

Nanotech Middle East 2020

International Conference

24 - 26 February 2020

Dubai - UAE

Book of Abstracts

Organizer



www.setcor.org

Nanotech Middle East 2020 Conference Program

Feb. 24 - 25, 2020 - Dubai, U.A.E

Feb. 24, 2020

Nanotech ME 2020 Session I:

Nanomaterials Fabrication, Characterization and Properties

Conference Room : Al Ain B

Session Chairs:

Dr. Maguy Abi Jaoude, Khalifa University of Science and Technology, UAE Prof. Daniel Choi, Khalifa University of Science and Technology, UAE

09:00 - 10:30	Registration + Welcoming Coffee - Al Multaqua Ballroom	
10:30 - 11:00	What makes lattice and spin dynamical together	Prof. Jonas Fransson, Uppsala University, Sweden
11:00 -11:30	Advanced Carbon-based Nanomaterials: Present and Future M. Al Fahim, L. Burchfield, R. Al Fahim, F. Delodovici, N. Manini, K. Askar and D. Choi	Prof. Daniel Choi , Khalifa University of Science and Technology, UAE
11:30 -11:45	Using Femtosecond Pulse Laser Nanomachining to Increase Surface Area and Emissivity to Values that Significantly Accelerate Cooling of Electronics by Radiative Heat Transfer V. Rivas and D. Zimmerman	Dr. Delore Zimmerman , Praxis Strategy Group, USA
11:45 - 12:00	Ultra-High Precision Diamond Machining of Nanostructured Rapidly Solidified Aluminium Alloys for Optical Applications K. Abou-EI-Hossein	Prof. Khaled Abou-El- Hossein, Nelson Mandela University, South Africa
12:00 - 14:00	Lunch Break / Posters Session I : Al Multa	aqua Ballroom
Session Chairs: Prof. Jonas Fransson, Uppsala University, Sweden Prof. Junais Mokkath, Kuwait College of Science And Technology, Kuwait Prof. Daniel Choi, Khalifa University of Science and Technology, UAE		
14:00 - 14:30	Effects of synthesis parameters on the structure, optical properties and photocatalytic activity of TiO2-CeO2-Bi2O3 nanocomposites for solar-driven water disinfection M. Abi Jaoude, S. Sood, K. Polychronopoulou, E. Alhseinat and M. Stefancich	Dr. Maguy Abi Jaoude , Khalifa University of Science and Technology, UAE
14:30 - 15:00	Advanced photocatalysts for water treatment and antifouling/self- cleaning coatings G. Palmisano	Dr. Giovanni Palmisano, Khalifa University of Science and Technology, UAE
15:00 - 15:15	A Simulation Study for ABS 3D Filament Doped with Nanoparticles for Thermal Neutrons Applications E. Banogitah, E. Elmoujarkach , F. Nadwi and A. Alhawsawi	Mr. Ezzat Elmoujarkach, King Abdulaziz University, Saudi Arabia
15:15 - 15:30	Different charge ordering states in Niobium diselenide under strain and with metal adsorbates F. Cossu , I. di Marco, and A. Akbari	Dr. Fabrizio Cossu , Asia Pacific Center for Theoretical Physics, Rep. of Korea
15:30 - 16:00	Coffee Break / Posters Session I - Al Multa	aqua Ballroom
16:00 - 16:15	Electrosprayed Aerogel/PCM Embedded PTFE Microporous Materials for Thermal Protection M.Venkataraman , J. Militký, X. M. Xiong and M. Petrů	Dr. Mohanapriya Venkataraman, Technical University of Liberec, Czech Republic
16:15 - 16:30	Integration of functional oxides on silicon A. Benamar , G. Agnus, G. Saint-Girons, C. Magen, S. Schamm- Chardon and P. Lecoeur	Mr. Abdelnour Benamar, Paris-Saclay University, France
16:30 - 16:45	Challenges for High Performance of Polyaniline / Nanocomposite as Super Hydrophobic Coatings via Electrochemical Polymerization Technique	Prof. Zeinab abdel Hamid, CMRDI, Cairo, Egypt.

