes that include current direction. We investigated the phase separation structure in solution by using pure tap water without controlling water quality like conductivity by DC process. This fundamental data would be required when designing the optimal decomposition process of refractory organic compounds.

Keywords: Atmospheric pressure, DC glow discharge, Electrolysis, charge transfer, Advanced oxidation process.

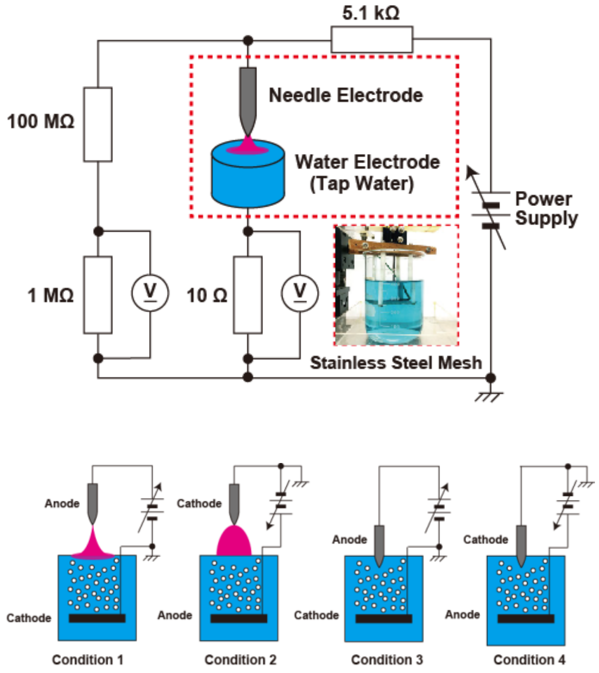

Figure 1: Experimental setup for the atmospheric pressure glow discharge and electrolysis with a tap water as the electrode.

References:

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Glucose Effect on Controlling TiO_2 Physicochemical Properties for CO_2 Reduction by UV/Vis Light Irradiation

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Abstract:

Photocatalytic reduction of CO_2 is an attractive approach to produce fuels. Moreover, semiconductor titanium dioxide (TiO_2) has engrossed much attention for photocatalytic reduction of CO_2 due to good stability, high activity and abundantly available. However, wide band gap and rapid electron hole recombination still hinder and limit its efficiency. Hence, better efficiency could be achieved by doping TiO_2 with metal or/and non-metal. In this study, glucose has been adopted as a dopant to modify the physical and chemical properties of TiO_2. Glucose/TiO_2 was synthesized by hydrothermal method for photoreduction of CO_2 to methanol under UV/Vis light irradiation. The properties of TiO_2 doped glucose were characterized using photoluminescence (PL), diffuse reflectance ultraviolet-visible spectroscopy (DRUV-Vis) and high-resolution transmission electron microscopy (HR-TEM). The performance of glucose/TiO_2 efficiency was observed for 2 h and analyzed using gas chromatography-flame ionization detector (GC-FID). Results showed that the optical properties of TiO_2 changed after doping with glucose and reduced the rate of recombination between electron and hole. The efficiency of glucose/TiO_2 increased two-fold compared to bare TiO_2 with 19.5 $mmolg_{cat}^{-1}h^{-1}$ of methanol yield. This could be attributed to the association of TiO_2 and glucose through ligand-metal charge transfer (LMCT). LMCT phenomena is due to electron donor-acceptor that occurs between TiO_2 and glucose during the synthesis of glucose/TiO_2. The time of electron excitation could be prolonged at the covalent band resulting in high yield of methanol.

Keywords: biomass, glucose, TiO_2 photocatalyst, methanol, carbon dioxide, photoreduction.

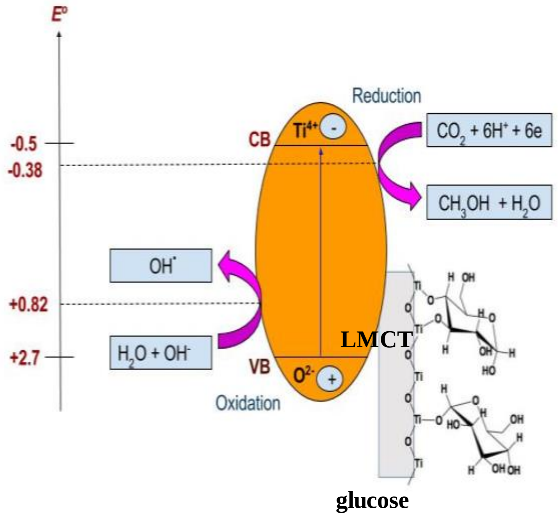

Figure 1: Illustration of ligand-metal charge transfer (LMCT) phenomena between TiO_2 and glucose.

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Various Nanocatalysts for Catalytic Furfural Hydrogenation

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Abstract:

With the increasing demand for eco-friendly products and the associated replacement of petroleum-based chemicals, the interest in biomass conversion has also increased. As unsaturated oxygenate species are abundant in decomposed biomass components, the catalytic conversion of biomass derivatives, such as heterocyclic molecules containing alcohol or aldehyde moieties, is important not only for the energy industry but also to improve the fundamental understanding of various catalytic processes. Furfural (FAL) as a model compound is catalytically converted into furan (F), tetrahydrofuran (THF), 2-methylfuran (MF), furfuryl alcohol (FA), and tetrahydrofurfuryl alcohol (THFA) through distinct reaction pathways depending on the type of catalysts and their surface properties. Various nanocatalysts including metal and metal oxide nanoparticles with controlled shape and size, porous materials with highly ordered pore strucutres as supports, and metal-organic frameworks are diversly used and the role of nanocatalysts is demonstrated in furfural hydrogenation.

$LaMnO_3$ perovskite/reduced graphene oxide nanocomposites for supercapacitor electrode application

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Abstract:

$LaMnO_3$ (LMO) perovskite, with the typical ABO_3-type structure, has proven to be an effective pseudocapacitive materials due to its ability to store charges through anion intercalation mechanism (intercalation of oxygen ion inside the vacancies sites) [1-3]. However, concerning the practical application, $LaMnO_3$ suffers from many challenges, such as low conductivity, small surface area and low cycle stability [3]. Thus, solving these problems and bring $LaMnO_3$ from laboratory studies to real practical applications is considered as a current challenge. In this work, we describe a facile and novel strategy to prepare nitrogen-doped graphene (N-rGO)-wrapped $LaMnO_3$ perovskite (LMO/N-rGO). The process is driven by the electrostatic interactions between negatively charged LMO nanoparticles and positively charged N-rGO with the help of sonication process (Figure 1). The resulting LMO/N-rGO nanocomposite possesses flexible rGO sheets that effectively encapsulate the LMO particles. This unique hybrid structure can prevent the aggregation of LMO nanoparticles and maintain a high electrical conductivity of the electrode. In addition, both electric double layer (N-rGO) and faradaic (LMO) processes can be used to store charges. As a result, graphene-encapsulated LMO nanoparticles (LMO/N-rGO) exhibit a very high specific capacity (398 Cg^{-1} at 10 Ag^{-1}) (208 Cg^{-1} for LMO), with excellent cycle performance (76% retention after 2000 cycle at 10 Ag^{-1}) (55% for LMO). Thus LMO/N-rGO can be proposed as promising supercapacitor electrode materials.

Keywords: $LaMnO_3$ perovskite; Nitrogen-doped graphene; graphene nanocomposite; electric double layer capacity, pseudocapacitive, and supercapacitor.

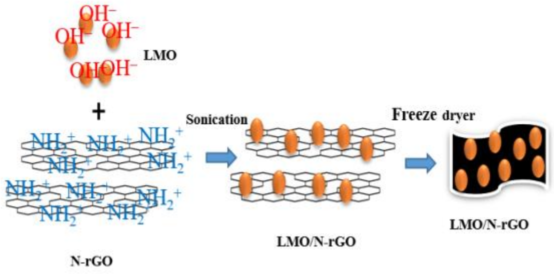

Figure 1: Figure illustrating the the synthesis technique used to prepare LMO/N-rGO nanocomposite.

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Scattering Parameters and Dielectric Properties of Nano Barium Ferrite Microwave Absorber Composite

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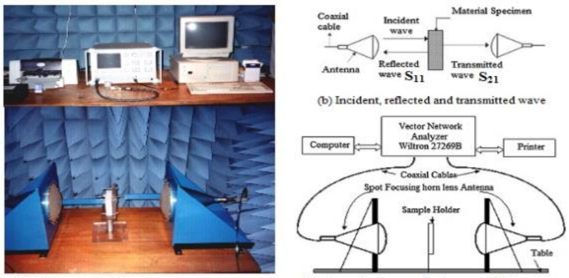
[2] King Khalid University, Vice Presidency for Project, Abha, SAUDI ARABIA

Abstract:

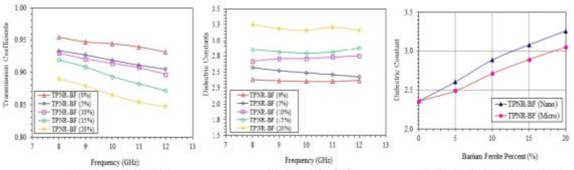
The speedy growth and development of electronic systems and telecommunications have contributed to an increased interest in electromagnetic and microwave absorption technology and materials. In the last decades, extensive research has been undertaken to develop microwave absorption composite through the use of non-magnetic polymer materials added to the granules of magnetic materials. Recently intensive research conducted to develop microwave absorber composite using polymers and incorporated magnetic filler in microscale such as Barium ferrite The chemical formula of Barium ferrite (BF) is $BaFe_{12}O_{19}$. This paper presented the improvement of the microwave scattering parameter (reflection coefficients S_{11} and transmission coefficients S_{21}) and complex permittivity (dielectric constant ε' and loss factor ε") of the thermoplastic natural rubber barium ferrite (TPNR-BF) composite when the size of BF filler changed from 3 μm to 55 nm. TPNR was prepared as hosting material, and the BF was used as filler. Five samples of the TPNR-BF were prepared with micro BF content range from 0% to 20%. The same procedure was used to prepare five samples using nano BF. Scattering parameters and dielectric properties were measured using free space microwave method presented in Figure 1. The results in Figure 2 indicate that the absorption of microwave signal (ε') increases with increasing BF content while the transmission of the signal (S_{21}) decreases. The use of nano BF enhances the absorption of the composite in compare with the micro BF. This result could be explained from the Scanning Electron Microscopy (SEM) in Figure 3 which shows a better dispersion of the nano BF in the TPNR matrix.

Keywords: microwave absorber, barium ferrite, dielectric properties, scattering parameters, nanomaterial.



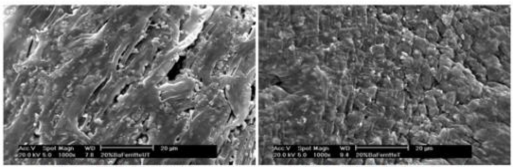
(a) Microwave NDT System (b) Incident, reflected and transmitted wave (c) schematic diagram of microwave NDT system

Figure 1: Free space microwave method used to measure the scattering parameters and dielectric properties of the composite.



(a) Transmission Coefficient (S_{21}) (b) Dielectric Constant (ε') (c) Effect of the size of BF on Dielectric Constant

Figure 2: Scattering parameters and dielectric properties of micro and nano TPNR-BF.



(a) SEM of TPNR-BF 20% (Micro) (b) SEM of TPNR-BF 20% (Nano)

Figure 3: SEM of micro and nano TPNR-BF composite.

References:

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Surface Oxygen Vacancy Assisted Visible Light-induced Photocatalytic Dye Degradation and Photocapacitive Performance of CeO_2-Graphene Nanostructures

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Abstract:

Cerium oxide nanoparticles (CeO_2 NPs) were fabricated and grown on graphene sheets using a facile, low cost hydrothermal approach and subsequently characterized using different standard characterization techniques. X-ray photoelectron spectroscopy and electron paramagnetic resonance revealed the changes in surface states, composition, changes in Ce^{4+} to Ce^{3+} ratio, and other defects. Transmission electron microscopy (TEM) and high resolution TEM revealed that the fabricated CeO_2 NPs to be spherical with particle size of ~10-12 nm. Combination of defects in CeO_2 NPs with optimal amount of two-dimensional graphene sheets had a significant effect on the properties of the resulting hybrid CeO_2-Graphene nanostructures, such as improved optical, photocatalytic, and photocapacitive performance. The excellent photocatalytic degradation performances were examined by monitoring their ability to degrade Congo red ~94.5% and methylene blue dye ~98% under visible light irradiation. The photoelectrode performance had a maximum photocapacitance of 177.54 Fg^{-1} and exhibited regular capacitive behavior. Therefore, the Ce^{3+}-ion, surface-oxygen-vacancies, and defects-induced behavior can be attributed to the suppression of the recombination of photo-generated electron–hole pairs due to the rapid charge transfer between the CeO_2 NPs and graphene sheets. These results displays the CeO_2-Graphene nanostructures revealed improved photocatalytic and photocapacitive performance that could be used for real applications.

Keywords CeO_2NPs; Ce^{3+}-ion; defects; graphene; photocatalysis; photodegradation; photocapacitance

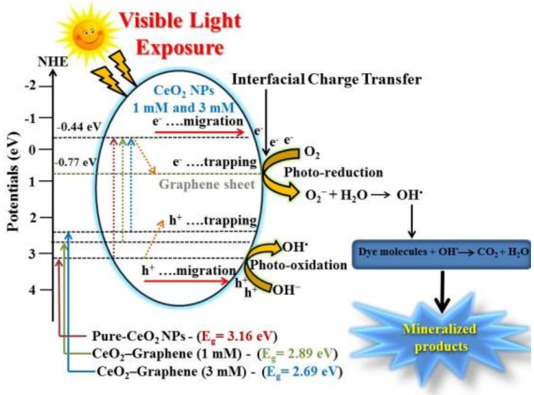

Figure 1: Proposed schematic diagram of the proposed mechanism for the photoexcited electron-hole separation and charge transport process at the CeO_2-Graphene nanostructures as a photocatalyst under visible light irradiation.

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Biowaste-derived carbon functionalized with polyaniline: Recycling to multifunctional applications

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Abstract:

Waste management systems are of prime concern now-a-days to reach the sustainable development goals. Reduce, reuse and recycle-these three `R´ factors are the building blocks towards managing waste products not only of the industries but also from households. Obviously, carbon based materials are the lion´s share of such waste products as well as of the raw materials. Here, waste carbon from cooking oven has been directly percolated into polyaniline (PANI), via in-situ polymerization procedure, without any prior chemical purification or modification. The excellent properties of π-electron delocalization at the backbone of conjugate polymer like PANI can be initiator of charge transfer mechanism with the incorporated carbon nanoparticles resulting tunibility of electronics dynamics within the composites.

Aim of our work is to develop novel strategies for recycling biowaste-derived carbon after functionalizing with PANI via simple cost-effective techniques towards multifunctional applicability. Based on the charge transfer mechanism between PANI matrix and waste carbon particles, composites have been used for next-generation charge trapping memory device, microelectrodes for supercapacitors, sensitive ion (Fe^{+3}) detectors etc. Such kind of advanced multifunctional materials derived from waste carbon-polyaniline by a cheap and eco-friendly process, having unique synergy in their physicochemical properties, can surely enrich the green technology towards sustainability.[1,2]

Keywords: Waste carbon, polyaniline, multifunctional materials, sustainability, green nanotechogy.

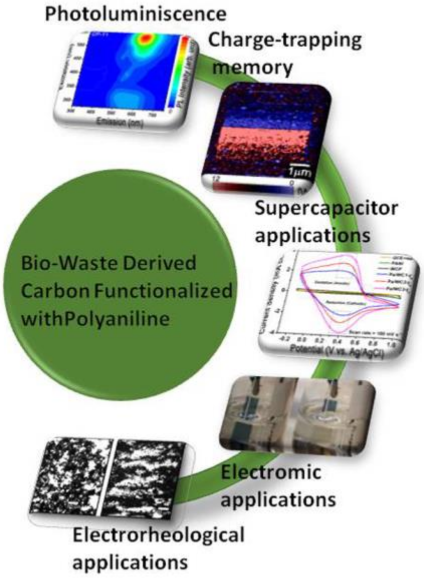

Figure 1: Figure illustrating the multifunctional applications of the composites composed of polyaniline-functionalized bio-waste derived carbon particles─A step towards sustainability development through green technology.

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Session III.C:
NanoMedecine/ Nanosafety

Short, long term fate and biodegradation of IONPs in vivo

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Abstract:

Once a nanoparticle (NP) is administered *in vivo*, it interacts with components of a physiological environment what results in a formation of so called biomolecule corona.[1] Surrounding the NP corona is mostly composed of proteins (hence the protein corona (PC) definition) and it can dramatically change the nanomaterial size, aggregation state and interfacial properties.[2] As a result NP acquires a new biological identity that would dominate the behaviour of NPs *in vivo*.[3,4] Therefore, investigation of the PC is a benchmark in understanding and controlling NPs performance *in vivo*. Moreover, long term studies encompassing the whole NP lifecycle are necessary to clarify the fears concerning NPs safety. Thoroughly, unravelling of the interactions of commonly known nanomaterials with living organisms could diminish the huge discrepancy between the produced numerous nanoscale size therapeutics and scarce clinical outcomes.

Here we report the effect of the superparamagnetic iron oxide NPs (IONPs) surface modification with two hydrophilic molecules, either glucose (Glc) or poly(ethylene glycol) (PEG), on protein adsorption, NPs fate and their biotransformation over 4 months. Although NPs@Glc and NPs@PEG bound similar amount of proteins *in vitro*, the differences found in the composition of both PCs corresponded to the NPs biodistribution *in vivo*. Whereas NPs@Glc were mostly accumulated in the liver and spleen, NPs@PEG were detected in various organs, including thymus or reproductive system organs. Moreover, by employing magnetic measurements we have found, that the biodegradation kinetic and therefore clearance of both NPs types was unequal. 4 months after the administration, NPs@PEG suffered a complete disaggregation and/or reduction of size, and were totally removed from the spleen, but not from the liver. On the other side, NPs@Glc clearance kinetic was higher in the liver than in the spleen, albeit here the degradation of the NPs in both organs was only partial. Interestingly, degradation tested *in vitro* was faster for NPs@Glc than for NPs@PEG demonstrating that the attached molecule is implicated in the protection against degradation in NPs with the same core-shell structure. The variation in the degradation rate observed *in vivo* could be therefore related not only with the attached molecules, but also with the associated PC, which composition may directly affect the degradation rate by lysosomal enzymes or indirectly by driving NPs accumulation in different cells.

Keywords: Magnetic nanoparticles, fate, hyperthermia, biodistribution.

References

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Nanoparticle delivery of drugs for Tuberculosis

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Abstract: Tuberculosis (TB) is an infectious disease caused by *Mycobacterium tuberculosis* (MTB) and one of the top ten causes of death worldwide. There were 10.4 million estimated new cases of TB in 2016 [1]. Drugs to treat TB are most commonly administered either orally or parentally. The oral route requires prolonged treatments with high drug concentrations with only small amounts reaching alveolar macrophages in the lung where bacteria are harboured. The high systemic exposure often results in adverse effects for the patients. On the other hand, parental route is painful and inconvenient. These factors undermine patient compliance, which ultimately might lead to the development of drug resistance [2].

There is an evident unmet medical need to improve TB therapy, not only by developing new drugs and optimising existing drug regimens, but also by designing and generating improved delivery systems [2,3]. Nanotechnology has proved to be an invaluable asset for the diagnosis and treatment of a variety of diseases. A range of nanocarriers have been developed to allow a safe, efficient and localised delivery of antibiotic regiments to reach and sustain antibiotic concentrations above the minimum inhibitory concentration for MTB in the target tissue. These include polymeric nanoparticles, nanoliposomes, nanomicelles, niosomes, cyclodextrin complexes, etc. Drawbacks associated with the use of nanocarriers include cytotoxicity depending on the chemical composition of the materials and the burst release of the encapsulated drugs [2]. With that in mind, we have developed a novel drug delivery system to enable targeted, controlled and sustained release of pharmaceuticals to treat TB. The key innovative feature of this system is to incorporate active pharmaceutical drugs into the chemical structure of the nanoparticle. Drug release occurs upon hydrolytic degradation of the nanoparticle, which solely generates biocompatible products. Pre-clinical evaluation shows the successful uptake of the nanoparticles by macrophages in a zebrafish model of Mycobacterial infection by confocal microscopy. Zebrafish experiments also showed that the nanocarried drug significantly reduced granuloma formation and decreased bacterial load when compared to the free drug.

Keywords: *Mycobacterium tuberculosis*, nanoparticles, drug delivery.

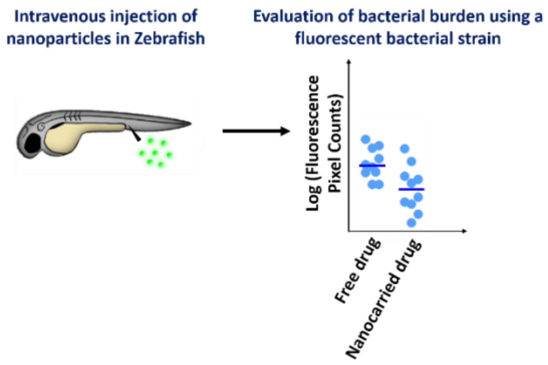

Figure 1: Illustration of nanocarried drug efficacy when compared to free drug in Zebrafish.

References:

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Synthesis of Gold Nanovehicles for Controlled Drug Delivery Applications

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Abstract:

Nanomedicines capable of specifically identifying and binding to target tissues are currently being investigated for imaging, sensing and drug delivery purposes. In order to probe these interactions, it is paramount to have maximum control over the interaction of the nanostructures with their surrounding environment.

Conventional nano-targeting approaches consist of modifying the surface of the nanoparticles with proteins (antibodies or ligands) known to be expressed on the target tissue.

It is well known that a nanoparticle's shape and size correlate closely to their optico/physico-chemical properties. Hence, when programming the nanoparticles with biological entities it is ideal to preserve the nanoparticle's baseline characteristics such as morphology and ensure their stability.

In this study, we synthesize gold nanostructures and characterize the nanosystem by transmission electron microscopy.

The results here presented provide an important quality control over the design of nanomedicines formulated for drug delivery.

Keywords: nanoparticle synthesis, bio-conugation, protein binding, , gold-based biomaterials, transmission elecron microscope, biomedical applications.

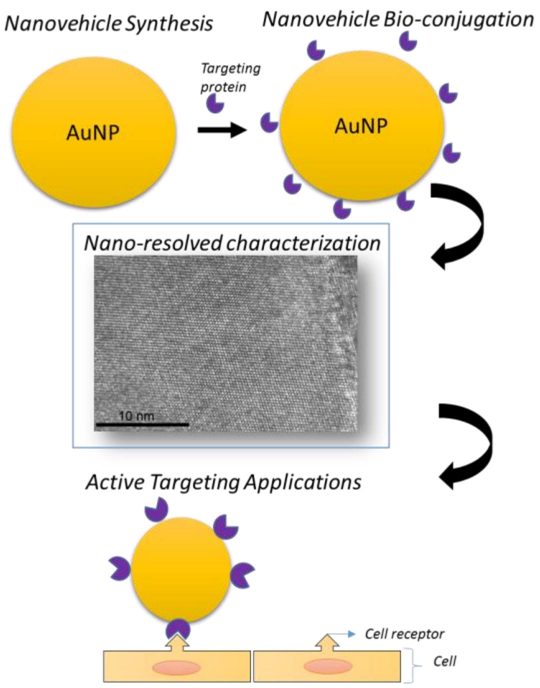

Figure 1: Figure illustrating the rational of the study; highlighting the importance of characterizing nanoparticles with imparted functionality to enable the design of platforms for controlled drug delivery.