Z. Abdel Hamid, M. Hasan Gomaa	S. S. Abd El Rehim, M.Abdel
Hamid and A.Ibrahim	

Feb 25, 2020 Nanotech ME 2020 Session II:			
Nanomaterials for Energy and Environment / Nano Electronics			
Conference Room : Al Ain B			
Session Chairs: Prof Ali Bumajdad, Kuwait University, Kuwait Prof . Taleb Ibrahim, American University of Sharjah, UAE			
09:30 - 10:00	Application of Graphene Oxide Derivatives in Industrial Pharmaceutical Wastewater Treatment M.Khamis and T.Ibrahim	Prof . Taleb Ibrahim , American University of Sharjah, UAE	
10:00 - 10:30	Modified graphene oxides as efficient electrode for Capacitive deionization K.A.Khalil , N.A. M. Barakat, M. Motlak and F.S. Al-Mubaddel	Prof. Khalil Abdelrazek Khalil Abdelmawgoud , University of Sharjah, UAE	
10:30 - 11:00	Coffee Break / Posters Session	II	
11:00 - 11:30	Nano-Additives for Green and Sustainable Construction Materials A. Bumajdad	Prof Ali Bumajdad, Kuwait University, Kuwait	
11:30 - 12:00	Surface Deposited Copper Particles on Composite Nonwovens J. Militký , M. Venkataraman, J. Večerník and M. Petrů	Prof. Jiri Militky, Technical University of Liberec, Czech Republic	
12:30 - 13:45	Lunch Break / Posters Session II : Al Mult	aqua Ballroom	

Nanotech ME 2020 Session III Nanomaterials for Energy and Environment			
Conference Room: Al Ain B			
Session Chairs: Prof. Khalil A.K. Abdelmawgoud, University of Sharjah, UAE Prof. Francesco P. La Mantia, University of Palermo, Italy Prof . Taleb Ibrahim, American University of Sharjah, UAE			
14:00 - 14:30	Optimized wet graphene transfer on SiO2/Si substrate using chem-ical surface treatment for potential solar cell application A.F. Abdelaal, B. Salhi and T. Laoui	Prof. Tahar Laoui , University of Sharjah, UAE	
14:00 - 15:00	Electric field hotspots of all-inorganic APbX\$_3\$ (A = Cs, Rb and X = Cl, Br, I) perovskite quantum dots J.H. Mokkath	Prof. Junais Mokkath, Kuwait College of Science And Technology, Kuwait	
15:00 - 15:15	Polymer and Nanoparticles as a New Method for Chemical Enhanced Oil Recovery P. Druetta and F. Picchioni,	Dr. Pablo Druetta, University of Groningen, The Netherlands.	
15:15 - 15:30	Antioxidant Gold nanoconjugates for the treatment of neurodegenerative diseases M.E. Piersimoni ,T. Casd and L. Ying	Ms. Maria Elena Piersimoni , Imperial College London, UK	
15:30 - 15:45	Shape-Stabilized Phase Change Materials for Solar Energy Storage: MgO doped CaCO3 mixed with Polyethylene Glycol S.K.S. Basamad, M. Hasan Zahir and M.M. Hossain	Dr. Md. Hasan Zahir , King Fahd University of Petroleum and Minerals, Saudi Arabia	
15:30 - 16:30	Coffee Break / Posters Session I - Al Multa	aqua Ballroom	

February 24 and 25, 2020 Posters Session Nanotech ME 2020

	Posters / Coffee break area - Al Multaqua Ballroom		
N.	Poster Title	Author/Affiliation/Country	
1	Effect of the Concentration of Graphene Nanoplatelets in the Pho-to- oxidation of the Polypropylene F.P. La Mantia , L. Botta, M.C. Mistretta and M. Ceraulo	Prof. Francesco P. La Mantia , University of Palermo, Italy	
2	Sub-millimeter-scale synthesis of chromium doped CdS nanosheets and their temperature-dependent excitonic emission D. J. Lee and D. Y. Kim	Dr. Dong Jin Lee , Dongguk University, Rep. of Korea	
3	Activation Energy of Hydrogen Evolution Reaction on Strontium modified TiO2 nanotubes K.M. Emran	Dr. Khadijah Emran , Taibah University, Saudi Arabia	
4	Efficient hydrogen production electrocatalytic using hydrothermal Synthesized Sn-TNT nanotubes K.M. Emran and RM. A. Alsahli	Ms. Rawan M. A. Alsahli , Taibah University, Saudi Arabia	
5	Synthesis of quaternary chalcogenide CPSS (CuPbSbS3) as a candidate absorber material for solar cells Y.T. Alharbi and D.J. Lewis	Mr. Yasser T. Alharbi , University of Manchester, UK	
6	Mechanical and electrical properties of GeSn nanowires and their application in NEM switches R. Meija , J. Kosmaca, M. Antsov, R. Sondors, J;D. Holmes and D. Erts	Dr. Raimonds Meija, University of Latvia, Latvia	

Nanotech ME 2020 Session I Nanomaterials Fabrication, Characterization and Properties

Advanced Carbon-based Nanomaterials: Present and Future

M.Al Fahimı, L. Burchfieldı, R. Al Fahimı, F. Delodovici2, N. Manini2, K. Askar3 and D. Chois

Alfields, Inc., Abu Dhabi, P.O. Box 279, UAE

2Dipatimento di Fisica, Universita degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

5Department of Mechanical Engineering, Khalifa University of Science and Technology, Abu Dhabi,

P.O. Box 127788, UAE

Abstract:

A new classification of carbon allotropes called, Novamene is the first release in a series which fall into an entirely new class of carbon in 20161. The basis of this new classification resides on the concept of combining hexagonal diamond (sp3 bonded carbon - lonsdaleite) and ring carbon (sp2 bonded carbon - graphene), provides the basis for the new carbon allotropes, whose properties have been found to be superior to graphene that has been introduced by Nobel Laureates Andrea Geim and Konstantin Novoselov in 2010. Since hexagonal diamond acts as an insulator and sp2 bonded rings act as conductors, these predicted materials can transform the electronic industry and have potential applications for transistors, other electronic components such as quantum computers and even energy applications. Following up the debut of Novamene, another new carbon allotrope named Protomene has been also introduced as a family of Novamene recently. It turns out that Protomene exhibits surprisingly electronic/optical/thermal outstanding properties compared to Novamene.2 As for the comparison with diamond and other carbon allotropes, thermal properties of Protomene can be differentiated. Since thermal expansion behaviors of Protomene are associated with interplane bonding, Protomene may experience structural phase change which can lead to a more rapid change in energy band gap and thermal expansion compared with diamond and silicon. Recently, another new third carbon allotrope has been developed as result of combining linear sp carbon chairs with sp3 bulk carbon and named 'Zayedene'3. It was

found that Zayedene exhibits several competing metallic, insulating and possibly even superconducting states of materials.

I will present our efforts of on-going development of fabrication techniques for new carbon allotropes including Novamene and Protomene based on both top-down and bottom-up approaches and modeling activities by means of Density Functional Theory (DFT) simulations.

- L. A Burchfield, M. Al Fahim, R. S Wittman, F. Delodovici, N. Manini, "Novamene: A new class of carbon allotropes" *Heliyon* 3, e00242 (2017).
- F. Delodovici, N. Manini, R. Wittman, D. Choi, M. Al Fahim, and L. Burchfield, "Protomene: A new carbon allotrope", *Carbon*, 126, pp574-579 (2018).
- 3. F. Delodovici, D. Choi, M. Al Fahim, L. Burchfield and N. Manini, "Carbon sp chains in diamond nanocavities", Phys. Chem. Chem. Phys., pp21814-21823 (2019).

Using Femtosecond Pulse Laser Nanomachining to Increase Surface Area and Emissivity to Values that Significantly Accelerate Cooling of Electronics by Radiative Heat Transfer

Victor Rivas1 and Delore Zimmerman2

¹ThermOptical Cooling Technologies, Ltd, Regina, SK, Canada ²Praxis Strategy Group, Grand Forks, North Dakota, USA

Abstract:

As consumer, industrial and space electronics become faster and smaller, overheating of the components such as microprocessors, batteries, and LEDs has become one of the key problems in the industry. Overheating leads to performance losses, failures in operation, and shortening of the device lifespan – and even to direct dangers, as heated batteries pose a risk of explosion. There is universal agreement that improved heat management is necessary for continued advancements in the performance of electronics.