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Nanopattern improves chondrogenesis for cartilage regeneration

Ignasi Casanellas[1,2], Anna Lagunas[3,1,*], Iro Tsintzou[1], Yolanda Vida[4,5], Daniel Collado[4,5], Ezequiel Pérez-Inestrosa[4,5], Cristina Rodríguez Pereira[6], Joana Magalhaes[3,6], Josep Samitier[1,3,2]
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Abstract:

Cell adhesion and differentiation processes are influenced by the nanoscale arrangement of the extracellular matrix (ECM), being more affected by local rather than global concentrations of cell adhesive ligands. We have created large-scale uneven nanopatterns of arginine-glycine-aspartic acid (RGD)-functionalized dendrimers that permit the nanoscale control of local RGD surface density changing the initial dendrimer concentration. The nanopatterning method presented here is very simple and can be extended to other ligands having density effects on cells.

Cartilage damage is the main cause of joint disorders. The cartilage inability to spontaneous repair has stimulated clinical and experimental research to promote damaged cartilage regeneration. Nevertheless, current surgical techniques are only suitable to treat small joint defects due to their limited regenerative capacity. Transplantation of mesenchymal stem cells (MSCs), which have a vast proliferative capacity and differentiation potential, has emerged as an attractive strategy to treat widespread joint defects. However, direct implantation of undifferentiated MSCs without any preconditioning lead to calcification of the implanted cells, fibrogenesis and heterotopic tissue formation in the cartilage. Therefore, in vitro stem cell preconditioning is required to direct cells to a particular differentiation pathway prior to implantation.

Moreover, since cartilage is a non-vascularized tissue, the establishment of a functional cell interconnectivity network (mainly through gap junctions, GJs) is of capital importance in cartilage architecture and well function. We here demonstrate that nanopatterned growth substrates facilitate the formation of a GJ connectivity network among human stem cells undergoing induced chondrogenesis. Results show that a specific nano-clustering concentration of RGD dendrimers, leading to intermediate cell-substrate adherence, promotes chondrogenic differentiation and formation of a GJ network. This is an important milestone for the development of a cell carrier with nanofeatures that allows cell preconditioning and implantation into osteoarthritis patients

Keywords: Dendrimer, nanopattern, arginine-glycine-aspartic acid (RGD), atomic force microscopy (AFM), cell adhesion, mesenchymal stem cells (MSCs), chondrogenesis.

References:

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Characterization of the interaction of graphene oxide with the mammalian sperm membrane

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Abstract:

The growing use of Graphene Oxide (GO) as a biomaterial has risen questions regarding its safety, including in terms of reproductive ability. It has been shown that graphene is able to interact with the cytoplasmic membrane [1, 2].

Previous work has shown that treatment with graphene oxide in a media enabling capacitation increases membrane fluidity, resulting in higher rates of capacitation and "*in vitro*" fertilization [3].

This lead us to question whether Graphene Oxide is changing the composition of the membrane or if this is due to the physical connection.

Thermogravimetric Analysis indicates that the effects exerted by GO is not directly related to its attachment to sperm membrane (data not shown). A cytofluorimetric study using Filipin III as a marker for cholesterol shows a decrease of this sterol in the samples treated with graphene oxide, in a concentration dependent fashion. Indicating that GO is extracting the cholesterol from the membrane. Furthermore, Differential Scanning Calorimetry study comparing GO with other molecules used to remove cholesterol, shows that it has a stronger effect than the traditionally used bovine serum albumin (BSA) but to a decreased effect compared to the toxic Methyl-β-cyclodextrin (MBCD).

Keywords: Graphene Oxide (GO), boar spermatozoa, capacitation, cholesterol, Cytoplasmic membrane.

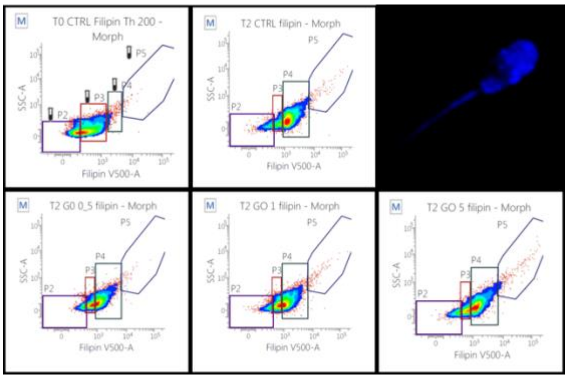

Figure 1: Cytofluorometry of spermatozoa incubated for 2 hours with different concentrations of GO (0,5µg/mL; 1 µg/mL; 5 µg/mL) stained with Filipin III to mark the cholesterol.

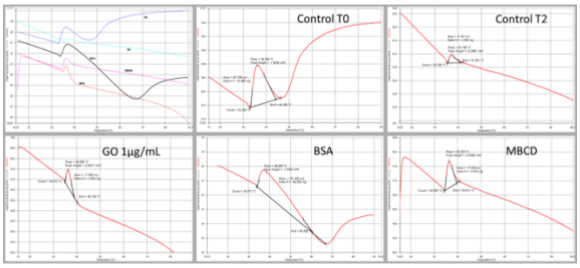

Figure 2: Differential Scanning Calorimetric analysis of the membrane response to a temperature scan. Comparison between GO and other cholesterol extractors (BSA and methyl-β-cyclodextrin)

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A Potential Approach to Assess and Control the Potential Risks Related to Nanomaterials

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Abstract:

Twenty-first century businesses will rely on nanoscience and nanotechnology. However, nanotechnology is making advance faster than the risk and safety assessment/management related to it. Consequently, we focus to establish adequate strategies to manage and communicate nano-related risks and safety issues in an appropriate way along the innovation chain (from initial idea to market).

The presented framework (Fig. 1) relates to existing practice of the current regulatory framework on the safe use of chemicals (i.e., REACH) and new advances towards regulation (e.g., ECHA, appendix to chapter R.7a) and is structured into two parts. The first part focuses on the creation of a risk profile for a given nanomaterial (e.g., classify which materials and/process operation pose greater risk, where these risks occur in the lifecycle, and the impact of these risks on society) using state-of-the-art safety assessment approaches/tools (ECETOC TRA, Stoffenmanager Nano and ISO 12901-2).

The second part emphases on giving concrete, practical guidance to industry and regulatory authorities (such as European agencies, scientific committees, national competent authorities) on how to deal with environmental health and safety (EHS) issues of manufactured nanomaterials (NMs) and nano-enabled products, including, as appropriate, legislation/sector specific issues. Risk mitigation actions focus on hazard/risk avoidance rather than address them as an exposure (e.g., "design out" physico-chemical parameters that are identified as being drivers of toxicity of NMs whilst retaining the functional aspects, "re-design" process and operational conditions, develop solutions for exposure reduction and personal protective equipment).

Use of the concept cannot prove safety or guarantee absolute safety. However, implementation of Safe-by-Design early in the development process can form an important cornerstone in making products and materials fit for a circular economy and offers a chance for smart innovation.

Keywords: risk assessment, nano-related risks, Safe-by-Design, nanotechnology, nanomaterials

Figure 1: Illustration of the proposed safety strategy

References:

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Tuball ™ Single wall Carbon Nanotubes: Health, Safety & Environmental issues

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Abstract:
The company OCSiAl is been founded in 2009 and is also the first SWCNT manufacturer who has completed his EU-REACH registration for a tonnage band of up to 10T/a. Later on this year we will be placed on the US-TSCA inventory, our PMN file will be dropped meaning we will have a signed consent order with the EPA.

Because Tuball™ is used and also tested in various applications on an ongoing basis, also receiving a lot of interests worldwide. That is why it is obvious that the company OCSiAl is establishing the necessary regulatory and quality standards worldwide.

The first part of this presentation will aim at providing a short introduction of our Tuball™ substance and his product line, a second part of the presentation will be an overview of the status and plans of the ongoing registrations an compliance. The third and last part of the presentation will focus on the health, safety and environmental aspects of our Tuball™ substance and the different applications.

As SWCNT manufacturer, OCSiAl is doing continues investments in improving our understanding of our different (new) Tuball products themselves and potential hazards through their (entire) life cycle. We are involved in generating additional test data and collaborating with industry associations and networks.

This presentation will describe the steps being taken by the company H&S Lead manager, Van Kerckhove Gunther to successfully introduce our carbon nanotubes (SWCNT's) regulatory status and outline our (future) plans for numerous of studies and qualifying our Tuball™ substance including the different kind of compositions.

REVIEW OF HUMAN HEALTH RISK ASSESSMENT MODELS CONSIDERING THEIR INPUT REQUIREMENTS AND APPLICABILITY DURING NANOMATERIAL PRODUCT DEVELOPMENT RESULTS FROM THE EU H2020 'CALIBRATE' PROJECT

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Abstract:

A selection of human health risk-assessment software tools to support innovation decision making was made. The tools are matched against stakeholder criteria at different stage of innovation (according to the Cooper stage-gate model).

In order to optimally implement Human Risk Assessment models along the innovation chain, requirement and objective performance criteria to accommodate different stage gates of innovation, exposure scenarios and stakeholder needs were identified. The applicability of 18 available tools was evaluated based on the identified stakeholder criteria. The evaluation resulted in a selection of most suitable models for each innovation stage and formed the basis for a gap analysis. This gap analysis has resulted in a guidance for futher improvement of the models based on the stakeholder criteria.

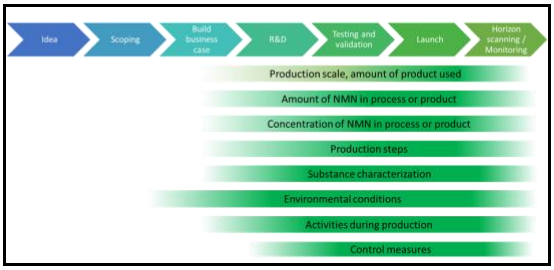
The following steps are explained:

- The inventory and selection of appropriate Human Risk Assessment tools based on previous experiences and expert knowledge
- Identification of requirement and objective performance criteria per stage-gate
- The matching of each of the models against these requirements
- Selection of the models that match best with the stakeholder requirements at different innovations stages
- Identified potential for further development and improvement of the models.

This approach gives a final selection of models per stage gate of innovation which can be used in the system of systems as to be developed in the H2020 caLIBRAte project. It can be concluded that the identified mismatches between the stakeholder requirements and performance criteria and the assessed tools can be overcome by further developing and calibrating the existing risk assessment tools. Furthermore many mismatches can be overcome by developing default scenarios and by linking the tools to standard scenario's and defaults for input values

Keywords: Safe innovation, safe by design, risk governance, human risk assessment models, caLIBRAte, nanomaterial safety

Figure: Availability of information relevant for human risk assessment along the Cooper stage gates of innovation



References:

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Session III.D: NanoMaterials for Food Applications

Nanotechnology in the Food Packaging Sector: Recent Applications and Future Trends

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Abstract:

Nanotechnology may be applied in all steps of the food chain in order to improve the quality and the safety of food, to extend food shelf life (active packaging and packaging with enhanced mechanical, optical, barrier or thermal properties) or as quality control (intelligent packaging). Nanotechnology may also be used to produce healthier foods with tailor-made nutritional characteritics.

One of the main obstacles for nanotechnology implementation is the lack of knowledge about the impact of nanomaterials on Human Health because they have different properties at nanoscale such as increased reactivity due to increased surface area. Nevertheless some nanoforms have already been authorized to be used in plastic food packaging in the European Union (EU) through Regulation EU No 10/2011 and its amendments[1]. Table 1 compiles some of the nanoforms evaluated by the European Authority for Food Science (EFSA) and authorized in the EU such as silicon dioxide (Food Contact Material substance number, FCM No, 504) and titanium nitride (FCM No 807).

In order to carry out a correct risk management of nanomaterials and to keep the legislation in this field updated, it is required a close and fruitfull collaboration among researchers, risk assessors, regulators and food and food packaging industry.

Recent applications of nano-based materials will be discussed within this presentation. Special emphasis will be given to nanoforms authorized in the EU. Finally, future trends on the application of nanomaterials to foods will be addressed. For instance, active compounds extracted from tomato and/or fruit by-prodcuts can be embedded into nanocarriers to control their release from films to foods.

Keywords: Nanotechnology, Food Packaging, Legislation, Nanoforms, Food Contact Naterial, Regulation (EU) no. 10/2011.

Figure 1: Examples of nanoforms evaluated by the European Authority for Food Science (EFSA) and authorized in the European Union.

FCM substance no.	**Substance name**
87	Silicon dioxide, silanated
411	Carbon black
504	Silicon dioxide
807	Titanium nitride, nanoparticles
859	(butadiene, ethyl acrylate, methyl methacrylate, styrene) copolymer crosslinked with divinylbenzene, in nanoform
998	(butadiene, ethyl acrylate, methyl methacrylate, styrene) copolymer not cross-linked, in nanoform
1016	(methacrylic acid, ethyl acrylate, n-butyl acrylate, methyl methacrylate and butadiene) copolymer in nanoform
1030	montmorillonite clay modified by dimethyldialkyl(C16-C18)ammonium chloride
1043	(butadiene, ethyl acrylate, methyl methacrylate, styrene) copolymer crosslinked with 1,3-butanediol dimethacrylate, in nanoform
1046	zinc oxide, nanoparticles, coated with [3-(methacryloxy)propyl] trimethoxysilane (FCM No 788)
1050	zinc oxide, nanoparticles, uncoated

References:

1. Commision Regulation (EU) No 10/2011, of 14 January 2011 on plastic materials and articles intended to come into contact with food. Official Journal of the European Union L 12/1-89 and its amendments.

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Active biopolymer film or coating for food packaging application: structure-properties relationship and shelf life extension

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Abstract:

Increasing environmental concerns regarding the use of syntetic packaging of petrochemical origin together with consumers demands for both higher quality and longer shelf life have led to increased interest in alternative packaging material research. Biopolymers, such as protein, polysaccharides and lipids, or their combination, have been extensively studied to prepare edible coating or films to preserve quality and extend shelf life. Best results in terms of shelf life extension can be obtained when the biopolymer material can be used as substrate to develop new active biobased film. Active material are designed to deliberately incorporate "active" components intended to be released into the food ot to absorb substances from the food (Regulation (EC) No 1935/2004; regulation (EC) No 450/2009). To properly design coating or film with desired functional properties a proper understanding of the role of constituents on network formation and on film structure is required. Among active compound, essential oil are interesting for their potential use as natural preservatives. In the present work the role of interaction between proteins and polysaccharides on film structure and on the active packaging functionality in terms of antioxidant activity will be discussed. The film structure have been investigated by scanning electronic microscopy analysis, rheological properties and particle sixe analysis of the film forming dispersion, dynamic mechanical properties and SDS-PAGE analysis. Fuctional properties of film have been studied in terms of water solubility, water vapour permeability, mechanical properties and antioxidant properties. The effect of the active biopolymer coating on shelf life extension will be discussed focusing the attention on minimally processed fruits and meat. Quality parameter such as respiration rate, transpiration rate, colour and mechanical properties of the product have been studied to quantify the effect of the new technology on product shelf life. Different concentration of protein and polysaccharides affect structure of the film and in turn the physical properties of the obtained blend film (1). The structure of the film have a significant effect on the particle dimension of essential oil and on its distribution in the film (2). As conseguence, the antioxidant activity of the film have been modified in terms of kinetics of release of the active compound. Active biopolymer film showed a positive effect on minimally processed fruits and meat shelf life, but the effect were functions of the films structures.

Keywords: biopolymer film, protein, polisaccherides, essential oil, film structure, film functional properties, active film, shelf life.

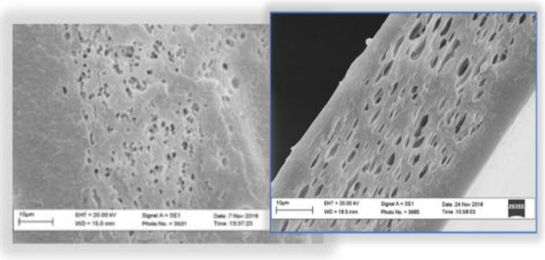

Figure 1: Effect of film composition on essential oil dispersion and particle size dimension.

References:

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PAA.PVA-PAMAM bio-nanocomposite films incorporating thymol for food packaging

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Abstract:

In alimentary sector, particulary for the manufacturing of food packaging systems, nanotechnology offers the opportunity for compact designs based on the high and selective surface area available at the nanoscale and the ability to integrate multiple functionalities into a single product[1,2]. In this work, amino-terminated fifth generation poly(amide-amine) dendrimer (PAMAM G5-NH_2) were grafted onto the surface of biodegradable poly(acrylic acid)/poly(vinyl alcohol) (PAA/PVA) electrospun fibres with the purpose of creating a host-guest architecture for the controlled delivery of the natural antioxidant thymol. The electrospun films consisted of uniform, straight and well-defined fibers that preserved their fibrous morphology after washing and functionalization. The amount of grafted dendrimer reached $2.25x10^{-6}\pm3.0x10^{-7}$ mmol PAMAM G5-NH_2/mg film and was higher for membranes with higher content of PAA. The amount of thymol loaded reached a maximum of $2.51x10^{-4}$ mol thymol/g film, from which 18% corresponded to the PAA/PVA base film. For the whole set of film, the amount of thymol hosted by the dendrimer was 37±5 molecules of thymol per molecule PAMAM. The films could be recharged without losing capacity. Computational modelling allowed determining the molecular details of the dendrimer-guest complex and the calculation of the number of loaded molecules. The results predicted 16 thymol molecules encapsulated around the dendrimer core or between dendrimer branches via hydrophobic interactions. 25 additional thymol molecules could be hosted at the dendrimer surface, although with lower binding energies than those encapsulated inside the dendritic cavities. Upon contact between thymol-loaded membranes and food simulants, we showed that the release behaviour was mainly driven by the pH of the medium. In 95 vol% ethanol the release of thymol took place at a relatively constant rate of ~$8x10^{-4}$ mmol thymol g $film^{-1}day^{-1}$. This it was below the overall migration limit of 10 mg/dm^2 established by EU Commission Regulation 10/2011. Based on the results of this study, PAA/PVA-PAMAM G5-NH_2 functionalized nanofibers loaded with antimicrobial thymol molecule hold great promise for their use as active food packaging material.

Keywords: biodegradable polymers, electrospinning, nanofibers, PAMAM G5-NH_2 dendrimer, natural extract, nanocomposite, active food packaging systems.

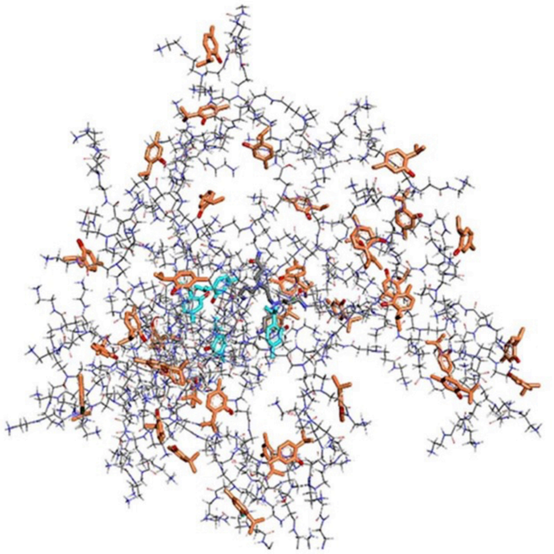

Figure 1: Docking model of the 41 thymol molecules associated to the G5 dendrimer. (The four thymol molecules located near the dendrimer core were coloured in blue.)

References:

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A novel antibacterial strategy based on oxide nanoparticles for medical and food-related polygraphy

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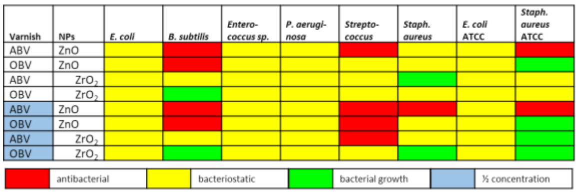
Abstract:

From the epidemiological point of view, two problems were recognised concerning printed materials used in the medical environment and in the food industry. First is the fact, that varnishes based on organic solvents are an excellent medium for bacterial growth. The second problem concerns possibility to transfer multiresistant bacterial strains that occur in the hospital environment through printed materials (such as brochures, flyers or packages). Here, a strong concern is for transfer of those strains out of the hospital regime. One of the solutions we propose for medicine is the use of nanolayers with antibacterial properties deposited by the ALD technique. However, from the point of view of printing this strategy would be extremly difficult to apply. Hence, we proposed application of nanopowders with antibacterial properties as an integral element of the vanish. Zinc oxide and Zirconium dioxide, nanoparticles with confimed antibacterial properties *in substantia* and/or as nanolayer [1], were added to the comercial vanishes of either aqueous (ABV) or organic (OBV) solvent base. They were printed on 240 g/m^2 paper sheets and then cut into 1 cm^2 samples in the sterile conditions. Antibacterial properties were evaluated according to the the modified agar disk diffusion method using both reference and wild type bacterial strains (latter were the isolates from the clinical cases). Samples were placed on the surface of the bacteria-covered medium. The efficiency of antibacterial activity of vanishes supplemented with Zinc oxide and Zirconium dioxide was evaluated by the measurement of the area in which bacteria growth was inhibited. According to the obtained results we can conclude that nanoparticles-enhanced vanishes showed antibacterial and bacteriostatic properties, therefore they can find potential applications in the polygraphy for medicine, broader health care and food industry.

Keywords: oxide nanoparticles, antibacterial properties, polygraphy, medical applications, food industry applications



Varnish	NPs	*E. coli*	*B. subtilis*	*Entero-coccus sp.*	*P. aerugi-nosa*	*Strepto-coccus*	*Staph. aureus*	*E. coli* ATCC	*Staph. aureus* ATCC
ABV	ZnO	🟨	🟥	🟨	🟨	🟥	🟨	🟨	🟥
OBV	ZnO	🟨	🟥	🟨	🟨	🟨	🟨	🟨	🟩
ABV	ZrO_2	🟨	🟨	🟨	🟨	🟨	🟩	🟨	🟨
OBV	ZrO_2	🟨	🟩	🟨	🟨	🟨	🟨	🟨	🟨
🟦 ABV	ZnO	🟨	🟥	🟨	🟨	🟥	🟥	🟨	🟥
🟦 OBV	ZnO	🟨	🟥	🟨	🟨	🟥	🟨	🟨	🟩
🟦 ABV	ZrO_2	🟨	🟨	🟨	🟨	🟥	🟨	🟨	🟩
🟦 OBV	ZrO_2	🟨	🟩	🟨	🟨	🟨	🟩	🟨	🟩

🟥 antibacterial 🟨 bacteriostatic 🟩 bacterial growth 🟦 ½ concentration

Table 1: Results showing antibacterial and bacteriostatic properties od nanoparticles-enhanced vanishes.

Acknowledgments:

NCN DEC-2012/05/E/NZ4/02994, NCN 20/0139/N/ST3/04189, 05-1/KNOW2/2015

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Posters Sessions

Posters Session I: Nanomaterials synthesis, characterization/Nanometrology and properties

Preparation and Characterization of AlOOH-based Nanocrystalline Film on Aluminum Alloy

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Abstract:

Al alloys have been used as an advanced structural material in automobile and railway industries because of their excellent physical and mechanical properties such as low density, high specific strength and ductility. Their low corrosion resistance, however, have restricted their application in a corrosive environment. It is necessary to develop a novel coating technology for improvement the corrosion resistance of Al alloys [1]. In this presentation, a control method of corrosion protection for Al alloys using steam will be discussed.