Using ultrafast pulse laser systems to form and create micro-nanostructures on metallic and nonmetallic surfaces significantly increases the surface area and emissivity to values that accelerate cooling by 100% plus (Rivas 2012). This makes radiative heat transfer highly significant and improves conduction and convection cooling in terrestrial and space thermal management systems

Laser surface functionalization to increase surface area and emissivity can complement, eliminate or augment conventional conduction and convection cooling methods involving fans or fluids. Unlike conventional cooling methods and nanotubes, nanowires and nanolaminates it involves no chemical processes, does not add weight and eliminates time consuming post processing steps resulting in single step machining.

Recent technical developments in the laser industry have scaled the technology to more than 1000W of power such that the combination of high-power lasers and high-speed scanner systems processes large substrates quickly and accurately. These concurrent developments now enable high-throughput manufacturing that makes this nano-structuring technique feasible for high volume manufacturing of thermal management components, such as integrated heat spreaders for microprocessors, heat sinks, heat pipes, cold plates and vapor chambers used in thermal management systems for terrestrial and space applications.

Laser surface functionalization to increase surface area offers alternative cost-effective thermal management solutions for critical, harsh environment space applications, such as those identified in the 2020 NASA Technology Taxonomy. These include numerous thermal control components and systems to provide capabilities that enable a space vehicle to maintain operational temperature limits.

In summary: The exponential growth in the number of processors, batteries and LEDs for computers, smartphones and IoT devices combined with the shrinking size of electronic components is leading to the significant rise in demand for thermal management solutions and systems in consumer, industrial, and space electronics. Laser surface functionalization to significantly increase surface area and emissivity can play an important role in meeting this demand for a variety of terrestrial and space applications.

- 1. Rivas, Victor. Nano machined materials using femtosecond pulse laser technologies to enhance thermal and optical properties for increased surface area to enhance heat dissipation and emissivity and electromagnetic radiation. United States Patent 8238098. 2012.
- 2. National Aeronautics and Space Administration. 2020 NASA Technology Taxonomy. TX14: Thermal Management Systems.

Ultra-High Precision Diamond Machining of Nanostructured Rapidly Solidified Aluminium Alloys for Optical Applications

K. Abou-El-Hossein

Preocsion Engineering Laboratory, Department of Mechatroncis, Nelson Mandela University, Port Elizabeth 6031, South Africa, email: <u>Khaled.abou-el-hossein@mandela.ac.za</u>

Abstract:

Aluminium alloys such as optical AA6061 are commonly used in the production of optical and structural components of aerospace and automative optical systems using ultra-high precision diamond machining. However. traditional AA6061 is produced through conventional foundry processes that involve slow solidification. Hence, they are made up of a coarse microstructure and relatively large grain sizes. Diamond turned AA6061 results in surface roughness values of approximately 10 nm. However, to achieve surface roughness withing the range of 1-3 nm, the microstructure of the machined material needs to be further controlled to avoid the presence of coarse grains. This resulted in the development of new aluminum alloys produced by rapid solidification casting. Rapidly solidified aluminium are characterized by their ultrafine nanometric structure (Figure 1) that results in highly improved mechanical and physical properties [1] and reduced diamond tool wear rates [2]. This study contributes to address the lack of machinability database on the most optimal diamond machining parameters during diamond turning. The author will report their findings on the effect of diamond cutting parameters such as cutting speed, feed rate and depth of cut on the nanometric optical surface quality of rapidly solidified aluminum. The study is based on running diamond turning experiments on an ultra-high precision machine to machine convex optical surfaces and measure surface roughness. The results show that surface roughness in the range of 3 namoters can be achieved on surfaces made from rapidly solidified alumnium. This can be attributed to the fact that material surface grain recovery after machining is minimal as a result of their ultrafine sizes.

Keywords: Ultra-high precision manufacturing, single-point diamod turning, optics manufacturing, nanostructure of materials, rapidly solidified materials, nanometric optical surface roughness



Figure 1: Material structure of rapidly solidified alimnium.



Figure 2: Surface roughness of Ra 3 nm achived on optical surface of rapidly solidified alumnium.

- 1. Salehi, M., Dehghani, K. (2008), Structure and properties of nanostructured aluminum A413 produced by melt spinning compared with ingot microstructure, *J. Alloys Compd.*, 457 (1), 357-361.
- Abou-El-Hossein, K., Olufayo, O., Mkoko, Z. (2013), Diamond tool wear during ultrahigh precision machining of rapidly solidified aluminium RSA 905, *Wear* 302 (1-2), 1105-1112.

Effects of synthesis parameters on the structure, optical properties and photocatalytic activity of TiO₂-CeO₂-Bi₂O₃ nanocomposites for solar-driven water disinfection

M. Abi Jaoude, 1-3* S. Sood, 1 Kyriaki Polychronopoulou, 3,4 Emad Alhseinat, 2,5 Marco Stefancich, 6

1 Khalifa University, Department of Chemistry, Abu Dhabi, UAE

² Center for Membranes and Advanced Water Technology, Khalifa University, Abu Dhabi, UAE

³ Center for Catalysis and Separation, Khalifa University, Abu Dhabi, UAE

4 Khalifa University, Department of Mechanical Engineering, Abu Dhabi, UAE

5 Khalifa University, Department of Chemical Engineering, Abu Dhabi, UAE

6 Research and Development Centre, Dubai Electricity and Water Authority (DEWA), Dubai, UAE

Abstract:

The advancement of the traditional TiO₂photocatalysis for water reclamation has been largely driven by the outstanding need to curtail the scalability costs of artificial UV illumination sources, via the use of more sustainable means such as solar energy [1].

Due to the poor visible-light harvesting ability of TiO₂ across the solar-spectrum (large bandgap and fast charge carrier recombination), extensive design and fabrication strategies involving nanoscale morphology regulation, and heterojunction coupling with narrower bandgap semi-conductor materials, have enabled the preparation of nanocomposites with desired optical and charge-transfer properties [1]. While the promotion of the photocatalytic efficiency in nanocomposites is often attributed to synergistic quantum physicochemical effects, design and synthesis guidelines that account for intercorrelations among various key material properties (surface area, crystal and interface structures, bandgap energy) remain hardly elucidated.

In this work, we examine the effects of critical parameters on the morphology, synthesis microstructure, and optical absorption properties of bismuth oxide (Bi2O3) -doped TiO2-CeO2 (75:25 mol/mol) nanocomposites (Figure 1), produced by a sol-gel assisted solvothermal method, in the presence of structure directing agents such as acetic and lauric acids. The sol-gel and solvothermal methodologies are typical topdown synthesis approaches, owing to their adapatability for mass production, and versatility for the fabrication of mixed systems, with extended composition ranges and high degree of homogeneity. As coupling semi-conductor oxide co-catalysts, CeO₂ has a superior oxygen exchange and storage capacity, while Bi2O3 can exhibit a thermodynamically stable, visible-light positioned absorption edge, depending on the processing temperature.



Figure 1: Selected area scanning electronmicroscopy and elemental analysis map for 5 mol% Bi-doped TiO₂-CeO₂ (75:25).

The incorporation of both materials with TiO2 significantly improves the solar-driven photocatalytic activity in the context of chlorophenols and rhodamine B degradation studies in water. The influence of the Bi₂O₃ doping concentration, presence and amount of structuring agents, as well as the calcination program on key physical properties and their correlations to the photocatalytic performance of the nanocomposite materials (including the photocurrent density, and % removal efficiency) are discussed.

Keywords: Solar-driven photocatalysis, semiconductor metal-oxide nanocomposites, TiO₂, CeO₂, Bi₂O₃, sol-gel process, solvothermal synthesis, structure and performance correlations, degradation of organic contaminants in water.