Al-Zn-Mg alloy was used as the substrate. The cleaned substrates were set in the autoclave with 20 ml of ultrapure water in order to produce steam. The autoclave was heated to a temperature of 373 to 453 K, and then held at this temperature for up to 48 h, resulting in the formation of anticorrosive films on Al alloy. The films were characterized by XRD, XPS, FE-SEM and electrochemical measurements.

FE-SEM images of film surfaces treated at 140ºC, 160ºC, 180ºC and 200ºC for 24 h using steam demonstrated that plate-like nanostructure was densely formed on the surface (Figure 1). XRD patterns indicated that the film formed on Al-Zn-Mg alloy by steam process was mainly composed of AlOOH crystals with the co-formation of Zn-Mg LDH (Layered Double Hydroxide). The potentiodynamic polarization curves of the film coated and uncoated substrates after immersion in the 5 wt% NaCl aqueous solution for 30 min revealed that the corrosion current density, j_{corr}, of the film coated substrates decreased by more than two orders of magnitude as compared to the uncoated substrates, indicating that the corrosion resistance of the Al-Zn-Mg alloy were improved by the formation of the film via steam process.

Keywords:

Aluminum alloy, layered double hydroxide, steam process, corrosion resistance, surface modification.

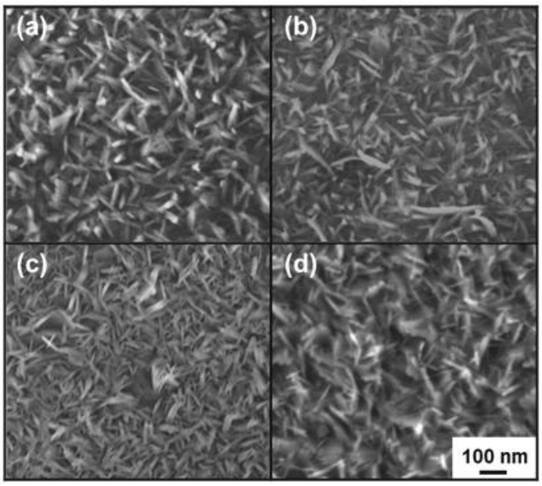

Figure 1: FE-SEM images of film surfaces steam processed at (a) 140ºC, (b) 160ºC, (c) 180ºC and (d) 200ºC for 24 h.

Acknowledgement:

This research was supported by Japan Science and Technology Agency (JST) under Industry-Academia Collaborative R&D Program "Heterogeneous Structure Control: Towards Innovative Development of Metallic Structural Materials" (No. 20100120).

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Dynamic behavior of water droplet on hydrophobic surfaces covered with two organic silane molecules with alkyl chain

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Abstract:

Control of wettability on the material surface is indispensable for various applications such as µ-TAS, automobile, and so on, because the technology holds the promise for considerably reducing energy consumption in their industries. Superhydrophobic surface with a water contact angle of more than 150° is known as a surface to repel extremely water. [1,2] The superhydrophobicity is created by two factors, i.e., low surface energy and nanostructure. The nanostructure is easily damaged by physical contact, resulting in the decrease in the water contact angle. Thus, it is required to create a novel surface that can control surface wettability after physical contact. Hydrophobic surface with a low contact angle hysteresis is considered to be an alternative surface, because the surface can control wetting behavior of water droplet. In addition, such a surface does not have nanostructure, so it is hardly affected by the physical damage. Thus, it is very important to develop a technology for creating hydrophobic surface with a low contact angle hysteresis. In this study, we aimed to prepare dewetting surface showing a low contact angle hysteresis by a simple process.
Hydrophobic surface was prepared on the cleaned Si substrate using mixed raw materials composed of trimethoxy(methyl)silane (TTMS), dodecyltrimethoxysilane (DDS) or hexyltrimethoxysilane (HXS), and octadecyltrimethoxysilane (ODS) by a chemical vapor deposition at 373 K for 24 h.

Fig 1 shows water contact angle hysteresis values as a function of ODS amounts in raw materials. The water contact angle hysteresis on the surface covered with HXS and ODS, and DDS and ODS were decreased with an increase in ODS amounts in raw materials. The contact angle hysteresis of the samples were approximately kept constant at 10°. The surface covered with HXS and ODS became water contact angle hysteresis of less than 10°. On the other hand, water contact angle hysteresis of the surface covered with TTS and ODS were approximately kept constant at 20°. These results indicate that the difference in the alkyl chain length of the raw material can affect the contact angle hysteresis.

Keywords: Wettability, contact angle hysteresis, dynamic behavior of water dloplet, CVD.

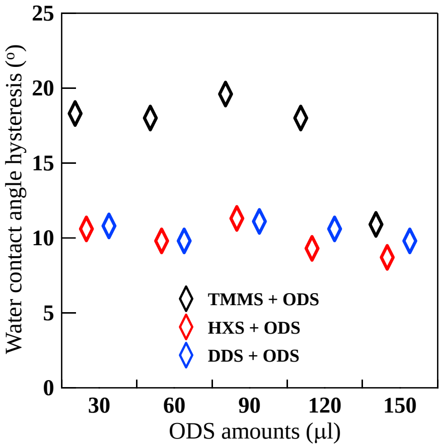

Figure 1: Water contact angle hysteresis values as a function of ODS amounts in raw materials.

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Acknowledgment:

This work was partly supported by Grant-in-Aid for Scientific Research (A) (No. 16H02400) from Japan Society for the Promotion of Science.

Quantitative analysis of point and lattice defects in $Si_{0.6}Ge_{0.4}$ alloys with thickness variation using Terahertz Pump probe measurement

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Abstract:

$Si_{1-x}Ge_x$/Si heterostructure have been studied for decades. One of the main topic in $Si_{1-x}Ge_x$/Si heterostructure is attempt of quantification of defects in strained $Si_{1-x}Ge_x$. Because of the larger lattice parameter of Ge than Si, $Si_{1-x}Ge_x$ on Si is under strain. At small thickness of $Si_{1-x}Ge_x$, It forms pseudomorphic structure and is fully strained on xy-plane and then finally relaxed at certain thickness called 'critical thickness'. $Si_{1-x}Ge_x$ has various types of defect and there are two main types of defect, one is point defect (vacancy, interstitial, substitial *etc*) other is lattice defect (misfit dislocation *etc*). We have evaluated time constants of carrier recombination of $Si_{0.6}Ge_{0.4}$ with various thickness using Thz 1D pump probe method. Photo-carriers can be made by absorbing pump beam and then decay to lower band. It is known that defect assisted transition process has tendency that has smaller time constant with increasing concentration of defects. After inverse Laplace conversion, we can evaluate of time constants of recombination of various $Si_{0.6}Ge_{0.4}$ samples which have thickness variation and we can conclude that point defects and lattice defects have different tendency of time constant. We have also studied qualitative analysis using AFM, TEM, XRD rocking curve, Hall measurement, DFT calculation. With these experiments, pump probe data can be supported qualitatively well.

Keywords: $Si_{0.6}Ge_{0.4}$, Thz-Pump probe, AFM, TEM, XRD, Hall measurement, DFT, Point defect, Lattice defect, Exitation, Decay, Time constant,

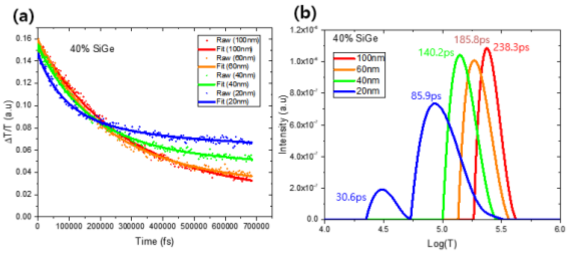

Figure 1: Figure (a) shows THz 1D-pump probe results of $Si_{0.6}Ge_{0.4}$ under variety of thickness (20nm, 40nm, 60nm, 100nm). Data has fs resolution using fs pump beam (800nm). Figure (b) shows time constants of various samples by inverse Laplace conversion method. Time constants are gathered within hundreds of ps

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A Combination of PVD and PECVD Techniques for Deposition of CrNx Coatings and Metal Oxide Top-Coats on Polymers

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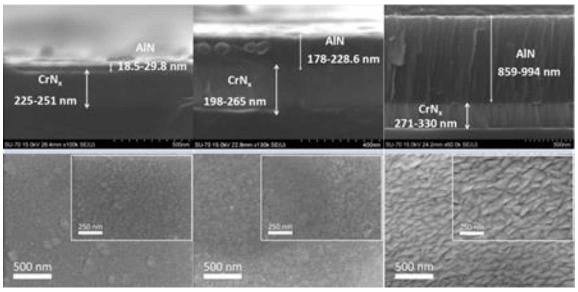
Abstract:

The electrochemical process is today the most common used method for the metallization of polymeric materials. However, this method produces highly toxic residues, in particular the hexavalent chromium (Cr^{6+}) and the trivalent chromium (Cr^{3+}), which are known to be carcinogenic to humans [1]. Thus, in accordance with European recommendations [2] we have choose the more environmental friendly and less toxic physical vapour deposition (PVD) process and refine it to allow the production of metallic looking CrN_x coatings on several polymeric materials. In addition, the PVD technique can be used to deposit top-coats on the metallic coating, to increase its chemical and mechanical resistance to humidity/corrosion and scratch, respectively.

For this innovative proposed process the treatment and coating of polymeric materials is carried out in a single cycle, using a combination of Plasma Enhanced Chemical Vapour Deposition (PECVD) and PVD techniques. We present preliminary colorimetry and surface morphology analysis of metal-oxides (TiO_2, Al_2O_3, AlN and ZrO_2) of various thickness, as protective films deposited on CrN_x coatings. Such bi-layered coatings were also characterized by their surface roughness using optical prephilometry. The results have shown uniform protective films with increasing grain size and surface roughness for the AlN and ZrO_2 films deposited for longer times. Also, the electrical resistivity (ρ) for the CrN_x coatings deposited on polyethylene terephthalate (PET) and polyamide (PA) substrates was measured using the four point probe method. The results have shown higher ρ values for the untreated PA substrates and a steady decrease for argon plasma treated PET and PA substrates when compared to untreated ones.

Keywords: Physical Vapour Deposition, metallization, polymeric materials, colorimetry, surface roughness, metal-oxides, protective coatings.



(a) (b) (c)

Figure 1: Scanning electron microscopy (SEM) micrographs for the AlN protective film on the CrNx coating, with different metal-oxide deposition time: (a) 5min; (b) 30min; (c) 180min.

References:

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2. European Chemicals Agency, press release ECHA/PR/11/27.

Hydrophobic/oleophobic coating of polydimethylsiloxane from modified silica nanoparticles

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Abstract:
Modified silica nanoparticles were prepared by hydrolysis and condensation with tetraethylorthosilicate (TEOS), and their surface was modified with an organic silane bearing a non-hydrolyzable functional group (e.g., alkyl, fluorinated alkyl). They were used to produce hydrophobic/oleophobic coatings on polydimethylsiloxane. Plasma treatment of the surface is required to promote the adhesion of the nanoparticules on the polydimethylsiloxane surface.

The hydrophobicity of the surface was confirmed by measurements of contact angle of water (128 °). The oleophobic character of the coating was also determined by measurements of contact angle of hexadecane (74 °).

The size of the nanoparticles and surface charge was determined by DLS, TEM and Z-Potential, respectively. The resulting coating was charactherized by SEM and perfilometry.

This method improved the preparation of modified silica nanoparticules being easier and cost-effective compared to those already described. Moreover, the resulted silica nanoparticules are transparent.

Keywords: sol-gel process; modification of nanoparticles; hydrophobicity; oleophobicity; alkylsilane; fluoroalkylsilane; polydimethylsiloxane; dynamic light scattering; Z-potential

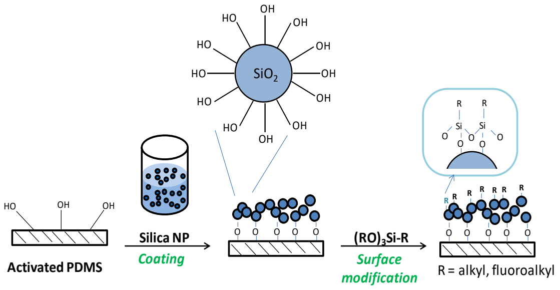

Figure 1: Hydrophobic/oleophobic coating of polydimethylsiloxane methodology involving three important steps: (i)activation of the polydimethylsiloxane surface by plasma treatment, (ii) coating of the polydimethylsiloxane surface and (iii) surface modification of silica nanoparticles with an alkyl and/or fluoroalkylsilane.

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The corrosion studies of Ni/Al_2O_3 and $Ni/Al_2O_3/PTFE$ composite coatings in anti-icing environments

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(topic - Nanostructured coatings, surfaces and membranes)
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Abstract:
The reduction of corrosion and tribological wear processes of vehicle's equipment parts working in anti-icing environments is one of the biggest problem in transport industry. Electrochemical composite coatings could allow for extend lifespan of automobile components due to their improved performance characteristics. The paper describes microstructure, microhardness and corrosion investigations of the nickel-alumina (Ni/Al_2O_3) and nickel-alumina-polytetrafluoroethylene ($Ni/Al_2O_3/PTFE$) composite coatings produced by electrochemical method in base and modified by organic additives Watts bath. Ductile nickel matrix provides a lot of advantageous mechanical properties, the built-in hard ceramic particles increases hardness and wear resistance and self-lubricant fluoropolymer reduces the friction coefficient and increases the anti-adhesive properties.

The main purpose of this paper was to elaborate the process parameters for producing $Ni/Al_2O_3/PTFE$ composite coatings in order to obtain layer with uniformly distributed disperse phase particles in nickel matrix and sufficient microhardness. Such coatings were subjected to corrosion studies by the electrochemical impedance spectroscopy and potentiodynamic methods in two anti-icing environments (sodium chloride NaCl and calcium magnesium acetate CMA). The choice of CMA is caused by gradual replacement of corrosive chlorides as a road anti-icing agent. The completed studies have shown that the $Ni/Al_2O_3/PTFE$ composite coatings produced in the base Watts bath are characterized by lower microhardness and higher corrosion resistance in NaCl solution compared to nickel and composite Ni/Al_2O_3 coatings. In the case of composite coatings deposited in a modified bath their microhardness is higher to pure nickel coatings and the best corrosion resistance showed the Ni/Al_2O_3 coating. All coatings tested in the NaCl were characterized by pitting corrosion. In contrast, the coatings exposed in the CMA environment were characterized by a slight change in microstructure in relation to the condition prior to the corrosion tests.

Keywords: composite coatings, Ni/Al_2O_3, $Ni/Al_2O_3/PTFE$, electroplating, corrosion resistance, anti-icing agent, EIS and potentiodynamic methods.

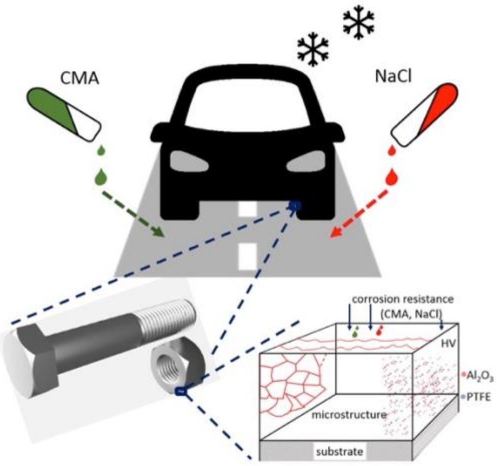

Figure 1: Figure illustrating problems of corrosion of vehicle's equipment parts in winter anti-icing environments and performed in the present paper studies.

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Adsorption and Penetration of Nano-dispersed Super Hydrophobic Colorants into High Molecular Weight Polyethylene

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[2] Yeungnam University, Department of Fiber System Engineering, Gyeongsan, Korea

Abstract:

A high molecular weight polyethylene fiber is a highly crystalline polymer with a linear aliphatic backbone. The fibrous material exhibits very strong tensile strength and modulus, which enables to be applied for various protective and high-resistant areas such as bullet-proof, knife-proof, cut-resistant safety gloves, to name a few. In addition, the fiber is extremely hydrophobic due to pure alkyl backbone comprising only carbon-hydrogen covalent bonds. Although this makes the fiber very resistant to humid and wet conditions, intended penetration of some chemicals and organic materials such as dyes and finishing agents into the fiber becomes very difficult and almost impossible in aqueous medium. To penetrate into the fibrous polymer, the chemicals must be also very hydrophobic. Introducing hydrophobic groups like long linear alkyl groups enhances the hydrophobicity of dyes and finishing agents. However, the long alkyl groups make the chemicals insoluble in an aqueous medium. Therefore, a dispersion of the chemicls is very important in the super hydrophobic material systems. A lot of super hydrophobic coloring materials were synthesized by introducing long linear alkyl substituents to practical chromophores. To apply in an aqueous medium, the super hydrophobic colorants were dispersed with doule-tailed cationic surfactants in average partical size of approximately a few hundred nanometer. Practically, anionic surfactants are used since they are cheap at mass production. However, in this study, mainly cationic were used to obtain very fine dispersions and dispersion stability during application process. The cationic surfactants can make a nano-sized vesicle structure in which fine colorants particles contained with high stability. At first, the dye-containing vesicles are adsorbed on the surface of high molecular weight polyethylene fibers and then disassembled thermodynamically to release the materials contained inside. At last, the dyes get into contact to the extremely hydrophobic fibers and penetate by thermodynamic diffusion process (Figure 1). Since the outer aqueous phase was hydrophilic, the super hydrophobic dyes would not diffuse out from the inside fibers.

Keywords: high molecular weight polyethylene, double-tailed cationic surfactant, dyes, nano-dispersion, super-hydrophobic, vesicle, thermodynamic diffusion.

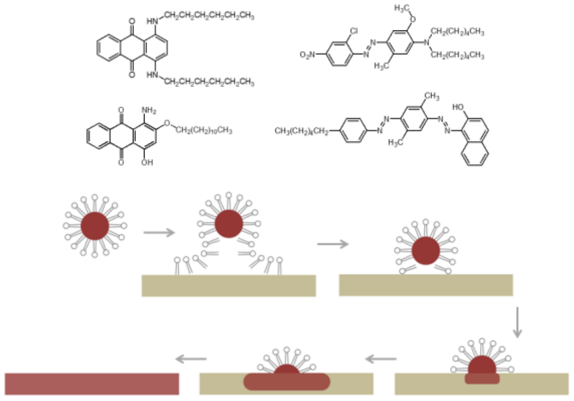

Figure 1: Fomation of vesicles of double-tained cationic surfactants containing super hydrophobic materials inside and releasing process of them toward extremely hydrophobic polyethylene polymer in an aqueous medium.

References:

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Enhanced Barrier Property of Poly(vinyl chloride) Film by Nanoconfinement effects of graphene oxide nanoribbons

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Abstract:

Considerable effort has been put in to designing better performance reinforcements for polymer composites, in order to make more lightweight, strong and thermo-stable polymer-based materials. Nanostructured carbon-based materials such as carbon nanotubes (CNTs) and graphene have attracted much attention as the reinforcement due to their outstanding physical properties and peculiar morphologies with high aspect ratio. In particular, graphene oxide nanoribbons (GONRs) fabricated by unzipping of CNTs have advantages of both CNTs and graphene as a reinforcement for polymer composites, such as low percolation threshold, large interfacial area and numerous edge sites with functional groups. In contrast, the chemically prepared GONRs possess numerous topological defects and multitudinous heteroatoms, which deteriorating their physical properties. Nevertheless, remarkable reinforcing effects of GONRs in polymer matrix were confirmed in the previous reports, and these results suggest that the significant enhancement of polymer properties by adding GONRs could be induced by indirect reinforcing behaviors rather than originate from a significant property gap between polymer matrix and GONRs.

In this study, we report a unusual indirect reinforcing phenomenon of highly defective graphene-based nanocarbons dispersed in poly(vinyl chloride) (PVC) matrix via densification of polymer packing originating from nanoscale confinement. Herein, chemically reduced graphene oxide nanoribbons (C-rGONRs) is employed as a nanofiller. The inclusion of defective and oxygen-functionalized C-rGONRs resulted in a dramatic densification of PVC host with extremely low C-rGONRs loading, largely exceeding the theoretical calculation from a rule of mixture. Along with the densification, glass transition temperature of PVC also increased by 28.6 °C at 0.1 wt.% filler loading. Remarkably, oxygen barrier property and mechanical toughness in tension of the PVC/C-rGONRs nanocomposite are maximized when the largest densification occurs. The structure-property relations of the nanocomposites will be discussed with an emphasis on the nanoscale confinement phenomenon.

Keywords: poly(vinyl chloride), gas barrier, nanoconfinement effect, nanocomposite, graphene oxide nanoribbon, carbon nanotube

References:

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Fabrication of polyaniline-graphene/polyvinyl alcohol nanocomposites for flexible gas sensor

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Abstract:

This correspondence presents the fabrication of a polyaniline-graphene (PANI-G) nanocomposite-coated polystyrene (PS) nanofiber mat for the purpose of generating a flexible and highly sensitive gas sensor. Preparation of the PANI-G nanocomposite and its deposition on the surface of the nanofiber mat were performed via in-situ chemical polymerization. The surface morphology of the prepared flexible films was investigated using SEM, AFM, and profilometry. Morphology studies reveal that the PANI-G nanocomposite forms a uniform coating on the surface of PS. Chemical properties analysis, carried out by FTIR and XRD, revealed the formation of a chemical interaction between the nanocomposites and the polymer fiber surface. The TGA study showed an increase in the thermal stability of the coated polymer fibers compared to the pure fibers. The effect of humidity on the nanocomposites was evaluated by checking the electrical resistivity at different humidity values. Adding the composite increased the electrical conductivity of the coated sample by the ninth order. The nanocomposite-coated PS flexible film was tested for its use in a sensor for carbon dioxide gas (20-100 ppm). Due to the higher surface area, the film shows a high sensitivity towards carbon dioxide gas; as the gas concentration increases the surface resistivity also increases. At the same time, the gas sensor shows good repeatability, low response time, and low recovery time.

Keywords: Nanocomposite, Electrospin nanofiber, insitu chemical polymerization, flexible thinfilm, gas sensor,

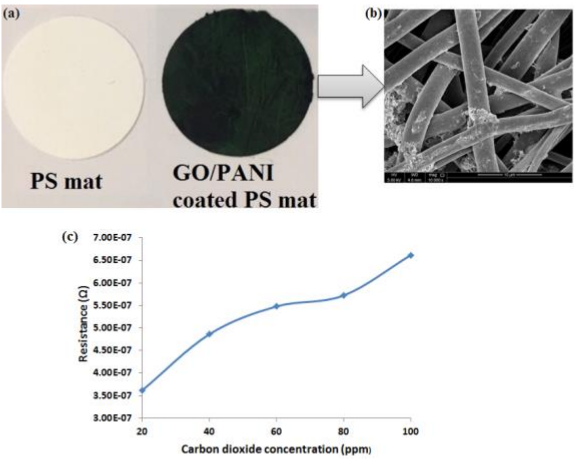

Figure 1: (a) Figure illustrating optical image of PS membrane, and PANI-G coated PS membrane, (b) SEM image of nanocomposite coated PS membrane, (d) Plot showing resistance as a function of carbon dioxide concentrations.