References:

1. Coronado, J. M., Fresno, F., Hernández-Alonso, M. D., Portela, R. (Eds.). (2013). Design of advanced photocatalytic materials for energy and environmental applications (pp. 1-348). London: Springer.

A Simulation Study for ABS 3D Filament Doped with Nanoparticles for Thermal Neutrons Applications

E. Banoqitahı, E. Elmoujarkachı, F. Nadwiı, A. Alhawsawiı,

1 King Abdulaziz University, Department of Nuclear Engineering, Jeddah, Saudi Arabia

Abstract:

The last decade witnessed a huge advancement in several fields of science and technology including 3D printing. 3D printing is utilized in a wide range of applications, from printing small personal items to full-size houses. This research aims to test the thermal neutron radiation attenuation when using ABS filament infused with Gadolinium, Boron, Gold and Cadmium using a Monte Carlo simulation toolkit. Simulations showed Boron infused filaments to have the potential to be a good thermal neutron shielding material and also be used in the manufacture of water equivalent phantoms. As for the Gadolinium filament, Results indicated it could be possibly used as a cover for detectors to discriminate against neutrons in a radiation mixed field. Adding Gold nanoparticles reduced the total dose compared to the ABS. However, the neutron dose remined unchanged. The use of Cadmium resulted in a stable reduction for total dose with changing the thickness while reducing the neutron dose better than the pure ABS.

Keywords: 3D-printing, simulation, nanoparticles, thermal neutrons.

References:

- X. M. Abdulraheem Kinsara, Essam Banoqitah, Fuad Nadwi, Ahmed El-Gizawy, "Dose Reduction of the Scattered Radiation from Medical Radiation Exposures using 3D-printed Organ-shaped Fillable Shields," 2016.
- 2. J. Ceh *et al.*, "Bismuth infusion of ABS enables additive manufacturing of complex radiological phantoms and shielding equipment," *Sensors (Switzerland)*, vol. 17, no. 3, pp. 1–11, 2017.
- M. F. Bieniosek, B. J. Lee, and C. S. Levin, "3D printing for cost-effective, customized, reusable multi-modality imaging phantoms," *IEEE Nucl. Sci. Symp. Conf. Rec.*, 2013.
- 4. T. S. Yoo, T. Hamilton, D. E. Hurt, J.

Caban, D. Liao, and D. T. Chen, "Toward quantitative X-ray CT phantoms of metastatic tumors using rapid prototyping technology," in *Proceedings - International Symposium on Biomedical Imaging*, 2011.

- C. Hazelaar *et al.*, "Using 3D printing techniques to create an anthropomorphic thorax phantom for medical imaging purposes," *Med. Phys.*, vol. 45, no. 1, pp. 92–100, Jan. 2018.
- 6. G. J. Schoessow, *Introduction to Nuclear Engineering*, vol. 12, no. 2. 2017.
- 7. Kate Cummins, "The rise of additive manufacturing," 2010. .
- 8. D. Sarrut *et al.*, "A review of the use and potential of the GATE Monte Carlo simulation code for radiation therapy and dosimetry applications A review of the use and potential of the GATE Monte Carlo simulation code for radiation therapy and dosimetry applications," *Med. Phys.*, vol. 41, 2014.
- S. Jan *et al.*, "GATE V6: A major enhancement of the GATE simulation platform enabling modelling of CT and radiotherapy," *Phys. Med. Biol.*, vol. 56, no. 4, pp. 881–901, 2011.
- O. Ozyurt, N. Altinsoy, Karaaslan, A. Bora, B. Buyuk, and Erk, "Calculation of gamma ray attenuation coefficients of some granite samples using a Monte Carlo simulation code," *Radiat. Phys. Chem.*, vol. 144, no. July 2017, pp. 271–275, 2018.