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Natural Polymer Gate Dielectrics for Low-voltage Organic Thin Film Transistors

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Abstract:

Natural polymer materials have excellent inimitable properties and are environmentally friendly. Natural polymers include cellulose, starch, protein, enzyme, and rubber. Of these, urushiol is suitable as an environmentally friendly gate dielectric material. The hydroxyl-rich, natural, unsaturated hydrocarbon resin Urushiol easily forms a dense thin film that can be useful in gate dielectrics. Urushiol film were fabricated by easy spin coating and thermal curing process (100 °C, 30 min) and gave a smooth surface ($R_q \sim 0.3$ nm) with a hydrophobic nature (44.6 mJ/m^2); Thermal curing of urushiol is possible due to unsaturated double bonds of long hydrocarbon side chains, unlike other catechol derivatives. The leakage current density values remained stable (5×10^{-8} A / cm^2 to -3 V). The thin urushiol gate dielectric OFETs exhibited good transfer and output characteristics with mobility of 0.07 cm^2 / Vs and negligible hysteresis (+2 ~ -3 V). This research are possible numerous opportunities in the field of gate materials and electronics, as well as on earth-rich materials and eco-friendly products.

Gas molecule sensing of van der Waals tunnel field effect transistors

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Abstract:

Van der Waals (vdW) heterostructures with two-dimensional (2D) crystals such as graphene, hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDCs) allow us to demonstrate atomically thin field-effect transistors (FETs), photodetectors (PDs) and photovoltaic devices capable of higher performance and greater stability levels than conventional devices. Although there have been studies of gas molecule sensing with 2D crystal channels, vdW heterostructures based on 2D crystals have not been employed thus far. Here, utilizing graphene/WS2/graphene (G/WS2/G) vdW heterostructure tunnel FETs, we demonstrate the rectification behavior of the sensitivity signal by tuning the WS2 potential barriers as a function of the gas molecule concentration and devise a fingerprint map of the sensitivity variation corresponding to an individual ratio of two different molecules in a gas mixture. Because the separation of different gas molecule concentrations from gas mixtures is in high demand in the gas-sensing research field, this result will greatly assist in the progress on selective gas sensing

Keywords: Van der Waals heterostructure, two-dimensional materials, field effect transistor, gas sensor

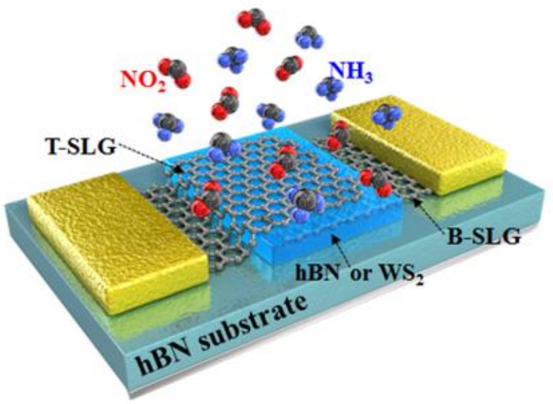

Figure 1: Schematic diagram of the tunnelling G/hBN/G or G/WS_2/G field effect transistor used for sensing the concentration ratio between donor(NH_3) and acceptor(NO_2) types of molecules in a gas mixture condition.

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Preparation and Luminescence of $(Ba,Sr)_{1.3}Ca_{0.7}SiO_4$:$Eu^{2+}$,$Mn^{2+}$, Dy^{3+} powders for Warm White Light-Emitting Diodes

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Abstract:

Multi-color-emitting phosphors with a single phase can be obtained by doping multi-activators and are useful for use in phosphor-conversion white light-emitting diodes. For example, Eu^{2+} and Mn^{2+} co-doping is well known to be suitable for multiple-photoluminescence (PL). In this study, we prepared $(Ba,Sr)_{1.3}Ca_{0.7}SiO_4$:$Eu^{2+}$,$Mn^{2+}$,$Dy^{3+}$ powders using a sol-gel-combustion process, and then investigated the effects of Sr^{2+} and Dy^{3+} substitutions on the PL properties of the powders. The PL spectra consisted of the green and red emission bands, which originated from Eu^{2+} and Mn^{2+} ions, respectively. Upon adjusting the ratio of Eu^{2+} to Mn^{2+} content, the green and red emission intensity varied in the opposite way from each other, confirming that the red emission occurred via an energy transfer from Eu^{2+} to Mn^{2+}. The substitution of smaller Sr^{2+} ions for Ba^{2+} ions caused a shift of the wavelengths of the red band toward the longer wavelengths, affecting the CIE chromaticity coordinates located in the warm white regions. The phosphorescence properties of the red emission band were also studied by co-doping Dy^{3+} ions.

Keywords: silicate, phosphors, sol-gel, luminescence, white light-emitting diodes, energy transfer.

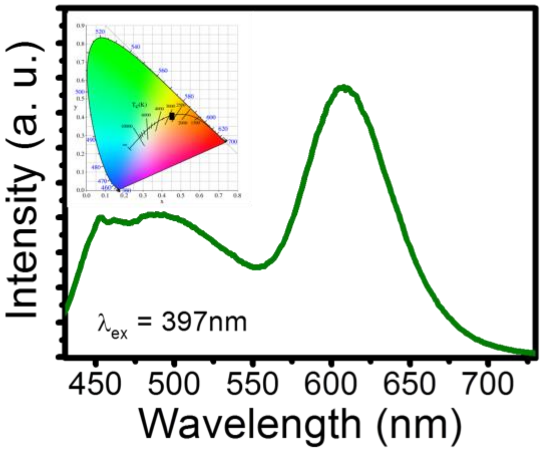

Figure 1: Photoluminescence spectra of $(Ba,Sr)_{1.3}Ca_{0.7}SiO_4$:$Eu^{2+}$,$Mn^{2+}$ phosphors. (Inset: CIE chromaticity coordinates)

References:

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Reliability of pre-deformed flexible-printed electrodes by silver nano-particle inks under temperature and humidity conditions

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Abstract:

Printed electronics is an emerging technology suitable for manufacturing the flexible electronics devices used for IoT and wearable applications. For the commercialization of these products by printed electronics technology, the reliability should be acquired. The reliability of devices in environmental conditions for temperature and humidity should be guaranteed. Moreover, the flexible devices can be used in the deformed state under various loading. Therefore, as a simple example of flexible-printed device, the result of reliability tests of pre-deformed printed electrodes on PET film under various temperature and humidity conditions by silver nano-particle inks is presented. For this study, the test apparatus for mechanical loading as well as environmental chamber capable of changing temperature and humidity is developed as shown in Fig.1. The test apparatus consists of several motors to give various kinds of deformations to the flexible electrodes such as bending, twisting, and shear. The environmental camber can adapt the temperature from 5℃ to 90℃ and humidity from 20% to 90%.as shown in Fig.1. Figure 2 shows the examples of test results for two cases of (a) non-deformation and (b) twisting load of 60degrees. As shown in these figure, even in the case of non-deformation, the resistance of electrodes increases with increase of temperature: about 8% during 20°C change. For the twisting load, the resistance increases by about 12% during 20°C change. The higher the humidity, the higher the increase of resistance as well. Therefore, we can conclude that even simple printed electrodes by silver nano-particle inks are very sensitive to temperature and humidity, moreover, the pre-deformation makes worse this effect.

Keywords: printed electronics, silver nano-particle inks, electrodes, reliability, deformation, temperature, humidity

Figure 1: The test apparatus is located inside the environmental chamber which can change the temperature and humidity.

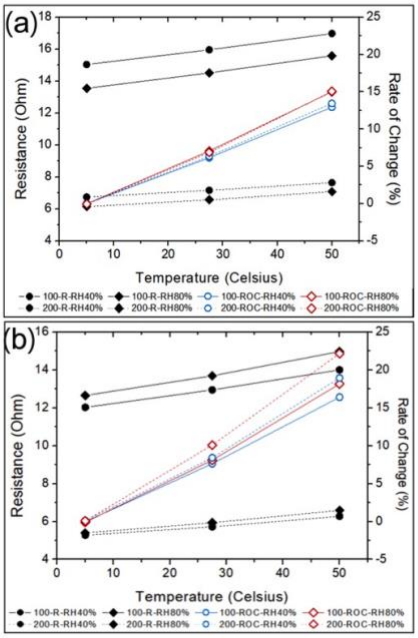

Figure 2: Results of environmental tests for printed electrodes under (a) non-deformation and (b) twisting load

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Influence of dispersion solvent in catalyst ink of polymer electrolyte membrane fuel cell on Ionomer distribution

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Abstract:

In this work, we study the influence of the dispersion solvents contained in the three DPG (Dipropylene glycol)/water mixture solutions containing 100, 50 and 0 wt. % contents of DPG on the morphology and distribution of ionomers using molecular dynamics (MD) simulations. Increasing the proportion of water in solvent leads to a gradual decrease in the Rg of the Nafion ionomer due to strong backbone hydrophobicity of the Nafion ionomer.

The solvation energies of the Nafion ionomers in the solvents indicated that a higher water content in the DPG/water mixture solvent results in the aggregation of the Nafion ionomer and subsequently aggravation of uniform dispersion in solvents. Moreover, the analysis of radial distribution functions (RDFs) reveals that the backbones (-CF_2CF_2-) in the Nafion ionomer are primarily enclosed with the DPG molecules, whereas the sulfonic acid groups (SO_3^-) of side chains mostly interacted with the water molecules because of the hydrophilic-hydrophobic property of ionomer.

Keywords: molecular dynamics, fuel cell, polymer membrance, ionomer, dispersion, solvent, distribution, catalyst ink, atomistic simulation, solvation energy, radius of gyration, radial distribution function

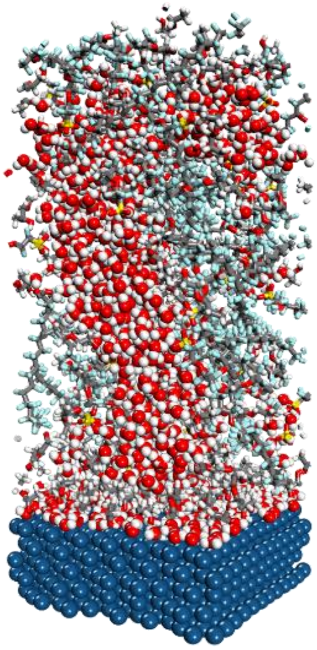

Figure 1. Model of Nafion ionomers in solvent on Pt catalyst. White, grey, red, cyan, yellow, navy color represent hydrogen, carbon, oxygen, fluorine, sulfur, platinum, repectively.

Acknowledgement:
This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (Nos. NRF-2016M1A2A2937151 and NRF-2015M1A2A2057129).

Influence of the Ti_xAl_y/a-Si:H Interlayer on the Adhesion of DLC Coatings on Stainless Steel Substrates

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Abstract:

Diamond-like carbon (DLC) coatings have been applied in several industrial applications due to their attractive properties such as high hardness, low coefficients of friction, high wear and corrosion protection, among others. Nevertheless, these coatings have a low adhesion on metal substrates (principally on steel alloys). This low adhesion is basically due to two reasons: the difference in coefficient of thermal expansion between the substrates and the DLC coatings and the high residual stresses in coatings. In order to increase the adherence of the DLC coatings on the steel surfaces, several techniques have been applied: surface thermal treatments to the substrates, doping the DLC with particles that decrease the residual stresses but lead to the reduction of the hardness of the DLC, and using several thin layers. Interlayers deposited using the sputtering techniques have been used in order to obtain high adhesion of DLC coatings on steel surfaces. In several papers, interlayers of Cr, Ti and others pure metallic elements were deposited using reactive sputtering techniques to improve the adherence of the DLC on different metallic surfaces. In this study, the influence of a single thin Ti_xAl_y/a-Si;H interlayer on the adhesion of DLC coatings on AISI 316L stainless steel substrate was investigated. The Ti_xAl_y coatings were deposited using a sputtering system, while the a-Si:H interlayer and DLC coatings were synthetized using a modified asymmetrical bipolar pulsed-DC PECVD system with an active screen. This additional cathode was used in order to accomplish plasma densification, while the active screen and the cathode were subjected to the same bias voltage. Thin Ti_xAl_y/a-Si;H interlayer produced a gradual change in the thermal expansion coefficients and contributed to reduce stress in the DLC coatings. The adhesion was analyzed using a conventional scratch test through a critical load measurement, using the Rockwell-C indenter. The applied load varied from 1 to 50 N, with a sliding distance of 5 mm and speed of 0.1 mm/s. The Lc1 and Lc2 critical load values were determined. SEM micrograph of the DLC surface deposited on steel substrate after the scratch test is presented in Figure 1. From the figure, it can see that high value of Lc1 of about 24 N and Lc2 approximately of 44 N were measured.

Keywords: DLC coating, stainless steel, adherence, interlayer, pulsed-DC PECVD, active screen, sputtering, scrach test.

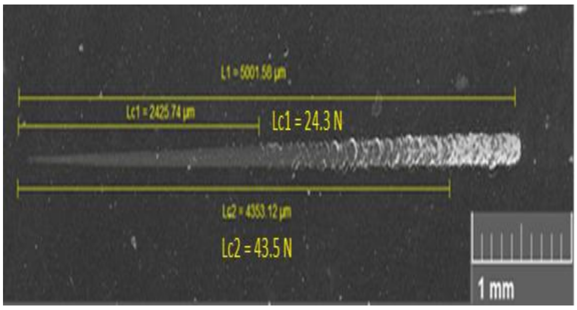

Figure 1: SEM micrograph of the DLC surface deposited on steel substrate after the scratch test.

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Nanoporous anodic alumina membrane modified with Chitosan and copper nanoparticles and its use as three-dimensional matrix for the degradation of the industrial dye Methylene Blue

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Abstract:
In recent years, there has been a tremendous development carried out in the shape and size selective synthesis of nano and microparticles because of their extraordinary and unique physicochemical properties

As a result of the diverse structures and properties of copper oxide nanoparticles, it is considered as an interesting material in modern research due to their applications in solar-energy conversion, magnetic storage, and gas sensors, DNA biosensor, lithium ion batteries, catalysis, cancer therapeutic and antimicrobial agent, hydrogen generation electronics, optics and electro-catalysis [1].

There are some recent reports on a successful synthesis of Cu-NPs using the biopolymer chitosan as a reducing and capping agent. It´s been reported that Chitosan acts as a stabilizer and has the ability to chelate metals, which makes a perfect material for Cu-NPs synthesis. The applicability of metal nanoparticles can show some drawbacks and limitations, mainly due to the tendency of aggregation and precipitation presented by these particles, especially in aqueous medium. One of the most promising strategies to solve this issue consists in the development of solid supports to immoblize and stabilize the nanoparticles. Also, nanoparticles supported into solid supports are easily recovered and recycled [2].

Nanoporous alumina membranes have important advantages, which make it an ideal material for the study of three-dimensional arrays. In the present work, we study the modification of nanoporous alumina membranes with Chitosan and copper nanoparticles for their use as catalytic support in degradation reactions of industrial dyes. These characteristics are expected to be highly attractive from both academic and industrial perspectives.

Keywords: Copper nanoparticles, Chitosan, nanoporous anodic alumina membrane

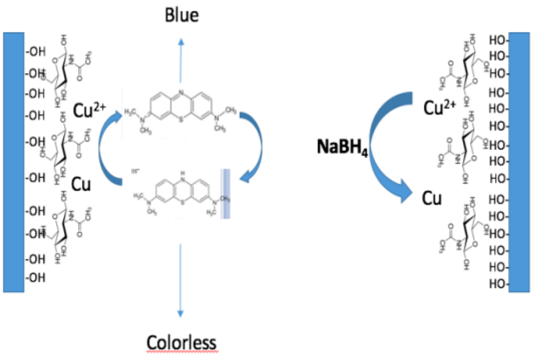

Figure 1: Squematic representation of anodic nanoporous alumina membrane modified with Chitosan and copper nanoparticles and their use as tridimentional array for the degradation of industrial dye Methylene blue.

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Effects of Halloysite on Morphological and Properties of Poly(3-hydroxybutyrate-co-3-hydroxyvalerate)/ Poly(butylene succinate) Blends

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Abstract:

In recent years, different types of biodegradable polymers have attracted much attention for developing various new polymeric materials with reduced environmental impacts. Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) is one of the most widely studied PHA polymers due to its potential use in packaging, automotive, biomedical, and agricultural applications. However, PHBV shows some drawbacks such as its high crystallinity and brittleness and difficulty in melt precessing. Blending PHBV with other polymers such as poly(butylene succinate) (PBS) represent interesting routes to control the properties of PHBV. PBS has good thermal and mechanical properties. It can be processed easily and it is thus a good candidate for blending with PHBV. This work carried out deals with the characterization of nanobiocomposites with PHBV/HNT and PBS/HNT prepared by melt blending. The morphological study showed through scanning electron microscopy that HNT was partially dispersed in the two polymers with the presence of some individual nanotubes in PBS. The presence of HNT in the PHBV does not modify the crystallization and the melting temperature contrary to an increase in the glass transition temperature Tg and the degree of crystallinity of the nanobiocomposite. In the case of PBS, the results indicate that the glass transition and melting temperature are not influenced by the addition of HNT, whereas an increase of the crystallinity temperature and the degree of Crystallinity with the introduction of the nanoparticules are obtained. Thermogravimetric analysis (TGA) releaved that the presence of halloysite decrease the thermal stability of the PHBV and PBS. A decrease of the thermal stability of the nanocomposite PHBV/ PBS/HNT compared to the neat blend was also observed.

Keywords: nanocomposites, Halloysite, Blends, thermal properties, morphology

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Biofunctionalized nanoscintillator for medical applications

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Abstract:

Applications of scintillating materials in medicine involve, in particular, imaging systems for medical diagnostics and medical therapy. X-ray induced photodynamic therapy (PDTX) uses tumor-destroying agents based on scintillating nanoparticles conjugated with photosensitizer molecules. The agent accumulates preferentially in the target cells. Subsequent external X-ray irradiation excites the scintillating nanoparticles, emitting secondary radiation, which activates the photosensitizer molecules [1]. Their deexcitation via non-radiative energy transfer leads to the production of the reactive oxygen species, where the singlet oxygen is believed to be the most cytotoxic. To observe a cytotoxic effect at therapeutic radiation doses, the light yield of scintillating nanoparticle, the efficiency of energy transfer to the photosensitizer and the cellular uptake of the nanoparticles, all need to be fairly well optimized [2].

We prepare highly prospective core-shell nanocomposites for PDTX based on $Lu_3Al_5O_{12}$:Pr^{3+} scintillating cores. The core is synthesized by the UV photochemical method [3], coated by amorphous silica using the sol-gel technique and biofuncionalized by attachment of the protoporphyrin IX (PpIX) molecules, acting as photosensitizers. Resulting three layer nanocomposite features uniform shell covering intensely luminescent core. We study luminescence and scintillation properties of prepared nanocomposites. Room temperature radioluminescence spectra as well as photoluminescence steady-state and time resolved spectra of the material confirm the non-radiative energy transfer from the core to the PpIX outer layer. The singlet oxygen generation in the system is demonstrated by the 3′-(p-aminophenyl) fluorescein (APF) chemical probe sensitive to the singlet oxygen presence. Quenching studies, using NaN_3 as an $^1O_2$ inhibitor, both additionally confirm the presence of $^1O_2$ in the system and rule out the parasitic reaction with OH radicals. Observed features of nanocomposite studied indicate its considerable potential for PDTX application.

Keywords: nanocomposites, bioconjugates, photodynamic therpay, scintillator, singlet oxygen, biomedical applications.

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Properties evaluation of Cu-based composite material by electroless plating

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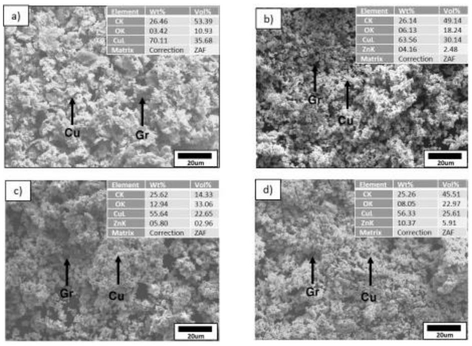
Abstract:

In this paper, Cu-coated graphite sintered body having high thermal conductivity was fabricated using electroless plating and pulsed current activated sintering process. First, 4 g of coarsening graphite powders, which was treated using an activation and wetting process, was added to an aqueous solution of copper (Cu) sulfate; also, 35 g of zinc (Zn) powders was added as a transposition solvent to the aqueous solution and stirred for 1 h for a transposition reaction. After the addition of the fabricated powders mixture to a 75 wt.% DI water : 10 wt.% H_3PO_4 : 10 wt.% H_2SO_4 : 5 wt.% mixture, tartaric acid was added to the aqueous solution to produce a passivating oxide film, followed by a drying for 24 h. The low-intensity oxide peak of the XRD pattern of the fabricated powders was due to the suitable Zn powder content. With the use of the Cu-coated graphite powder, direction control of graphite powder was carried out for high thermal conductivity. Cu-coated graphite sintered bodies were fabricated using a pulsed current activated sintering (PCAS) process. The Cu-graphite sintered bodies were sintered at 850℃ with heating rate each of step at 20 and 30℃/min, respectively. The Cu-coated graphite powders and sintered-bodies were evaluated using FE-SEM, EDS, XRD, TEM, particle analysis, Archimedes method.

Keywords: Electroless plating, Cu-coated graphite, Microstructures, Thermal conductivity, Electric conductivity



Element	Wt%	Vol%
CK	26.46	53.39
OK	03.42	10.93
CuL	70.11	35.68
Matrix	Correction	ZAF

Element	Wt%	Vol%
CK	26.14	49.14
OK	06.13	18.24
CuL	63.56	30.14
ZnK	04.16	2.48
Matrix	Correction	ZAF

Element	Wt%	Vol%
CK	25.62	14.33
OK	12.94	33.06
CuL	55.64	22.65
ZnK	05.80	02.96
Matrix	Correction	ZAF

Element	Wt%	Vol%
CK	25.26	45.51
OK	08.05	22.97
CuL	56.33	25.61
ZnK	10.37	5.91
Matrix	Correction	ZAF

Figure 1: FE-SEM images of Cu-coated graphite powders at different Zn contents; a) 24wt.%Zn, b) 40wt.%Zn, c) 45wt.% Zn and d) 50wt.% Zn

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Property evaluation of Ti-based target materials and their nitride nanocomposites coating layer

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Abstract:

To form a TiAlSiWN hard coating layer, Ti, Al, Si and W powders were mechanically alloyed and refined, TiAlSi and TiAlSiW coating targets were fabricated in a single process and in a short time from the PCAS process using the optimal sintering conditions. The coating targets were deposited on the WC substrate to form the coating layers of TiAlSiN and TiAlSiWN nitride nano-composite by applying the
AIP process.

The properties of the nitride nano-composite coating layers were compared in accordance with addition of W. In nitride nano-composite coating layer, the micro structural properties were analyzed, focusing on the distribution of crystalline phases and amorphous phases(Si_3N_4) and growth orientation of the columnar crystal depending on the addition of W. The mechanical properties of the coating layers were represented a hardness of approximately 3,000 kg/mm^2 and an adhesion of about 117.77 N in the TiAlSiN. In particular, at the TiAlSiWN showed excellent properties a hardness of more than 4,300 kg/mm^2 and an adhesion of about 181.47 N.

Keywords: Pulsed current activated sintering process, Mechanical alloying, TiAlSiW composites, Nano-composite materials, Arc ion plating

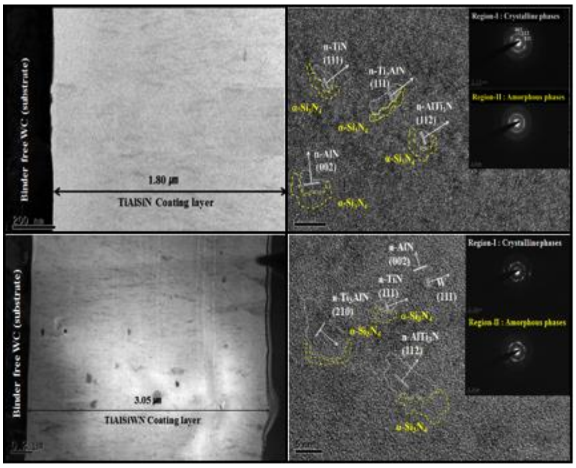

Figure 1: TEM images of TiAlSiN and TiAlSiWN coated layer : a) BF images of TiAlSiN, b) HR-TEM images and SAED patterns of TiAlSiN, c) BF images of TiAlSiWN and d) HR-TEM images and SAED patterns of TiAlSiWN

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Posters Session II: NanoBioMedecine / Nanosafety

Conductance measurements in Laponite-stabilized internally self-assembled particles in water.

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Abstract:

We showed the possibility of creating a dense cover around lipid-based liquid crystalline droplets using laponite nanoplatelets as stabilizer [1]. This is an interesting route for the design of new Colloid-ISAsome assemblies in which dense protective armours could be advantageous such as controlled delivery. The investigation of the structural by means of CRYO-TEM microscopy, DLS, and SANS with contrast variation conditions have been determined [2-4]. Herein, we use conductivity measurements as trigger to deduce the ratio between the free and the adsorbed laponite-stabilizer. Phytantriol (PT) is used as the lipid to create the nanostructured drops. The conductivity measurements have been performed in AC conditions (ranging from 60 Hz to 600 KHz) in order to check out the electrical response of the soft materials. The results help in understanding the concentration of free stabilizer which is requisite for further applications since this could have an important influence on the properties of such complex and interesting smart assemblies.

Keywords: laponite, nanoemulsions, active molecules, colloidal particules, cubosome, lipid, colloid, conductivity

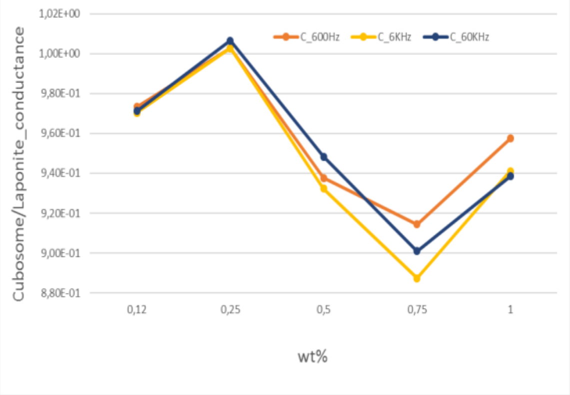

Figure 1: Figure illustrating laponite contribution in Cubosome conductance for f=600Hz, 60Hz and 60kHz.

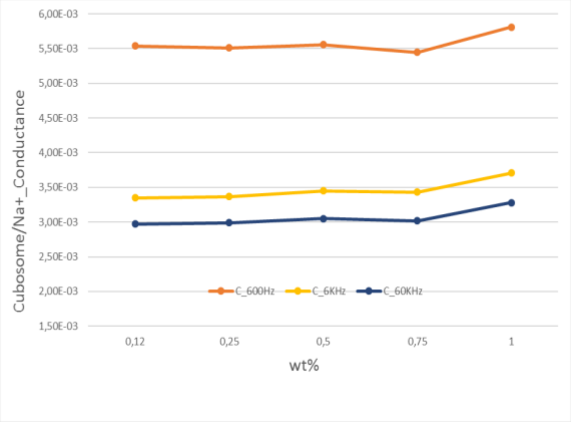

Figure 2: Figure illustrating Na+ contribution in cubosome solution for f=600Hz, 60Hz and 60kHz.

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Capture and growth of cells on the ligand modified polystyrene chips coated with agarose and agarose/gelatin

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Abstract:
Agarose gel can be used for 3D cell culture since it prevents cell attachment. The dried agarose film coated plate also allowed 3D growth of cancer cells. Agarose or agarose/gelatin film was coated on oxygen-plasma treated polystyrene chips. The sugar moieties of agarose were modified to aldehyde groups by periodate treatment. Poly-D-lysine (PL) was directly immobilized to the aldehyde group. The aldehyde-activated chips were further modified to maleimide groups for covalent attachment of the photoactivatable Fc-specific antibody binding protein (PFcBPs) and laminin-derived peptide (LDP) with terminal cysteine residues. The antibodies were covalently photocrosslinked onto the PFcBP-modified chips upon UV irradiation. The antibody modified chips with agarose coating could efficiently capture the target cells without nonspecific binding, and most captured cells grew 3D (spheroid) modes. The captured cells captured on the PL-modified also displayed 3D growing mode. In contrast, LDP modification of the agarose film slightly allowed the attached 2D (fibroblast) growth, even though most cells still showed 3D growth. No modified agarose/gelatin film showed almost no cell binding. In contrast, modification of antibody, LDP or PL induced efficient cell capture, and induced the 2D and 3D growth of captured cells. Although the gelatin film surface alone is not sufficient to induce attached cell growth, it may provide a synergistic effect for attached growth of the ligand captured cells. The ligand-modified agarose/gelatin film will be useful for 2D and 3D cultures of various cells.

Keywords: Agarose/gelatin film coating, Surface modification with ligands, 2D and 3D cell growth.

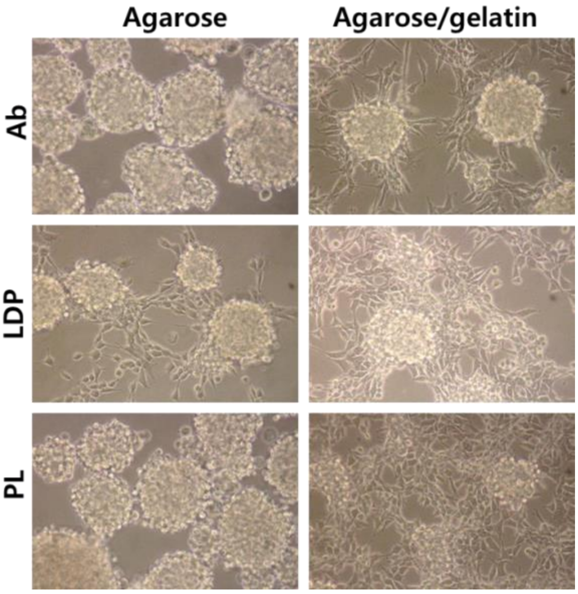

Figure: Cell growth of the ligand captured cells on the agarose or agarose/gelatin coated polystyrene chips. NIH-6T6.7 cells were captured on the indicated chips, and cell growing modes were analyzed using phase-contrast microscope at a 200x magnitude. Ab: anti-HER2 monoclonal antibody, LDP: laminin-derived peptide, and PL: poly-D-lysine.

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Selective Claudin-4 Targeting of Clostridium Perfringens Enterotoxin (CPE)-conjugated Poly-sialic acid Nanoparticles for effective pancreatic cancer therapy

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Abstract:

Recently, the advances of nanotechnology has led to the development of cancer diagnosis and treatment. However, pancreatic cancer is still remain to be difficult to treatment due to its aggressive growth and rapid development of metastasis. Moreover, the complexity of the microenvironment of pancreatic cancer reduces the efficiency of drug delivery with nanoparticles. To overcome these problems, there are many studies of biomarkers that can target pancreatic cancer. One of them, Claudin-4, which is known to overexpress pancreatic cancer, can be targeted to increase drug delivery efficiency. To target Claudin-4, Clostridium Perfringens Enterotoxin (CPE) was conjugated with the poly-sialic acid based nanoparticles (HPSA), which accumulated about 2.5 folds in pancreatic cancer compared to non-conjugated nanoparticles **(Figure 1**). CPE-conjugated HPSA (CHPSA) successfully delivered the drug (Doxorubicin) to pancreatic cancer and inhibited the progression of cancer. This study introduced a new method for the treatment of pancreatic cancer using nanoparticles.

Keywords: Poly-sialic acid nanoparticles, Claudin-4, Clostridium Perfringens Enterotoxin (CPE), pancreas cancer, Tumor targeting, Pancreas targeting

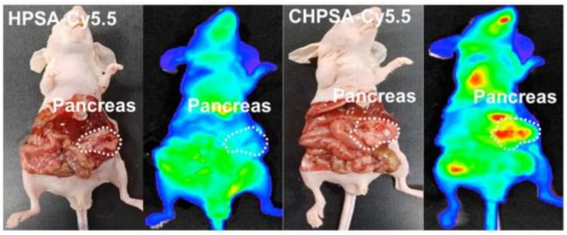

Figure 1: Targeting effects of Clostridium Perfringens Enterotoxin (CPE)-conjugated nanoparticles on pancreatic cancer. CPE-conjugated poly-sialic acid nanoparticles (CHPSA) has accumulated about 2.5 folds more in pancreatic cancer than non-conjugated nanoparticles (HPSA).

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Silver-Polyvinyl Pyrrolidone (Ag-PVP) Nanoparticles Exhibit Antibacterial Activity against *Chlamydia muridarum* in Mouse J774 Macrophages

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Abstract:

Infection with *Chlamydia trachomatis*, the most sexually transmitted bacterial diseases globally, often lead to pelvic inflammatory disease and infertility in women and sterility in men without early intervention. With growing reports of clinical isolates exhibiting resistance to antibiotics we need alternative treatment strategies. We previously published that silver-polyvinyl pyrrolidone (Ag-PVP) nanoparticles exerted anti-inflammatory actions in mouse macrophages by inhibiting several inflammatory mediators. We hypothesize that Ag-PVP anti-inflammatory action on *C. muridarum*-induced inflammation is due to its capacity to reduce bacterial replication in cells. Mouse J774 macrophages were exposed to various concentrations of 10 nm Ag-PVP (3-12 μg/mL) and infected with *C. muridarum* at a multiplicity of infection (MOI) of 0.05 to 0.4 for up to 48 hr. We used TaqMan qRT-PCR to quantify the mRNA gene expression of *C. muridarim* major outer membrane protein (MOMP) as a marker of bacterial load. Our qRT-PCR data showed that Ag-PVP reduced MOMP expression by 70% with no toxicity to cells at all tested concentrations of Ag-PVP, suggesting that nanoparticles potentially reduced chlamydial bacterial load in macrophages. We further demonstrated by immunofluorescence microscopy that Ag-PVP markedly reduced *C. muridarum* inclusions forming units (IFUs) in infected macrophages. Our data shows that the ability of Ag-PVP to inhibit *C. muridarum* bacterial load maybe a potential mechanism of its anti-inflammatory actions in macrophages.

Keywords: Ag-PVP nanoparticles, mouse J774 macrophages nopartilces, TaqMan qPCR,

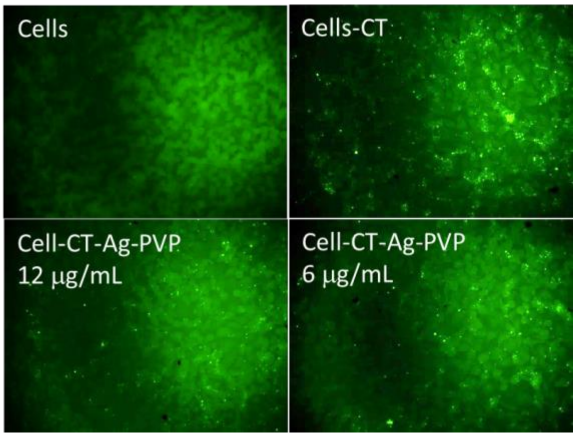

Figure 1: Imunofluorescence microscopy shows that Ag-PVP reduces chlamydial bacterial load (green fluorescences) in macrophages.

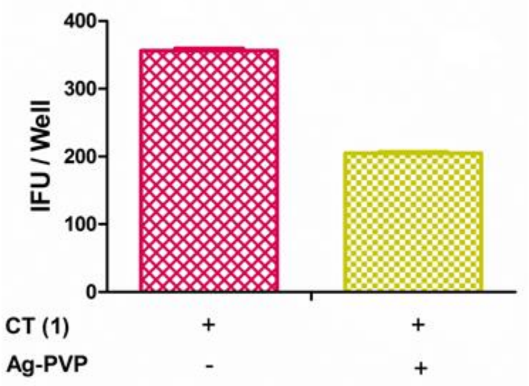

Figure 2: Ag-PVP reduces the numbers of *C. muridarum* inclusions forming units (IFU) in infected macrophages.

Reference

Yilma AN, Singh SR, Dixit S, Dennis VA. Anti-inflammatory effects of silver-polyvinyl pyrrolidone (Ag-PVP) nanoparticles in mouse macrophages infected with live *Chlamydia trachomatis*. Int J Nanomedicine. 2013;8:2421-32. doi: 10.2147/IJN.S44090.

Numerical optimization of the carboplatin encapsulation into Boron Nitride nanotubes

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Abstract:
Since several years, drug-delivery systems are widely investigated through many different applications. Among them, Carbon nanotubes (CNT) have gained significant interest thanks to their "unique" properties, but were also limited for medical usages due to important cytotoxic effects. Boron Nitride nanotubes (BNNT) are analog to CNT in terms of physical properties but are well suited for biocompatibility, making them very promising substitution candidates to be used as nanovector for cell therapy.

In order to develop news drug nanocarriers using BNNT, we report here a full numerical study of the encapsulation of Carboplatin, a common anticancer drug, inside BNNTs. For this purpose, we used armchair BNNT of five differents radii, ranging from 5,5 to 11Å.

Both molecular dynamic (MD) and density functional theory (DFT) simulations were used providing complementary informations.

DFT simulations allowed us to investigate chemical reactivity between the drug and its nanovector and to study potential barriers at the entrances of the BNNT. We showed that no chemical bonding was possible during the simulation. Moreove, these entrance barriers were proved to at best inexistent, at worst negligible. Manual exploration of the most favorable configurations also gave us an estimation of the potential wheel depth when the molecule is encapsulated in the nanotube.

Then, to simulate a realistic biological environment for the nanovector, MD were conducted in a water solvent. Both outside and encapsulated adsorptions were considered for the different systems. Our results were also compared with similar simulations on CNTs to highlight the differences between these two different nanostructures. This allows us opening the discussion about how BNNTs can be used efficacy for drug targetting purpose.

Keywords: Boron Nitride Nanotube, Carboplatin, Drug delivery system, Nanocarrier, Molecular Dynamic, Density Functional Theory, adsorption energy.

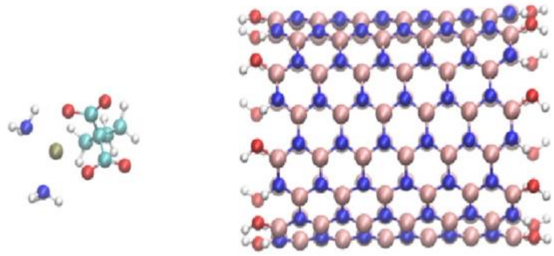

Figure 1: Illustration of the DFTs simulations, showing a Carboplatin molecule on the right and a functionnalized Boron Nitride Nanotube on the right

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A new neural-cell specific peptide for targeted delivery of drug-loaded nanoparticles

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Abstract:

Efficient delivery of therapeutics to the brain is extensively limited by the blood brain barrier (BBB).[1] Cell penetrating peptides have gained recognition for enhancing the uptake of conjugated payloads into various cell types, however the non-specific manner is not suitable for expensive or toxic drugs. The neural cell targeting peptide, rabies virus-derived peptide (RDP), has shown the ability to specifically enable the delivery of a conjugated cargo to the central nervous system *in vivo*.[2]

In taking advantage of the easily modified surface properties of polymeric nanoparticles (NP), we previously reported how RDP, conjugated to poly (lactic-co-glycolic) acid NP, could specifically target a cytotoxic payload into neural cells via the nicotinic acetylcholine receptor (nAChR).[3]

Here we report the optimization of RDP into a new 18-mer peptide, DAS, following *in silico* modelling with the nAChR (Figure 1). The new ligand, DAS, displayed a better stability profile than RDP in human serum at 37°C. DAS retained the ability to selectively enhance the uptake of conjugated doxorubicin-loaded NP in neural cell types only, leading to a larger decrease in cell viability in comparison to untargted NP treatment. This innovative, new targeting peptide may be developed further for application within nanoparticulate drug delivery systems to treat a wide range of neurological disorders.

Keywords: polymeric nanoparticles, peptide targeting, blood brain barrier, drug delivery, neural-specific, nicotinic acetylcholine receptor, rabies virus derived peptide, serum stability.

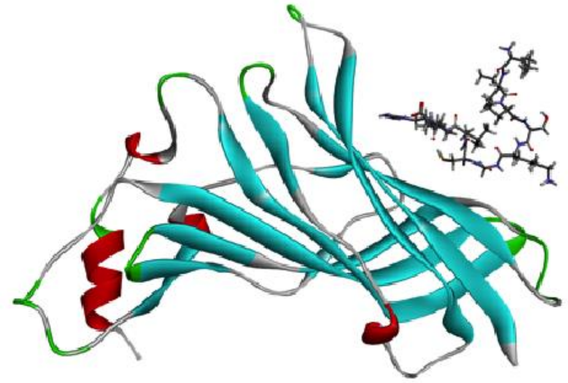

Figure 1: Figure illustrating the molecular dynamics simulation of a fragment from RDP (stick form) with the nicotinic acetyl choline receptor (ribbon form). Residues in contact with the receptor surface were identified and incorporated into a new 18-mer sequence, which would then be tested for serum stability and efficacy as a neural cell-specific targeting ligand.

References:

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Cationized Polymer (*d*CatAlb) Encrusted Nanoformulation enhance chemotherapeutic activity of Doxorubicin

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Abstract:
Aim: Glioblastoma is the most rapaciously growing cancer within brain, wherein an average life span is only 12-15 months with mere 3-5% 5 year survival. Doxorubicin (DOX) is used as a first line anticancer drug in several carcinomas including neuroblastomas. However, due to its hydrophilic nature, blood brain barrier restricts its entry into the brain thereby lowers its bio-efficacy against glioblastoma[1]. Biodegradable poly (lactic-co-glycolic acid (PLGA) polymer provides sustainable drug delivery to glioblastoma [2]. **Methodology:** *d*CatAlb was synthesized by -COOH activation method and characterized by MALDI-TOF and zeta potential. The synthesized *d*CatAlb was then encrusted on DOX-loaded PLGA nanoparticle core (*d*CatAlb-PLGA-DOX NPs) using an optimized one step desolvation protocol. The developed *d*CatAlb-PLGA-DOX NPs was characterized by particle size, surface charge, *in vitro* drug release, pH-dependent activity, cytotoxic study, cellular transport study, hemolytic assay, cellular uptake studies and apoptosis assay using U87MG glioblastoma cancer cell line. The BBB permeation efficacy was evaluated using bEnd.3 cell assay. **Results:** The *d*CatAlb-PLGA-DOX NPs was successfully formulated with an optimum particle size of 156±10.85 nm (surface charge, ʒ, 22±2.1mV) with 27±2.5% drug entrapment. *d*CatAlb-PLGA-DOX NPs showed an unique pH-dependent DOX release profile with rapid burst release under acidic tumor pH conditions. Notably, *d*CatAlb-PLGA-DOX NPs showed higher drug uptake and anticancer activity in U87MG glioblastoma cells. Moreover, a superior trans-epithelial permeation transport of DOX across monolayer bEnd.3 cells was noticed with cationized formulation as compared to the conventional PLGA-DOX NPs formulation. The *d*CatAlb-PLGA-DOX showed a better compatibility as compared to plain DOX as well as PLGA-DOX NPs formulations as evinced from its low hemolysis index.

The developed formulation approach also affirmed higher anticancer activity primarily through caspase-mediated apoptosis mechanism (2.93, 3.16 and 5.346 fold higher level of caspase-3 gene of Dox-solution, PLGA-DOX NPs and dCatAlb-PLGA-DOX NPs respectively; $p<0.05$) when studied in U87MG cells.**Conclusion:** The developed dCatAlb-PLGA-DOX polymeric nanoformulation improves the penetration, cellular uptake, tumor specific drug release potential and offer superior anticancer activity towards glioblastoma therapy. The developed strategy is versatile and can be extended to other nanoplatforms for delivery of other neuroactive compounds, gene therapeutics, diagnostics etc. **Keywords:** Glioblastoma, blood-brain tumor barrier, nanoparticles, PLGA, cationic polymer.

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Self-assembled Polymeric Nanoparticles for Targeting Mitochondrial Complex II

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Abstract:

In drug delivery fields, targeting subcellular compartments (e.g., cytosol, nucleus, and mitochondria) is very significant because therapeutic effects are generating at the subcellular level. Especially, mitochondria-targeting drug delivery systems have garnered more attention with the pivotal roles of the mitochondria (e.g., controlling the homeostasis of vital physiological functions, synthesizing bioenergy molecules, etc.). We focused more on mitochondrial Complex II (succinate dehydrogenase, SDH) because Complex II binds with succinate to tune its intracellular levels and is specifically known as a tumor suppressor in cancer cells. In this study, we designed novel mitochondrial Complex II-targeting polymeric nanoparticles composed of succinated poly(ε-caprolactone) to distinguish mitochondrial Complex II-mediated tumor/non-tumor character and to kill cancerous cells (Figure 1). Succinic anhydride was chemically linked with the hydroxyl group at two ends of low molecular weight poly(ε-caprolactone) (PCL), resulting in succinate-PCL-succinate (snPCL) polymers. The snPCL polymers had an amphiphilic character because of hydrophobic PCL and hydrophilic succinate and were self-assembled in aqueous solutions, constructing snPCL nanoparticles (NPs). The NPs had 30-100 nm in diameter and -40 mV as zeta-potentials. Interestingly, snPCL NPs represented dual targeting characters (pH and receptor) for faster cellular internalization and killed tumor cells but not normal cells, suggesting tumor suppressor-targeting anti-tumor nanodrugs. Specially, snPCL NPs were capable of loading hydrophobic doxorubicin (DOX) as an anti-cancer drug and DOX@snPCL NPs efficiently kill tumor cells. In conclusion, the designed mitochondrial complex II-targeting NPs would have a potential as nanodrugs and drug carriers for adverse effect-free anti-cancer therapy.

Keywords: drug delivery, nanoparticles, mitochondria, mitochondria-targeting, complex II, succinate dehydrogenase, poly(ε-caprolactone), self-assembly, nanodrugs, subcellular targeting, intracellular drug delivery.

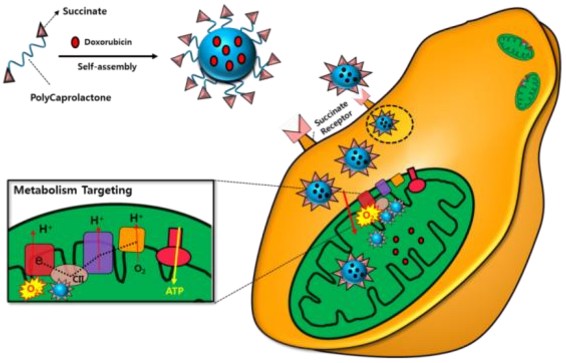

Figure 1: Design concept of mitochondrial metabolism-targeting nanosized drug delivery systems.

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Abstract:

In this study Gold nanoparticles (AuNPs) with an estimate diameter of 25 nm have been synthesized in water using sodium citrate as both reducing and stabilizing agent at high temperature (~95 °C) and in presence of sodium hydroxide. The obtained AuNPs were characterized using ultraviolet-visible spectroscopy (UV-Vis), dynamic light scattering (DLS) and Zeta potential measurements. Additionally, AuNPs were coated with D2B, a monoclonal antibody raised against an extracellular epitope of the human prostate specific membrane antigen (hPSMA), that has been tested in PSMA-prostate cancer xenografts (1). PSMA is expressed on the cell surface of prostate epithelial cells and overexpressed in higher grade carcinomas (2). Interestingly, binding of antibodies to PSMA induces endocytosis of the latter, thereby marking PSMA as a docking site for the delivery of therapeutic agents. To attain a stabilized and a high affinity binding of D2B to AuNPs, the mercapto group (SH) in cysteine of the D2B was used. Moreover, amino groups of the antibody might also help in anchoring the latter onto the negatively charged AuNPs-Citrate surface. The successful attachment of D2B onto AuNPs was confirmed by UV-Vis, DLS and Zeta potential. In fact, as shown in figure 1, addition of D2B to AuNPs-citrate colloidal solution caused a red shift (higher wavelength) by about 15 nm in the UV-Vis spectra, this might be due to the change in the refractive index around the AuNPs as a result to the attachment of D2B onto AuNPs (3); furthermore, dynamic light scattering (DLS) showed an increase in the AuNPs size from ~25 to about ~63 nm as a confirmation of the successful conjugation of AuNPs-Citrate with D2B. On the other hand, Zeta potential measurements revealed an increase from ~ -45 mV for AuNPs-Citrate to -23 mV.

The cytotoxicity of our D2B-AuNPs was circumvented using the WST-1 cell proliferation assay and the agarose gel DNA fragmentation method. Finally, the specific delivery and binding of our customized NPs was tested using flow cytometry and western blot.

Our results pave the way for further research using our coated NPs as vehicles for drug delivery in both in vitro and in vivo models.

Keywords: Gold nanoparticles, antibody, bioconjugation, drug delivery, cellular uptake, prostate cancer, water, biomedical applications.

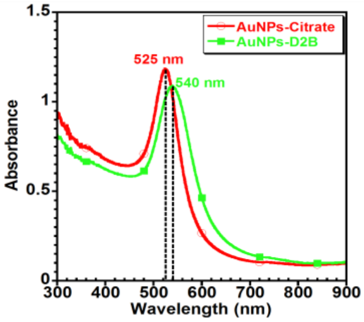

Figure 1. UV-Visible spectra of AuNPs-Citrate (~25 nm) before and after bioconjugation with D2B.

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Exploitation of the liposome-biomolecular corona for early detection of pancreatic cancer

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Abstract:

We developed a novel liposome-enabled blood (LEB) test for pancreatic ductal adenocarcinoma (PDAC) detection. Blood samples from PDAC patients and subjects without malignancy were let to interact with liposomal formulations leading to the formation of a biomolecular corona (BC) at the liposome surface. Protein patterns were characterized by one-dimensional (1D) sodium dodecyl sulphate polyacrylamide gel electrophoresis (SDS PAGE). Densitometry analysis (DA) of electrophoretic gels, followed by principal component analysis (PCA) of DA results distinguished controls and PDAC patients with a total discriminate correctness rate of 90%. As Figure 1 clearly shows, PDAC patients and healthy subjects were strongly separated in the plane of the principal components (PC1, PC2). The LEB test exhibited 85% sensitivity and 100% specificity. The prediction ability of the LEB test was compared with that feasible by means of routine blood testing. To this end, PCA and LDA were replicated using 24 hematological input parameters (e.g. levels of total protein, CEA, CA 19.9 etc.). When the 24 hematological values were used as variables for the PCA, much lower sensitivity and specificity were achieved (60% and 20% respectively). Total correctness decreased to 52%. Our data suggest that exploitation of liposome-BC could be an exciting new tool for early diagnosis of PDAC.

Keywords: biomolecular corona, liposomes, pancreatic cancer, early diagnosis, sodium dodecyl sulphate polyacrylamide gel electrophoresis, principal component analysis.

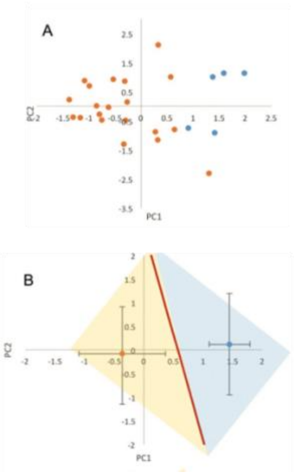

Figure 1. Principal components (PC1, PC2) calculated from SDS PAGE protein profiles. Orange and blue circles refer to the pancreatic cancer and healthy patients, respectively. (B) Centroids of the distributions of panel A. The straight line separates the healthy volunteers group from the pancreatic cancer patients group, according to the results of the linear discriminant analysis (LDA).

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Enhanced Gene Transfection by Multifunctional Properties of Polymeric Vitamins

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Abstract:

Vitamins are well-know as an antioxidant for the removal of reactive oxygen species (ROS) in the cells and has been used to improve cell viability in damaged cells.[1] However, their applications have been limited because of their hydrophilicity, short half-life in blood and/or poor water solubility.[2] In this study, in order to expand their biological applications, polymeric vitamins [poly(ascorbic acid 2’-phosphate) (pAAP) and poly(pyridoxal 5’-phosphate) (pP5P)] were synthesized by a coupling reaction in the presence of EDC. Interestingly, the phosphate groups in the designed polymers buffered protons in the endosomal pHs. Thus, polymeric vitamins were incorporated into nanosized drug carriers to overcome intracellular barriers of polymer-based gene delivery. pAAP- or pP5P-loaded gene complexes showed 100-fold or 20-to-80-fold higher gene transfection efficiency than pAAP- or pP5P-free complexes, respectively. The findings come from multifunctionality of polymeric vitamins. First, the phosphate groups in pP5P represented proton buffering capacity in endosomal pHs, leading to endosomal escape of nanocomplexes. Second, polymeric vitamins promoted nuclear uptake (1.5-to-2-fold higher) of the delivered gene. Third, the anti-oxidant property of polymeric vitamins improved viability (~20%) in ROS-treated cells. Based on these results, the applicability of polymeric vitamins could be extended to an antioxidant, an endosomolytic agent and a nuclear translocation promoter.

Keywords: gene delivery, non-viral vector, polymeric vitamin, endosomolytic materials, nuclear translocation

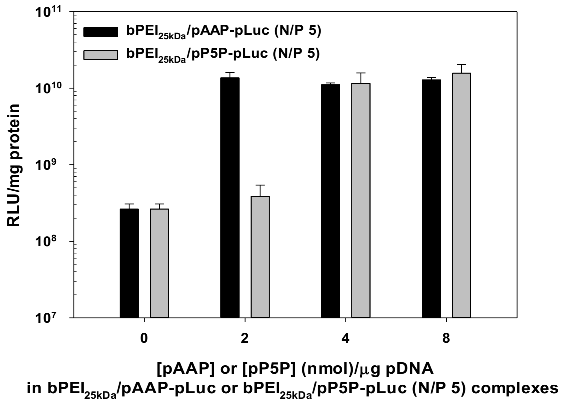

Figure 1: Transfection Efficiency of polymeric vitamins containing gene complexes in HEK293 cells.

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Preparation and physicochemical characterization of nanostructured iron(III) hydroxyphosphates as potential vaccine adjuvants

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Abstract:
Vaccine adjuvants are components of inactivated vaccine formulations that potentiate the immune response against antigens. Widely used adjuvants in routine human vaccinations are aluminium(III) oxyhydroxide and hydroxyphosphate. However, these adjuvants have certain limitations (low efficacy for some antigens, selective induction of Th2 type immune response and ineffective induction of Th1 type cytotoxic immune response, stimulation of eosinophilia, production of specific and total IgE antibodies, etc.) which is the major motivation for the search of alternative adjuvants with better efficacy and safety. In our previous work [1] we studied the physicochemical characteristics of mixed Fe/Al hydroxyphosphates as potential vaccine adjuvants, because ferric-based adjuvants are known to induce both humoral and cytotoxic T-cell response [2], which is advantageous compared to aluminium-based adjuvants. Here, we report on the physicochemical characterisation of nanostructured Fe(III) hydroxyphosphates of various composition as potential ferric-based alternatives of aluminium adjuvants. We synthesized various nanostructured iron(III) hydroxyphosphates with different composition. The obtained materials were characterized for elemental composition, crystal structure, isoelectric points, protein adsorption, and dissolution rate in sodium citrate solution, which are important physicochemical characteristics to be studied in the early adjuvant development stages.

Keywords: iron, phosphate, nanoparticles, vaccines, adjuvants, immune response

References:

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Acknowledgments:
Authors are grateful to Operational programme "Science and Education for Smart Growth", project BG05M2OP001-2.009-0028.

Gold nanoparticle-based colorimetric immunosensor for estradiol

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Abstract:
In recent years, the nanoparticles have stimulated a great scientific interest due to their physical and biochemical properties. The tiny size (1-100 nm) makes them very valuable for all kinds of practical uses compared to the bulk materials. Among many applications, the nanoparticles find a widely use in bio-sensing field. In particular, the gold nanoparticles (AuNPs) coupled with a specific bio-element, as the antibodies, make them a powerful optical biosensor. Indeed, the aggregation between functionalized AuNPs and corresponding antigens causes an increase of the clump size and, hence, a redshift of their absorption spectrum. The technique we use to functionalize the AuNPs is the Photochemical Immobilization Technique (PIT) [1] that consists in the irradiation of the antibodies by UV to bind them covalently and upright. Colloidal solution of colorimetric biosensors, functionalized by PIT, shows remarkable long-term stability as well as propensity to preserve their properties even after stressing steps of the procedure like the centrifugation aimed at removing free antibodies. In previous experiments, we have already observed that these biosensors are able to detect human IgG at a concentration level lower than 100 ng/mL [2]. The whole approach is depicted in Figure 1 and is here extended to 17β-estradiol in blood in view of its involvement in several hormonal [3] and carcinogenesis processes [4]. Proposed biosensor is easy to fabricate, it is fast, simple, reliable and very specific for detection of 17β-estradiol at low concentrations in blood. These advantages make the biosensor superior towards available tests and sensors for detection of 17β-estradiol, and make it very attractive in biomedical applications (menopause symptoms, ovaries and breast cancer, gynecomastia, in pregnancy or infertility treatments, etc.).

Keywords: biosensors, gold nanoparticles, antibodies, colorimetric test, colloidal solution, functionalization, medical application.

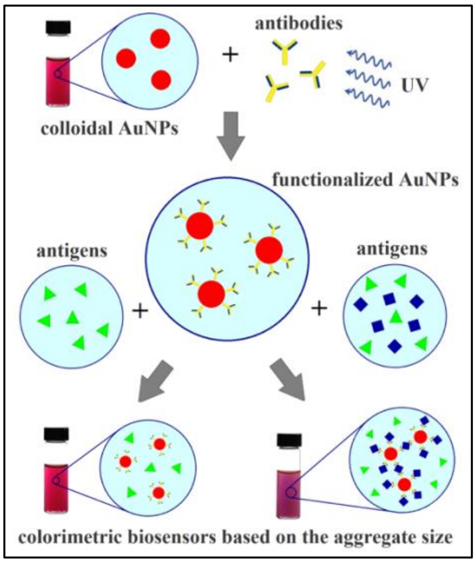

Figure 1: Scheme of the antigen detection by using AuNPs functionalized with antibodies through PIT.

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Big Instrument- and Chaotropic Detergent-Free Assay for Ultrasensitive Biomolecule Nucleic Acid Isolation and Detection Via Binary Nanomaterial

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Abstract:

Nucleic acid-based diagnostics are widely used for clinical applications due to their powerful recognition of biomolecule properties. Isolation and purification of biomolecules such as DNA and RNA in the diagnostic system have been severely hampered in point-of-care testing because of low recovery yields, degradation of biomolecules due to the use of chaotropic detergent and high temperature, and the requirement of large instruments such as centrifuges and thermal controllers. Here, we report a novel big instrument- and chaotropic detergent-free assay via binary nanomaterial for ultrasensitive biomolecule isolation and detection from cells (eukaryotic and prokaryotic). This binary nanomaterial couples a zinc oxide nano-multigonal shuttle (ZnO NMS) for cell membrane rupture without detergent and temperature control and diatomaceous earth with dimethyl suberimidate complex (DDS) for the capture and isolation of nucleic acids (NA) from cells. The ZnO NMS was synthesized to a size of 500 nm to permit efficient cell lysis at room temperature within 2 min using the biological, chemical, and physical properties of the nanomaterial. By combining the ZnO NMS with the DDS system, the biomolecule extraction could be completed in 15 min with high quantity and quality. Subsequently, the detection sensitivity of this binary nanomaterial in diverse cells was measured as 100 times higher than that of conventional methods. We believe that this binary nanomaterial will be a useful tool for rapid and sensitive biomolecule isolation and detection without instruments and detergent in the field of molecular diagnostics.

Keywords:
Nucleic Acid Isolation, Binary nanomaterial, ZnO NMS, DDS, Molecular diagnostics

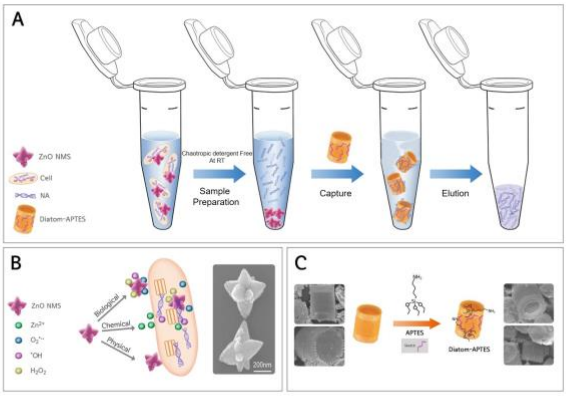

Figure 1:
The schematic of an innovative instrument- and detergent-free assay in a single tube for ultrasensitive biomolecule isolation and detection via binary nanomaterial. (A) In situ sample processing involves ZnO nano-multigonal shuttle (NMS) and diatomaceous earth (diatom) with dimethyl suberimidate (DDS) in a single tube. (B) A schematic of ZnO NMS for breaking of cell membrane based on biological, chemical, and physical properties of ZnO. ZnO NMS was used for cell lysis at RT for 15 min without detergent and thermal incubation. (C) The schematic of the DDS complex for isolation and extraction of NA (RNA and DNA) without centrifuges and vortexes. In a slightly acidic condition, the amine-modified diatom (diatom-APTES) captured NA and dimethyl suberimidate with high quantity and quality. Subsequently, the NA extracted from cells using the binary nanomaterial assay can be detected with highly sensitivity in downstream analysis.

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Fabrication of Highly Sensitive Ammonia Sensor: Potential Use for Diagnosis Purpose

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Abstract:

Ammonia sensor has been extensively used in a wide range of application areas such as emission detection from vehicles, passenger cabine air control, leakage alarm, and breath analysis [1]. For instance, ammonia sensor was considered as a facile tool to diagnose ulcers or kidney disorder by detecting trace amount of NH_3 gas included in patient's breath [2]. In this study, we fabricated and characterized a highly sensitive ammonia sensor which can be potentially used for diagnosis purpose, which consisted of composite thin films of reduced graphene oxide (RGO) and polyaniline (PANI) deposited on a microelectrode by the Langmuir-Schaefer (LS) method. The microelectrode included interdigitated Cu fingers of microscale dimensions sputtered on SiO_2 substrate (Figure 1). The PANI was prepared as emeraldine salt by a typical polymerization process from aniline. We prepared four different sensors having different thin films of hydrazine-reduced RGO, pyrrole(Py)-reduced RGO, PANI, and Py-reduced RGO/PANI composite, respectively, and characterized them by employing Raman spectroscopy, FTIR, SEM and AFM. We then examined their NH_3 gas detection performance using a typical set-up of a computer-interfaced multi-channel source meter and a gas chamber equipped with mass flow controllers. As main results, the sensor of the Py-reduced RGO/PANI composite thin film showed the highest response to small amount of NH_3 gas existed in the carrier gas of N_2 among the tested. It also yielded highly sensitive response and linear sensitivity in the range of 1 to 20 ppm of NH_3 gas included in the simulated exhale air of (containing 76.3% N_2, 15.2% O_2, 4% CO_2, 3.1% water vapor, and 0.83% of trace amount of argon and helium, etc) (Figure 2). Thin film characterization results by Raman and FTIR indicated that the Py-reduction increased the density of C=C bonding in the RGO and thus increased the binding sites to NH_3 gas molecules, and the PANI enhanced detection sensitivity because of plentiful protons on the molecular backbone, doped in the acidic preparation procedure [3].

Keywords: ammonia sensors, reduced graphene oxide, pyrrole, polyaniline, Langmuir-Schaefer films, breath analysis.

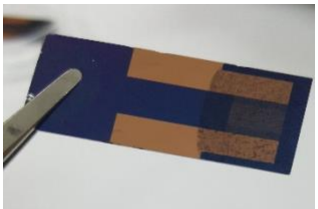
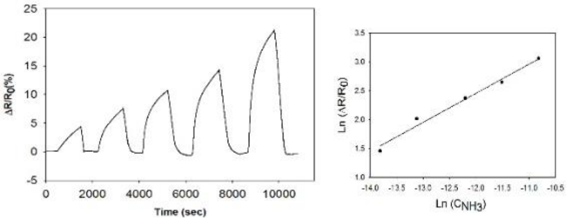


Figure 1. Microelectrode with interdigitated Cu fingers of microscale dimensions on SiO_2 substrates, and composite thin films of Py-redcued RGO/PANI.



(a) (b)

Figure 2. (a) Response profiles (1 to 20 ppm) and (b) linear sensitivity (R^2=0.9913) of the ammonia sensor of Py-reduced RGO/PANI thin film in the simulated exhale air.

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Rapid and Sensitive Detection of pathogen diagnosis based on Microfluidic Enrichment with a Label-free Nanobiosensing Platform

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Abstract:

Rapid and sensitive detection of low amounts of pathogen in large samples is needed for early diagnosis and treatment of patients and surveillance of pathogen spreading. In this study, we report a microfluidic platform for detection of low pathogen levels in a large sample volume that couples a Concanavalin A or Magainin-1 (AMPs) based microfluidic platform for pathogen enrichment and recombinase polymerase amplification (RPA) sensors for simultaneous pathogenic DNA amplification and detection in a label-free and real-time manner. After optimization of enrichment with Concanavalin A and detection conditions, we demonstrated that *Salmonella enterica* serotype *Typhimurium* could be detected in urine samples (10 mL) at a concentration as low as 5 CFU/mL in real-time using a label-free method. The detection limit of this platform by using magainin-1 was found to be 20 times more sensitive in 10 ml urine with *Salmonella* and 10 times more sensitive in 10 ml urine with *Brucella* than that of real-time PCR without the enrichment process. This platform provides rapid enrichment and detection of pathogens such as *Salmonella enterica* and *Brucella ovis* within 60 min. This system will be useful as it has the potential for better diagnosis of pathogens by increasing the capture efficiency of the pathogen in large samples, subsequently enhancing the detection limit of pathogenic DNA.

Key words: Microfluidic, Pathogen enrichment, Nanobiosensor, RPA, Molecular Diagnostics.

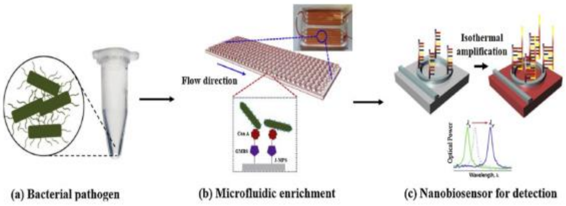

Figure 1: Principle of the microfluidic enrichment method combined with the DNA-based nanobiosensor for rapid and efficient bacterial detection

Reference:

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Development of X-shaped DNA as an immune adjuvant for the cancer immunotherapy through dual activation of TLR9 and inflammasomes

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Abstract:
We developed X-shaped double-stranded oligodeoxynucleotides (X-DNA) to investigate if they had immunostimulatory activity and thereby could be used for anti-cancer immunotherapy. A single unit of X-DNA (X_S-DNA) was composed by four strands of oligodeoxynucleotides while a ligated X-DNA complex (X_L-DNA) was formed by crosslinking each X-DNA to the other through complementary ACGT sequence. We found that these X-DNAs induced the activation of MAPKs and NF-κB leading to the generation of immune cytokines and co-stimulatory molecules in mouse primary dendritic cells differentiated from bone marrow cells. Dendritic cells stimulated by X_L-DNA were able to induce the differentiation of naïve CD^{4+} T cells to T_H1 cells. Intravenous injection of X_L-DNA to mice led to the increase of serum IFN-γ and IL-12 levels, of which potency was comparable with that of ODN1668, a well-known CpG DNA. These indicate in vivo activation of T_H1 cells and dendritic cells by X_L-DNA. Co-treatment of X_L-DNA greatly enhanced the therapeutic efficacy of anti-cancer drug, doxorubicin, in AOM/DSS-induced colon cancer mouse model. X_L-DNA associated with TLR9, thereby activating signaling pathways in dendritic cells. Immunostimulatory activities of X-DNA were abolished in TLR9-deficient dendritic cells. In addition, X-DNA induced activation of inflammasome exhibiting caspase-1 degradation and IL-1β secretion in primary wild-type dendritic cells, but not in caspase-1-deficient dendritic cells. These demonstrate the role of X-DNA as a dual activator for TLR9 and inflammasome and that X-DNA can be used as an excellent immune adjuvant for the cancer immunotherapy to enhance therapeutic efficacy of anti-cancer drugs by activating innate immune receptors such as TLR9 and inflammasome.

Keywords: Immunostimulatory DNA; pattern recognition receptor; colon cancer; inflammasome; dendritic cells.

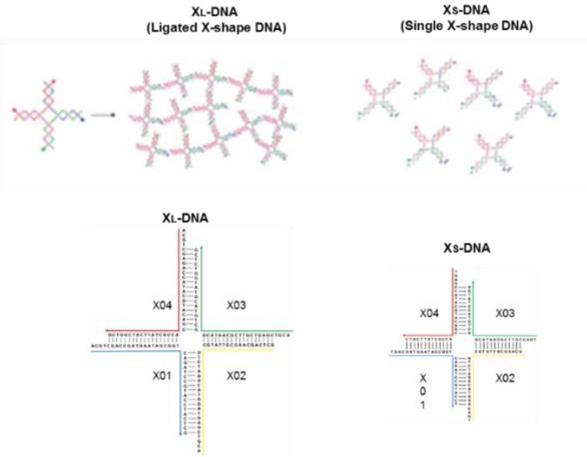

Figure 1: Figure illustrating the structure of X-shaped double-stranded DNA (X-DNA). X_L-DNA forms a ligated complex through self-ligation due to ACGT sequence at the end of the strand. X_S-DNA which does not have the ACGT sequence exists as a single module.

Reference:

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The Studies of Interaction Between Influenza Viruses and Surface of Nanocomposite PolyGraphene.

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Abstract:

It was discovered that expanded graphite – Nanocomposite of PolyGraphene (PG) obtained after hydro-termic treatment of modified graphite became to be able to interact as sorbent PG with influenza A and B viruses apart from antigenic properties of surface proteins.

Introduction. Wide circulation of substances harmful and toxic for people, pathogenic microorganisms including viruses, raises a question of deactivation and removal them from environment. It is known that for removal of viruses from solutions there are two methodical approaches – ultracentrifugation and their sorption on sorbents. Carboniferous substances can be one of such sorbents. In particular, absorbent carbon is an active sorbent as for the toxic substances which are present both at gases, and at liquids. Therefore it was important to investigate the newest carbon substance as a sorbent - the PolyGraphene (PG) received from the modified graphite by means of hydroheat treatment. The flu viruses possessing an external fibrous casing with various anti-gene properties were taken in qualities of the occluded substance.

Materials and methods. For studying of interaction of a virus with a sorbent PG reference and epidemic influenza strains of A(H1N1, H3N2) and B, and other strains, isolated during the period 1977-2005, possessing various structure of surface proteins and respectively properties, and also, the immune rat serums prepared for them were taken. All viruses were taken from a collection of the Center of Ecology and Epidemiology of Flu of Scientific Research Institute of Virology of the Russian Academy of Medical Science. Viruses were cultivated in chicken embryos, cleared in a gradient of concentration of sucrose of 10-50% at 22 000 rpm., are concentrated at 25 000 rpm within an hour. For definition of a virus in solution used the reaction of the hemagglutinating activity (RHA), for definition of antibodies in serums – the reaction of braking of the hemagglutinating activity (RBHA). In reactions applied 0,75% a suspension of erythrocytes of 0 (1) blood types of human. Determination of concentration of protein in preparations was carried out on Louri's method.

Results and Conclusions. Showed researches of sorption of different strains of viruses of flu A and B on a sorbent PG, all viruses successfully interacted with a sorbent irrespective of anti-gene properties of surface proteins. Viruses of flu A and B were occluded on PG from a virus-containing liquids: buffer solutions, liquid of chicken embryos.

The sorption of virions was took place rather active in range of temperature 8-34ºC during 15 min and more. The HA titer of viruses in solution decrease after contact with PG from 4 to 256 times. The immobilized viruses were able to interact with homological antibodies from immune sera. The desorption of viruses from PG was extremely small.

Thus, it is established that PG is capable to occlude in short time in the wide range of temperatures viruses of flu A and B irrespective of their anti-gene structure. The immobilized viruses kept opportunity to connect to the antibodies containing in the immune serums prepared for flu viruses. The obtained data can be used in the serological reactions for determination of specificity of antibodies to a flu virus, and also for removal of viruses from the tanks infected with avian flu viruses. It is very important and it has a big scale for realisation as in recent years transfer of flu viruses is growing from animals to people with serious consequences.

Keywords: PolyGraphene, influenza viruses.

Posters Session II: NanoMaterials for Energy and Environment / Nanoelectronics / NanoPhotonics

Boron-doping effect on photovoltaic performances of silicon nanoparticle/organic polymer hybrid solar cells

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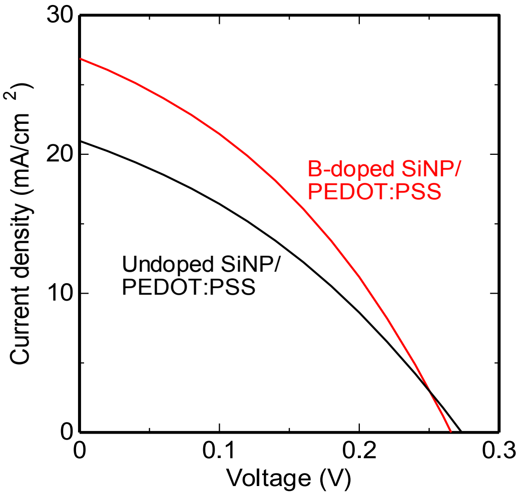
Abstract:

Inorganic/organic hybrid solar cells that combine silicon nanoparticles (SiNPs) with organic conducting polymers have been developed as an alternative to commercial Si-based solar cells.[1,2] The advantages of the hybrid solar cells are to enable not only the selective absorption of solar spectrum by controlling the optical bandgap width due to variation of the SiNP sizes but also the reduction of the manufacturing costs by solution-based approaches. In the design of such hybrid solar cells, the electrical conductivity of the SiNPs is of crucial importance so as to achieve the efficient transport of photogenerated charge carriers, which is directly relating to power conversion efficiency (PCE). We focus on the boron (B)-doping into the SiNPs in order to enhance the carrier transport efficiency. In this presentation, we report the influence of the B-doping on the photovoltaic performances of the hybrid solar cells consisting of the SiNPs with mean diameter of approximately 3.4 nm and poly(3,4-ethylenedioxythiophene):poly-(styrenesulfonate) (PEDOT:PSS). Figure 1 shows the current density-voltage characteristics of the B-doped SiNP/PEDOT:PSS hybrid solar cell and the undoped SiNP/PEDOT:PSS hybrid solar cell. The undoped SiNP/PEDOT:PSS hybrid solar cell exhibited a short circuit current density (J_{sc}) of 21.0 mA/cm^2, an open circuit voltage (V_{oc}) of 0.273 V, a fill factor (FF) of 0.342 and a PCE of 1.96%. The incorporation of the B atoms into the SiNPs resulted in the enhancement of PCE to 2.57% with an increase in a J_{sc} to 26.9 mA/cm^2 and a FF of 0.360. This improved photovoltaic performance was attributable to the efficient transport of the photogenerated charge carriers in the SiNPs layer due to the high conductance (7.06 mS) of the B-doped SiNPs compared to the undoped SiNPs having the conductance of 6.44×10^{-2} mS. Therefore, the B-doping into the SiNPs becomes the most important factor in the performance improvement of the inorganic/organic hybrid solar cells.



Keywords: silicon, boron doping, nanoparticle, organic polymer, inorganic/organic hybrid solar cell

Figure 1: Current density-voltage characteristics of the B-doped SiNP/PEDOT:PSS hybrid solar cell and the undoped SiNP/PEDOT:PSS hybrid solar cell.

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Acknowledgments:

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Enhanced performance of non-fullerene ternary organic solar cells

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Abstract:
In this study, three kinds of materials were designed to broaden the absorption spectrum and applied to the preparation of non-fullerene ternary organic solar cells. The active layers of the cells were prepared in different proportions and amounts of additives. It was found that the morphologies of binary and ternary active layer were quite different. The performance of ternary active layer in the UV-vis absorption and fluorescence quenching behaviors was better than those of binary active layer. The PBDB-T were introduced into the J51: ITIC binary system at the ratio of J51/PBDB-T/ITIC=0.2/0.8/1 and DIO was added at 0.75%, which effectively improved the performance of the solar cells. The best optoelectronic performance and the highest energy conversion efficiency was 8.86%. Due to the high degree of crystallinity of PBDB-T, the surface roughness of the blend membrane was slightly increased. However, by adding an appropriate amount of DIO, the ITIC was agglomerated with DIO that caused the improvement of overall membrane properties and thus reduced the surface roughness. Therefore, we concluded that by introducing the high crystalline PBDB-T to J51: ITIC binary system could effectively improve the film-forming property. In addition, adding the appropriate amount of additives could enhance the material uniformity and get a better optoelectronic performance.

Keywords: non-fullerene ,organic solar cells

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Polysilsesquioxane-Derived Hybrid Gel Polymer Electrolytes for Lithium Ion Batteries

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Abstract:
Over the past couple of decades, there have been immense research efforts to mitigate the safety concerns of liquid electrolytes in Li batteries, while maintaining practical battery performance.[1] To combat problems of leakage from Li batteries, a series of ladder-like structured polysilsesquioxanes were first synthesized through a controlled hydrolysis-polycondsation reaction. These ladder-like structured polysilsesquioxanes were then utilized as crosslinking gelation agent for conventional liquid electrolytes. Through extensive studies, only a mere 2 wt % was required to completely solidify the liquid electrolyte solution. Due to the minscule 2 wt % required to gelate the liquid electrolyte, exceptionally high ionic conductivity (~6 mS/cm) was obtained, which was on par with that with neat liquid electrolyte (~ 7.2 mS/cm), while having high electrochemical stability (~ 5V). [2] Li batteries fabricated with these materials showed that these materials performed exceptionally well at various C-rates for over 100 cycles, retaining 98.5% Coulombic efficiency.

Keywords: gel polymer electrolytes, polysilsesquioxanes, lithium ion batteries

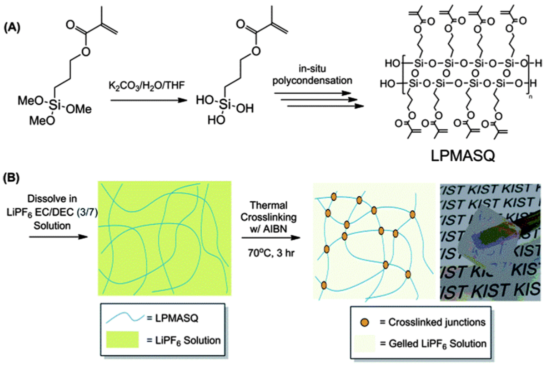

Figure 1: (a) Synthesis of crosslinkable polysilsesquioxane and (b) Fabrication schematic of hybrid gel polymer electrolytes through thermal crosslinking of liquid electrolytes.

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Novel modulating the concentrations of zinc oxide nanowires using electron beam

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Abstract:
Zinc oxides are attracting more attention because of their wide direct bandgap (Eg =3.37 eV) and their large exciton binding energy (about 60 meV), which can be used for gas sensors, surface acoustic wave devices, varistors, and transparent electronics such as display devices [1] [2]. The large surface area of the quasi-one dimensional ZnO structures can be very advantageous for environmental sensors. The significant role of defects in the electrical properties makes it difficult to predict the device characteristics, which should be completely understood for the application of the electronic devices. The sol-gel method was adopted for the sample preparation. After forming metal pads on the SiN substrate to bond the samples selectively opened area wre made after the development process of electron resists by electron beam lithography technique. ZnO nanowires were selectively grown in the opend areas. The in-situ current-voltage characteristic of ZnO nanowire devices under the electron beam was measured at room temperature. In this report, the deliberate treatments of the adsorbed ions by exposure to the high energy of electrons were introduced for clarifying the role of adsorbed ions on the electrical properties [3] [4]. The irradiation of the electron beam on ZnO nanowires enhanced the conductance, explained by the detachments of the anion adsorbed on the surface of ZnO nanowires such as O-, O2-, releasing the electrons. The increase in the available electrons can enhance the conductance of the ZnO nanowires. The slow recovery of the conductance by exposing to the air indicates the slow diffusion of the healing process by the adsorption. The cleaning & doping process using the electron beam may be used to reset the surface oxide states of the nanowires to tune the electrical properties prior to the passivation process.

Keywords: electron beam, ZnO nanowires, gas desorption / adsorption, concentration, passivation process, recovery

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Heterostructures of metal oxide/sulfide nanoparticles as efficient solar active photocatalysts

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Abstract

Harvesting the solar light with a full spectrum from UV to NIR regions would present real candidates as environmental pollutions tools. The idea of this work is to design a systematic nano heterostructures that are capable of harvesting the solar light with a full spectrum from UV to NIR. In our proposed system, n-type wide direct band gap CeO_2 NPs was coupled with n-type Ag_2S and p-type Cu_2S narrow indirect band gap semiconductors. The choice of Ag_2S or Cu_2S was based on their capability of extending the photo response CeO_2 NPs to the NIR region and also due to their longer charge carrier life times compared to direct gap ones. The prepared nano heterostructures were fully characterized via XRD, XPS, BET, UV-Vis, PL, TEM and HRTEM techniques. The TEM images showed that the synthesized nanoparticles are spherical in shape with an average particle size of 10 nm. Also the photocatalytic activities of the designed photocatalysts were tested toward the photodegradation of Rhodamine 6B dye under natural solar irradiation. The results obtained showed an extreme enhancement of the photodegradation rate in case of Cu_2S/CeO_2 and Ag_2S/CeO_2 compared to bare CeO_2 NPs.

Keywords: Nanoheterostructures, Semiconductor, solar irradiation, photodegradation

The Synthesis & Analysis of Two Long Lasting Phosphorescent Compounds: $SrAl_2O_4:Eu^{2+},Dy^{3+}$

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Abstract:

this research project focussed on specific compounds, whereas a literature review was completed on the broader subject of long lasting phosphorescence. For the review and subsequent laboratory work, long lasting phosphorescence compounds were defined as materials that have an afterglow decay time greater than a few minutes. The decay time is defined as the time between the end of excitation and the moment the light intensity drops below 0.32mcd/m2. This definition is widely used in industry and in most research studies. The experimental work focused on known long lasting phosphorescence compounds – strontium aluminate (SrAl2O4:Eu2+,Dy3+). at first, preparation was similar to literary methods. Temperature, dopant levels and mixing methods were then varied in order to expose their effects on long lasting phosphorescence. The effect of temperature was investigated for SrAl2O4:Eu2+,Dy3+, and resulted in the discovery that 1350°C was the only temperature that the compound could be heated to in the DSC in order to achieve any phosphorescence. However, no temperatures above 1350°C were investigated. The variation of mixing method and co-dopant level in the strontium aluminate compounds resulted in the finding that the dry mixing method using a Turbula mixer resulted in the longest afterglow. It was also found that an increase of europium inclusion, from 1mol% to 2mol% in these compounds, increased the brightest of the phosphorescence. As this increased batch was mixed using sonication, the phosphorescent time was actually reduced. which produced green long lasting phosphorescence for up to 20 minutes following 30 minutes excitation and 50 minutes when the europium content was doubled and mixed using sonication.

Keywords: long lasting phosphorescence,europium, excitation .

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CMOS Compatible Sensor for the Electrostatic Selectivity of Volatile Organic Compounds

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Abstract:

Growing demand for the development of miniature, low-power, highly selective and sensitive sensing technology, as a means of alert against the dispersion of hazardous materials, important for monitoring safety, pollution, and healthcare. Although there are several categories of gas sensors, but most of them suffers from the limitation of chip-scale miniaturization and low-power operation. By far, complementary metal–oxide–semiconductor (CMOS) compatible silicon nanowires (SiNWs)-based field-effect transistor (FET) technology have emerged as a promising candidate in overcoming power consumption, size limitations, and sensitivity. However, due to the inherent in-deterministic design of SiNWs it is not possible to mass-produce them. A new paradigm of gas sensing, termed Electrostatically-Formed Nanowire (EFN) was developed by our group that was inspired by the sensing performance of SiNWs. It is fabricated using standard very large scale integration (VLSI) techniques, where the nanowire is not physically-shaped but is electrostatically defined nano-scale size channel of a transistor induced by four biasing gates. The size and shape of the nanowire conducting channel are defined and tuned by controlling the bias applied to the surrounding gates (junction and back gates). The volatile organic compounds (VOCs) sensing occur *via* the modulation of drain-source current as a result of channel surface potential change due to the interaction of surface adsorbed gas in the linear amplifying region of the transistor. The "electrostatic selectivity" of homologous and different functional groups containing VOCs, is achieved by a single device without any surface modification. High selectivity (~90%) toward specific VOC is achieved by training machine-learning based classifiers using the calculated changes in the EFN sensor parameters (threshold voltage and drain-source on current), obtained from systematically controlled biasing of the surrounding gates of the FET (Figure 1). To the best of our knowledge, such a technology is novel for the sensing community as it has significant advantages relative to the state of the art: low cost, miniaturization, stability and robustness, low power consumption and high selectivity.

Keywords: electrostatic selectivity, electrostatically formed nanowire sensor, field-effect transistors, volatile organic compounds, selective detection, threshold voltage, transistor parameters, machine learning classifiers.

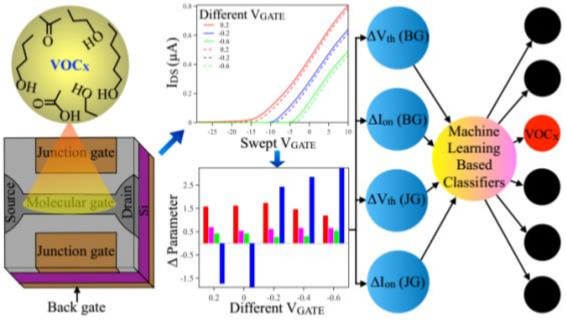

Figure 1: Schematic representation of "electrostatic selectivity" of the targeted VOC using FET-based EFN sensor with machine learning based classifiers.

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Effect of Mg-doping on synthesis of lithium iron phosphate as cathode materials for lithium-ion batteries

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Abstract:

Lithium iron phosphate, $LiFePO_4$, have been a good cathode material for lithium-ion batteries because of its high theoretical capacity, low cost, and environmental friendliness. In this study, Mg-doped lithium iron phosphate/carbon ($LiFe_{1-y}Mg_yPO_4/C$) composite cathode materials were synthesized by the solid-state reaction under H_2/Ar (5%/95%) atmosphere. Different Mg-doped concentrations (y=0, 0.02, 0.04, 0.06) were used in the synthesis of $LiFe_{1-y}Mg_yPO_4/C$ cathode materials. The crystalline phase and morphology of synthesized $LiFe_{1-y}Mg_yPO4/C$ particles were performed by powder X-ray diffraction, scanning electron microscopy, and transmission electron microscopy. The electrochemical studies were carried out by a coin cell. The cell was fabricated by using the $LiFe_{1-y}Mg_yPO_4/C$ as cathode and lithium foil as anode. The cell performance was measured on a computer-controlled multichannel charge/discharge apparatus. The experimental results showed that the synthesized cathode materials had a high crystalline intensity with an orthorhombic olivine structure. The primary particle sizes ranged from a few tens nanometers to one micrometer. Mg-doping did not affect the crystalline structure of the $LiFe_{1-y}Mg_yPO_4/C$ composites. No significant differences in morphology were observed with changing Mg-doped concentration. The highest initial discharge capacity of 150 mAh/g at 0.1 C-rate for $LiFe_{1-y}MgyPO_4/C$ cathode materials was obtained at y=0.04.

Keywords: Mg-doped lithium iron phosphate, solid state method, cathode materials, carbon coating, charge/discharge capacity.

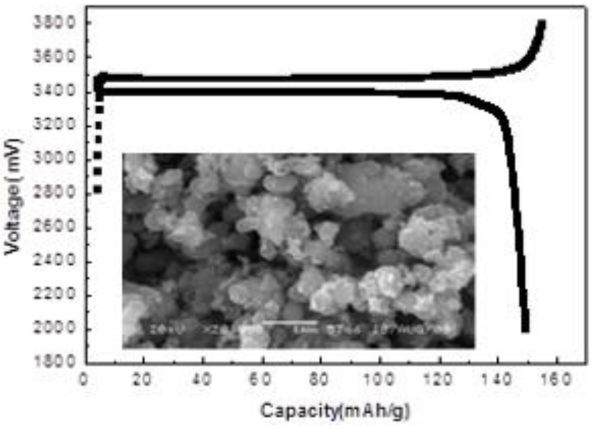

Figure 1: The initial charge-discharge curves at a fixed charge rate of 0.1 C and SEM image for the $LiFe_{0.96}Mg_{0.04}PO_4/C$ cathode materials. The initial discharge capacity is 150 mAh/g at 0.1 C and the as-prepared $LiFe_{0.96}Mg_{0.04}PO_4/C$ cathode materials show a irregular morphology and nano- to submicron-sized particles.

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New Synthetic Route for the Preparation of Highly Ordered Multilayer Metal Membranes

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Abstract:
Highly ordered metallic porous membranes containing Fe and Zr in different layers have been fabricated by successive physical vapour deposition of these metals on a typical porous anodic alumina oxide (AAO) membrane. Two different configurations were studied: Fe/Zr/AAO and Zr/Fe/AAO membranes.

The morphology of these multilayer metal membranes has been characterized by Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). As a result, the metal nanoholes replicate the structure of the AAO membrane used as template (see Figure 1), although a partial reduction of the pore diameter was observed depending on the thickness of the different metals deposited. X-ray diffraction (XRD) experiments and Rutherford backscattering spectrometry (RBS) were performed to study the structure and composition of the membranes. The RBS analysis of the membranes allowed to determine the real depth profile of the atomic composition. The asymmetry and long tails observed for the metal peaks in the RBS spectra (see Figure 2) indicate the different pore fillings during the PVD. The RBS fitting provides a model of the growing of the metallic membranes. Interestingly, Fe/Zr/AAO and Zr/Fe/AAO multilayer metal membranes followed different behaviours.

Keywords: Anodic Alumina Oxide membrane, Rutherford Backscattering Spectrometry, Fe/Zr/AAO, Zr/Fe/AAO.

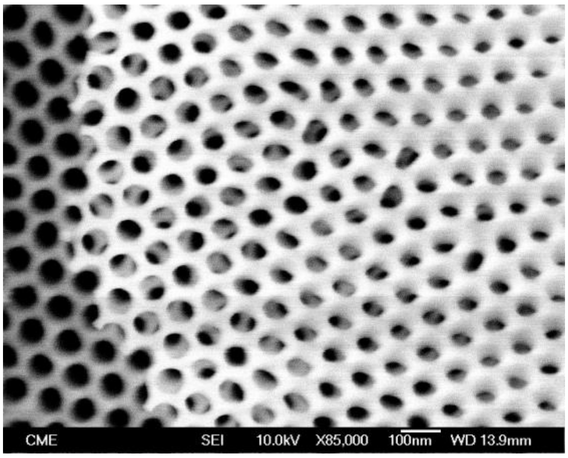

Figure 1: SEM image of a Zr/Fe/AAO membrane.

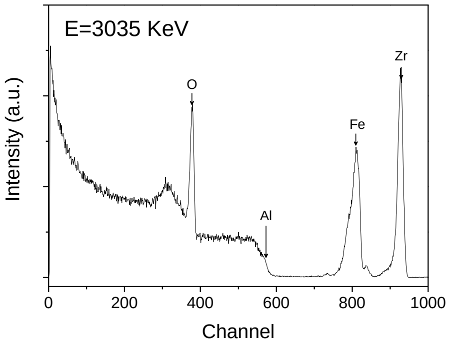

Figure 2: RBS spectrum of a multilayer Zr/Fe/AAO membrane.

Mustard Seed based Triboelectric Nanogenerator

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Abstract:

Mechanical energy from a local domain is seldom recovered due to its fluctuating amplitude and low frequency, and is therefore usually designated as “unsystematic” energy. With several new ideas and device schemes introduced by Z. L. Wang and coworkers as well as others, it has now become feasible to tap such energy systematically. Herein we introduce an idea of using mustard seeds as a vehicle for construction of a green Triboelectric Nano Generator (TENG). There have been only a few attempts to make such devices using natural materials.[1,2] Mustard seeds shells charge highly by friction and hence are susceptible to charge separation, a property that we have utilized in our device.

ITO coated-PET and aluminum sheet were employed as electrodes in TENG for achieving flexibility. The whole process of TENG fabrication is natural, cost-effective and environmental-friendly. For the first time, a specifically chosen natural seed with rich surface texture is introduced in this respect. The seeds were dispensed on an Araldite film as an active friction surface for TENG operation. Mustard seeds and Polyvinyl di fluoride)PVDF(were used in the construction of the flexible nanogenerator.

The flexible TENG furnished an impressive output voltage of 50 V and a maximum current of 5.25 µA. The seed-TENG with good adaptability rendered the maximum output power of 45µWcm^{-2}, which is capable of driving advertising LEDs and commercial electronic temperature sensors.

Keywords: energy harvesting, environment friendly, Natural seeds, triboelectric nanogenerators

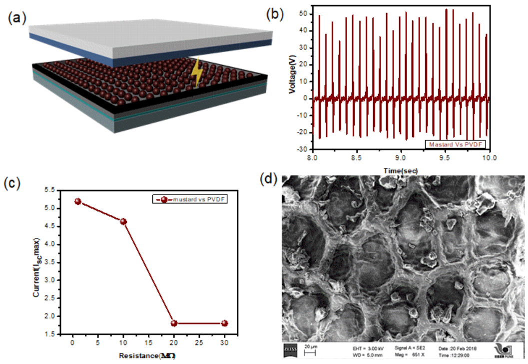

Figure 1: (a) illustrates a schematic diagram of Seed-TENG fabrication; (b), (c) displays Output voltage performance and maximum current variation with resistance (d) shows SEM of mustard seeds.

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Endurance measurements of Li_xCoO_2-based ReRAM cells

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Abstract:

The conductivity of Li_xCoO_2-based cells can be modified by the application of adequate voltages. It is thus possible to switch {electrode/film/electrode} cells reversibly from a high-resistance state R_{High} (initial and highest state of a cell) to a low resistance state R_{Low} (lowest achievable resistance), with a R_{High}/R_{Low} ratio over 2 orders of magnitude. It is also possible to obtain several intermediate resistance states [1]. Hence, this switching behaviour observed in lithium cobalt oxides appears very interesting, towards nonvolatile resistive memories (Re-RAM) in the field of nanoelectronics.

Here, we report preliminary results obtained on endurance, which is defined as the maximum number of write/erase cycles possible to achieve without degradation (Fig. 1 shows an example of endurance > 1000 cycles, with a R_{High}/R_{Low} ratio > 100). Pulse characteristics and cell current compliance play an important role: a better control of such parameters allows higher endurance towards potential application to nonvolatile memories [2].

Keywords: resistive switching, lithium cobalt oxides, thin films, non volatile resistive memories (ReRAM), write/erase cycles, endurance.

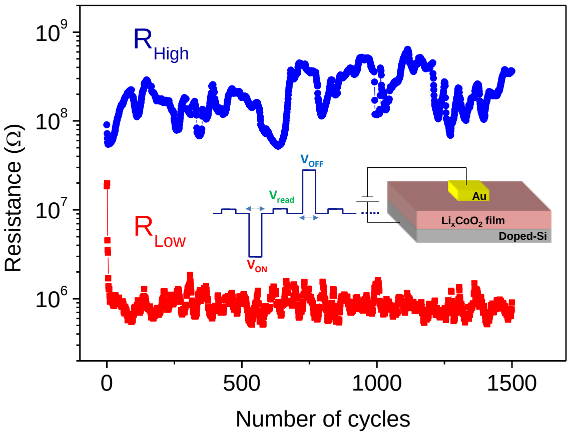

Figure 1: Endurance of a 100x100 µm² {Au / Li_xCoO_2 / doped Si} device. The inset shows the shape of pulses used to switch the device and to measure R_{Low} and R_{High} (at a lower read voltage).

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Effect of nanofluidic electrolytes on the electrochemical reaction of vanadium redox flow batteries

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Abstract:

The limitation of energy storage capacity in vanadium redox flow battery impedes further commercialization of the battery. The concept proposed in this study is to overcome the limit by using nanofluidic electrolytes. Multi-walled carbon nanotubes (MWCNTs) are chosen to disperse in electrolytes due to their high surface to volume ratio. Three nanofluidic electrolytes with different weight percentage of MWCNT (0.05, 0.1, 0.2 wt%) have been tested and compared with pristine electrolyte. Half-cell test with cyclic voltammetry has shown that the electrochemical reaction performance is proportional to the content of MWCNT in nanofluidic electrolytes. The redox reaction of nanofluidic electrolytes are enhanced by the increased electrochemical activity, reversibility and lower polarization effect. Meanwhile, single-cell test reveals that the optimum weight percent of nanofluidic electrolytes is 0.1% of MWCNT because the electrolyte containing 0.2% of MWCNT induces the unwanted precipitation at the electrodes during the electrochemical reaction. After completion of 62 charge/ discharge cycles, nanofluidic electrolyte with 0.1% MWCNT retains specific discharge capacity of 31.7 Ah L^{-1} while pristine electrolyte does 26.0 Ah L^{-1}. This corresponds to 22% enhancement of energy storage by using the nanofluidic electrolytes. We conclude that the nanofluidic electrolytes can considerably improve the energy storage capacity with optimized content of MWCNT.

Keywords: Nanofluidic electrolyte, Nanofluid electrode, Vanadium redox flow battery, Flow battery power density,

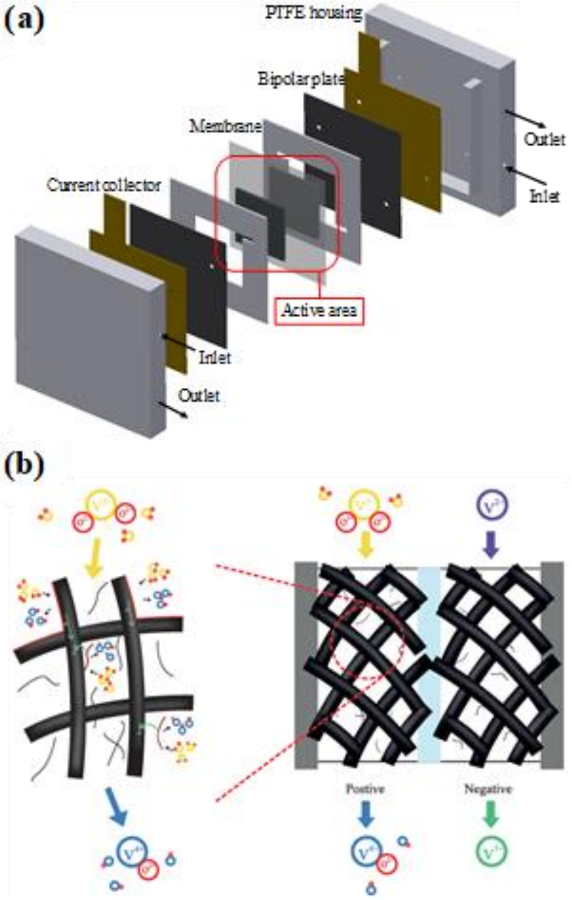

Figure 1: (a) Schematic diagram of 25 cm^2 in-house single cell. (b) Schematic illustration of MWCNT nanofluidic electrolytes in battery active area.

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Flexible thermoelectric devices for body temperature control

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Abstract:
A flexible thermoelectric device using body heat get attention as a power source for wearable device. And growing interests in self-powered wearable mobile electronics provoke the necessity of wearable thermoelectric devices. [1, 2].

We designed and fabricated a flexible thermoelectric device and evaluated performance of them by using our own testing system. Flexible printed circuit boards (FPCB) were used as the substrates. FPCB consists of Cu foil, adhesive layer and PI (polyimide) layer. Cu Electrodes were made on the PI substrate by wet etching method. The fabrication processes of FPCB has already been established and are low-cost.

We developed flexible thermoelectric devices using bulk-type thermoelectric materials and thermoelectric thin films by co-evaporation method. Bismuth telluride thin films for n-type thermoelectric legs and Antimony telluride thin films for p-type thermoelectric legs were deposited. Patterning of thermoelectric p-type and n-type legs were carried out by using metal masks which have the 50 um thickness.

The testing system was developed and is composed of plunger, load cell, vacuum chamber, power supply, measuring block, heater and water cooling system. Plunger is used to load pressure on thermoelectric devices, and the pressure is measured by load cell. We have characterized the performance of the flexible thermoelectric device through the testing system. We obtained power output-load resistance and voltage-current curves.

We carried out the body temperature control test using the flexible thermoelectric devices. The current of 0.65 A was applied to the thermoelectric device for body temperature control test. In case of the warming, body temperature was increased by about 3 ℃ in 1 second. In the case of the cooling, body temperature was decreased by 2 ℃ in 1 minute. The results show the feasibility of flexible thermoelectric devices in applications for controlling body temperature.

Keywords: flexible thermoelectric device, Bismuth telluride, Antimony telluride, performsance evaluation system, body temperature control

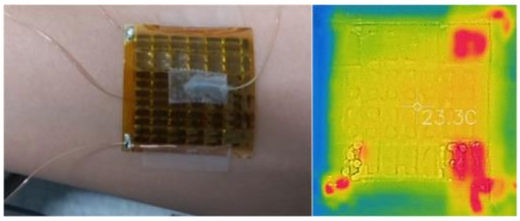

Figure 1: Body temperature control by flexbible thermoelectric devices

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Ethanol steam reforming on Pd/$ZnMgAl_2O_4$ catalyst

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Abstract:
The Pd-Zn bimetallic catalysts have been of interest in ethanol steam reforming reaction. Generally, ZnO has the problem of melting or expanding crystals at temperatures of 600 °C or more. Therefore, it is preferable that a catalyst has high temperature stability and a relatively low expansion coefficient in thermal catalytic reactions. In order to overcome this problem, this study confined the ZnO component, as the main catalytic species, in a $MgAl_2O_4$ support spinel crystal. The Pd component, at 3.0 mol.% of the ZnO concentration, was added simultaneously to improve ethanol steam reforming. In particular, the main aim of this study was to minimize carbon deposition while achieving a high H_2 yield in ethanol steam reforming reactions, at relatively low temperatures of 300–600 °C compared with the conventional reforming temperatures of 500–800 °C. Eventually, we have designed a catalytic system to stably produce large amounts of H_2 gas at low temperatures during ethanol steam reforming. A $Pd_{0.01}Zn_{0.29}Mg_{0.7}Al_2O_4$ catalyst, in which 0.01 mol of Pd and 0.29 mol of Zn had been simultaneously and stably inserted into the $MgAl_2O_4$ spinel structure, was assessed in the ethanol steam reforming reaction. The H_2 production ability during ethanol steam reforming for 30 h at 450 °C decreased in the following order: $Pd_{0.01}Zn_{0.29}Mg_{0.7}Al_2O_4 > Zn_{0.3}Mg_{0.7}Al_2O_4 > MgAl_2O_4$ (figure 1). In the case of the $MgAl_2O_4$ spinel catalyst, the hydrogen yield was as low as 40%, the amount of deposited coke was high, and carbon lumps and CNTs were deposited as carbon species over the surface of the catalyst. Unexpectedly, however, the CO-WGS was not activated in the $Zn_{0.3}Mg_{0.7}Al_2O_4$ catalyst, because Zn was stably embedded in the spinel structure of $MgAl_2O_4$. However, the yield of hydrogen was improved to 68%. Finally, the catalytic activity with 80% H_2 yield over $Pd_{0.01}Zn_{0.29}Mg_{0.7}Al_2O_4$ increased dramatically owing to significant CO-methanation and partial CO-WGS; additionally, there was no deterioration of the catalyst owing to coke deposition or sintering between particles, and no change in the properties of the catalyst after the reaction could be found. Consequently, we conclude that the simultaneous introduction of Pd and Zn into the stable structures of ethanol steam reforming catalysts has a favorable effect, allowing stable production of high levels of H_2 gas with significantly less catalytic deactivation caused by catalytic sintering and less catalytic poisoning by CO molecules.

Keywords: Ethanol stem reforming, CO-WGS, H_2 production, Zn, Pd, $MgAl_2O_4$

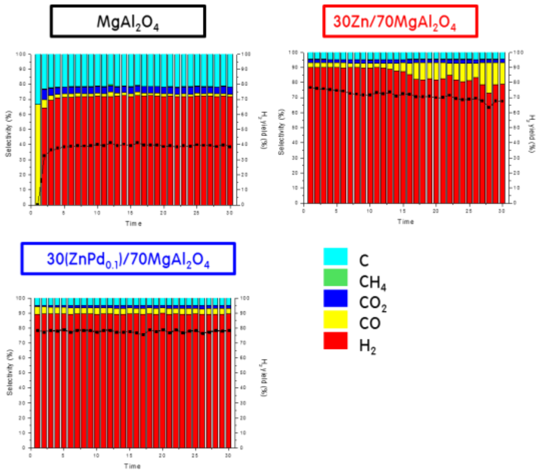

Figure 1: ESR reaction results of catalysts

References:

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Oxygen transfer capacity on a spinel typed $Cu_xMg_{1-x}Mn_yAl_{2-y}O_4$ oxygen carrier

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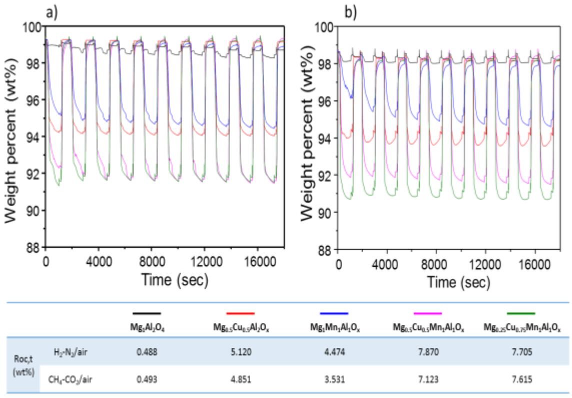
Abstract:

This study focused on $Cu_xMg_{1-x}Mn_yAl_{2-y}O_4$ oxygen carrier which simultaneously anchored by Cu^{2+} and Mn^{3+} ions instead of Mg^{2+} and Al^{3+} ions into the spinel structure of $MgAl_2O_4$ for chemical looping combustion of methane. Despite the Cu 75% and Mn 50% substitution, the spinel structure remained unbroken, but there was the low angle of movement of the XRD peak, which implies a loss of oxygen in the lattice. CH_4 and CO gases were significantly adsorbed on the surface of $Cu_xMg_{1-x}Mn_yAl_{2-y}O_4$ particles. There was a great increased and the $Cu_{0.75}Mg_{0.25}Mn_{1.0}Al_{1.0}O_4$ particles in H_2-N_2 and CH_4-CO_2/air redox systems exhibited 7.71% and 7.61% oxygen transfer capacities, respectively. The fact that the oxygen transfer capacities are nearly similar in both systems means that there is little poisoning to CO in the $Cu_xMg_{1-x}Mn_yAl_{2-y}O_4$ particle. The rate in the redox reaction was proportional to the concentration of Cu^{2+}. In particular, Mn^{3+} was found to contribute to CH_4 burning at high temperatures and Cu^{2+} influenced the oxidation of CO at low temperatures. As a result, it was found that Cu^{2+} influences the rate of oxygen transfer in the redox reaction but affects both Cu^{2+} and Mn^{3+} in the amount of oxygen delivery. From the XPS results, it can be seen that during the redox reaction, Cu^{2+} is completely reduced to Cu^0 but Mn^{3+} is reduced to Mn^{2+}. On the other hand, it was also confirmed that these metal species were stably fixed to the spinel structure, and remained stable without sintering each other even after the redox cycle at a high temperature. Furthermore, the oxygen defects in the spinel structure helped these species to act as long-time oxygen carriers by donating oxygen to these species. finally, this study concluded that the active metal species of Cu^{2+} and Mn^{3+} ions were stably anchored into the spinel structure, led to the reversible oxygen vacancy in spinel structure, resulted that an excellent oxygen transfer capacity could be maintained for a long time.

Keywords: $MgAl_2O_4$, Chemical Looping Combustion, Spinal, Oxygen carrier, Oxygen transfer, Copper, Iron.



		$Mg_1Al_2O_4$	$Mg_{0.5}Cu_{0.5}Al_2O_x$	$Mg_1Mn_1Al_1O_x$	$Mg_{0.5}Cu_{0.5}Mn_1Al_1O_x$	$Mg_{0.25}Cu_{0.75}Mn_1Al_1O_x$
Roc,t (wt%)	H_2-N_2/air	0.488	5.120	4.474	7.870	7.705
	CH_4-CO_2/air	0.493	4.851	3.531	7.123	7.615

Figure 1: Redox cycle curves for $Cu_xMg_{1-x}Mn_yAl_{2-y}O_4$ particles in the a) H_2-N_2/air and b) CH_4-CO_2/air redox systems.

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Significant COS adsorption ability on K-AC composite and adsorption mechanism analysis

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Abstract:
Despite the recent trend of renewable energy, interest in clean coal technology is increasing as the use of coal has increased recently. This is because of the Integrated Gasification Combined Cycle using coal, is a combined power generation system that reacts coal with oxygen and steam under high temperature and high pressure to produce syngas. It has been attracting attention as an eco-friendly clean power generation technology because it has high efficiency and low pollution emission compared to existing coal fired power. The problem is the treatment of the sulfur component that occurs during the gasification process. Among them, it is very important to remove COS. Many techniques for removing COS such as hydrogenation, adsorption and hydrolysis have been studied. Until recently, several types of adsorbents have been studied, including metal oxides containing a support, zeolites exchanged with metal ions, and activated carbon. Among them, activated carbon is very attractive because, considering all the synthesis routes, the coal-based activated carbon adsorbent is inexpensive, has an excellent adsorption ability by itself, and its adsorption ability can be further improved with transition metal impregnation to be. Therefore, based on the results of the above studies, we considered one idea in this study. In order to adsorb the COS as much as possible, we introduce activated carbon with a large surface area into the basic adsorption matrix and modifying the surface with KOH, a basic component that can be a fairly effective COS adsorbent at low temperatures. In the end, we have tried to synthesize a porous type material mixed with K and C to use this material as low temperature adsorbent for COS removal. The adsorption temperatures were tested in the range of 50~210 °C. The crystal state of the synthesized adsorbents was observed through XRD, and the morphology of the surface and the ratio of the elemental components were determined through SEM and EDS. Then, the specific surface area was analyzed by nitrogen gas adsorption, and the correlation between the specific surface area and COS adsorption were examined. Furthermore, we used the FT-IR, XPS, and MASS spectra to determine how the COS is adsorbed/desorbed on the adsorbent and identify the mechanism.

Keywords: Intergrated Gasification Combined Cycle, COS adsorption, K-AC composite, adsorption mechanism.

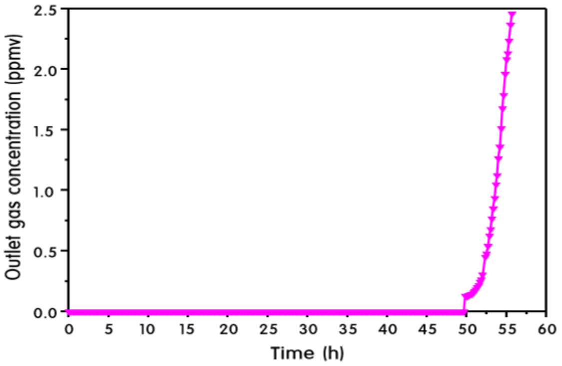

Figure 1: Performance of COS removal for K-AC at 200 ℃

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Spin Hall Effects in Antiferromagnets

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Abstract:

Recent experiments demonstrate that antiferromagnets exhibit a spin Hall effect. Calculations also indicate that the intrinsic contribution is important in determining the magnitude of the spin Hall angle. However, we do not know how the mean free path, exchange interaction, and spin-orbit coupling govern these results and how these factors might influence our understanding of experiments. To address these questions, we consider a minimal model of an antiferromagnet. We numerically compute the spin Hall conductance as a function of impurity concentration, exchange energy, and spin-orbit coupling. We find that the spin Hall conductance is considerably larger in antiferromagnetic systems compared to normal metals. This opens yet another avenue of using antiferromagnets in spintronics devices.

Preparation and characterization of poly(vinyl chloride) - montmorillonite clay composite membranes for water purification

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Abstract:

Despite the many efforts that have been devoted to developing new membranes in order to improve the membrane performance for water purification, the membrane cost is still a great concern for the worldwide applications. In this work, a low-cost poly (vinyl chloride) (PVC) polymer and montmorillonite (MMT) clay composite membranes were fabricated at different loading level (0-10%) using phase inversion method, in order to improve the PVC membrane physicochemical properties and performance.

Besides the membrane thermal, fourier-transform infrared spectroscopy, hydrophilicity, and morphology studies, X-ray diffraction studies revealed the formation of a mixture of the intercalated structure. Moreover, the experimental performance results demonstrated an enhancement regarding water flux and salt rejection up to a loading of 10%. The membrane containing 10% MMT exhibited about 100 % enhancement in water flux at the same low applied pressure. Moreover, it demonstrated an improvement of about 26% in the salt rejection for NaCl, Na_2SO_4 and about 33% for $MgSO_4$ and LiCl, compared to the pure PVC membrane.

Keywords: PVC, MMT, membrane, water purification.

Pavement Material Incorporated Nono Fly Ash Filler

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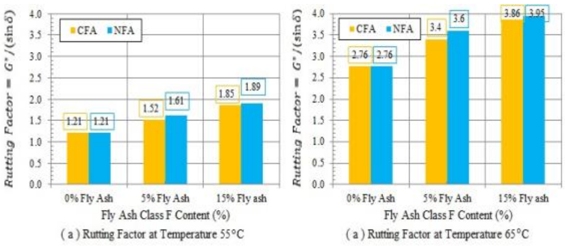
Abstract:

Asphalt and cement are binding materials used for road and pavement construction. Asphalt is used in bituminous flexible pavement while cement is used in concrete rigid pavement. Fly ash is an industrial waste and need to recycle this waste or dispose it in a proper manner. Intensive research conducted to investigate the enhancement of both asphalt and Portland cement concrete using fly ash. Very limited research investigate the use of nano fly ash in both pavement materials. In this paper conventional fly ash with average particle size equal to 10 mm from electrical power plant was used. Reducing the size of fly ash to about 500 nm were performed using Ball milling for 10 hours.wo pavement material was used. These material were asphalt AC60/70 and Portland cement type I. The characteristic of fly ash, asphalt and cement are given in Table 1. Cement paste were prepared using cement to water ratio equal to 0.5. asphalt and cement were replace by 0%, 5% and 10% by weight using both conventional and nano fly ash. Compressive strength of cement paste were measured at 7 and 28 days. The rutting factor of asphalt material were measured at different fly ash content and type. The results show that rutting factor of asphalt material improved significantly when replace CFA by NFA. This trend were observed at temperature 55°C and 65°C (Fig. 1). Also NFA improve compressive strength of cement paste at 7 and 28 days of curing in compare with CFA (Fig. 2).

Keywords: pavement material, asphalt, cement, conventional fly ash, nano fly ash.

Table 1: Asphalt properties properties

Test (property)	Asphalt AC 60/70
Density	1.02
Penetration @25°C, 10/mm	66
Softening Point (°C)	53
Ductility at 25°C (cm)	> 100
Flash Point (°C)	> 250
Solubility in Disulfide % wt	> 99.5
Weight Loss by Heating % wt	< 0.2
Penetration Loss by Heating %	< 20

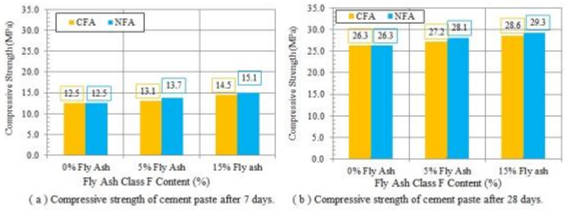


(a) Rutting Factor at Temperature 55°C
(a) Rutting Factor at Temperature 65°C

Figure 1: Rutting Factor of CFA and NFA Asphalt Material.

Table 2: Fly ash and cement properties

Chemical Composition	Cement	CFA
SiO2		20.5
Fe2O3		32.1
Al2O3		9.11
CaO		26.9
K2O		2.61
Na2O		1.10
SO3		1.50
MgO		2.16
LOI		2.95



(a) Compressive strength of cement paste after 7 days.
(b) Compressive strength of cement paste after 28 days.

Figure 2: Compressive strength of cement paste concrete is containing CFA and NFA.

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