Different charge ordering states in Niobium diselenide under strain and with metal adsorbates

F. Cossu1*, I. di Marco1,2,3, and A. Akbari1,3,4

Asia Pacific Center for Theoretical Physics, Pohang, Republic of Korea
 ² Department of Physics and Astronomy, Uppsala University, Sweden
 ³ Department of Physics, POSTECH, Pohang, Republic of Korea
 ⁴ Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang, Rep. of Korea

Abstract:

Transition metal dichalcogenides (TMdC) are layered van der Waals materials being tested as core constituents for electro-catalysis, energy storage1,2, nano-transistors3 and quantum computing4,5. In metallic TMdCs, charge density waves (CDWs) can coexist with superconductivity at low temperatures. Determining the nature of these collective electronic excitations in thin layers is crucial in view of their manipulation. We present a study of functionalisation of NbSe2 single layers by metal adsorptions and strain. In bulk NbSe2 a 3×3 CDW with triangular symmetry is observed; at the surface, impurities are present due to the high reactivity of NbSe2. We demonstrate6 that Co and Mn induce a triangular-hexagonal CDW transition, and the resulting CDW beats suggest a change of modulation. In addition, we find that a plethora of CDW modulations is possible for a NbSe2 pristine single layer under strain. We support, via ab-initio calculations, the recently observed stripe phase7,8 sided by the usual triangular phase and infer the coupling strength₉.

Keywords: transition metal dichalcogenides, charge density waves, phonon spectra, electronic structure, stripe phase, correlation, superconductivity.

References:

- Zhu J., Alshareef H. N. and Schwingenschlögl U. (2017) "Functionalized NbSe₂ as cathode for Liand Na-ion batteries", *Appl. Phys. Lett.*, **111**, 043903.
- 2. Chhowalla M., Shin H. S., Eda G., Li L.-J., Loh K. P. and Zhang H. (2013), "The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets", *Nat. Chem.*, **5**, 263.
- 3. Wang Q. H., Kalantar-Zadeh K., Kis A., Coleman J. N. and Strano M. S. (2012),

Electronics and optoelectronics of twodimensional transition metal dichalcogenides Nat. Nanotechnol. , **7**, 699.

- 4. Clarke J. and Wilhelm F. K. (2008), "Superconducting quantum bits", *Nature* **453**, 1031.
- Hsu Y. T., Vaezi A., Fischer M. H. and Kim E.-A. (2017) "Topological superconductivity in monolayer transition metal dichalcogenides", *Nat. Commun.* 8, 14985.
- Cossu F., Moghaddam A., Kim K., Tahini H. A., di Marco I., Yeom H.-W. And Akbari A. (2018) "Unveiling hidden charge density waves in single-layer NbSe₂ by impurities", *Phys. Rev. B* 98, 195419.
- Soumyanarayanan A., Yee M. M., He Y., van Wezel J., Rahn D. J., Rossnagel K., Hudson E. W., Norman M. R. and Hoffman J. (2013), "Quantum phase transition from triangular to stripe charge order in NbSe₂", *Proc. Natl. Acad. Sci.* **110**, 1623.
- Gao S., Flicker F., Sankar R., Zhao H., Ren Z., Rachmilowitz B., Balachandar S., Chou F., Burch K. S., Wang Z., van Wezel J. and Zeljkovic I. (2018), "Atomic-scale strain manipulation of a charge density wave", *Proc. Natl. Acad. Sci.* 115, 6986.
- Cossu F, di Marco I. and Akbari A. (2019), "Strain-induced stripe phase in charge ordered single layer NbSe₂", arXiv:1906.11142.

Electrosprayed Aerogel/PCM Embedded PTFE Microporous Materials for Thermal Protection

M.Venkataraman,1,* J. Militký,1, X. M. Xiong,1, M. Petrů2

¹ Technical University of Liberec, Department of Material Engineering, Faculty of Textile Engineering, Liberec, Czech Republic

² Technical University of Liberec, Institute for Nanomaterials, Advanced Technologies and Innovation, Department of Machinery Construction, Liberec, Czech Republic

Abstract:

As a gel composed of a porous solid where the dispersed phase is a gas, silica aerogel is an extremely light weight nanoporous material that has high specific surface area, high porosity, low bulk density and extremely low thermal conductivity [1]. Silica aerogel particles are readily commercially available, which enables an easy management to be incorporated in textile structures or polymer composites for the purpose of improving thermal insulation ability or thermal protection. Another attractive material for thermal protection is phase change material (PCM), which functions by absorbing external incoming heat flux as a shield for the protection from heat. The simultaneous use of aerogels and PCMs coated on a multilayer fabric structure have been found to offer superior thermal protection and comfort [2]. In this work, aerogels and **PCMs** were incorporated with polytetrafluoroethylene (PTFE) via electrospray technique (as seen in Figure 1). PTFE was selected for electrospray because it has many unique characteristics such as outstanding chemical stability and good thermal stability under high temperature. The use of electrospray technique allows easy incorporation of various particles with PTFE for performance modification. Therefore, fabrication of aerogel and PCM embedded PTFE microporous materials via electrospraying is preferred and the resultant material may combine the advantages of microporous membrane (porous, high pack density and ease management), PTFE (chemical and thermal stability) and thermal protection of aerogels and PCMs. Also, Kevlar fabrics coated with aerogel were prepared. Laser radiations revealed surface temperatures of the aerogel coated Kevlar fabrics to be lower than that of the uncoated fabric. Kevlar fabrics coated with silica aerogel provides better thermal protection under high temperature

Keywords: Silica aerogels, phase change materials, PTFE microporous materials,

electrospray technique, Kevlar fabric, laser irradation, thermal protection, infrared thermography.



Figure 1: Figure illustrating the scanning electron microscopy image of PTFE microporous layers which was electrosprayed with a 20min deposition time.

Acknowledgment

This work is supported by the Ministry of Education, Youth and Sports of the Czech Republic and the European Union (European Structural and Investment Funds - Operational Programme Research, Development and Education) in the frames of the project "Modular platform for autonomous chassis of specialized electric vehicles for freight and equipment transportation", Reg. No. CZ.02.1.01/0.0/0.0/16_025/0007293.

- 1. Pierre, A. C. and Pajonk, G. M. (2002). Chemistry of aerogels and their applications. *Chem. Rev.*, 102(11), 243-4265.
- 2. Shaid, A., Wang, L., Padhye, R. (2016). The thermal protection and comfort properties of aerogel and PCM-coated fabric for firefighter garment. *J. Ind. Text.*, 45(4), 611-625.

Integration of functional oxides on silicon

Abdelnour Benamarı, Guillaume Agnusı, Guillaume Saint-Girons2, César Magen3, Sylvie Schamm-Chardon4, Philippe LECOEUR1

¹Centre de Nanosciences et de Nanotechnologies, CNRS, Univ. Paris-Sud, Université Paris-Saclay, C2N, 91120 Palaiseau, France

2Ecole Centrale de Lyon, INL-UMR5270-CNRS, 69134 Ecully Cedex, France

3Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC-University of Zaragoza, Zaragoza, Spain

4Centre d'Élaboration de Matériaux et d'Etudes Structurales, UPR 8011-CNRS, 31055 Toulouse,

France

Abstract:

Functional oxides share the ABO₃ perovskite structure as a common crystal framework. Depending on the type of atoms occupying the A and B sites and potential dopants, they exhibit a wide range of physical properties such as ferromagnetism, ferroelectricity and superconductivity [1-2]. For example, comparing to Pt, LSMO has a high thermal coefficient near ambient temerature TCR = 1310-3 K-1, and low thermal conductivity coefficient k = 1.6 W/m.K [3].

The fabrication of MEMS structures based on epitaxial perovskite oxide consist in a very interesting way to take advantage of those exceptionnal properties. However, such realization requires (i) integrating crystalline perovskite on silicon to be able to use standard clean room fabrication processes and (ii) controlling the epitaxial and thermomechanical stresses that appear during the hetero-epitaxy of the perovskites on Si substrates. First, this stress plays a crucial role in the crystalline quality of the material and thus its physical properties. Many of this properties can be changed by varying the interatomic distances in the crystal lattice by applying stress [4]. Then, the stress relief induced by the releasing can highly reduce the fabrication yield.

As a consequence, we performed a detailed study on the stress level in these materials integrated on Si by:

- Transmission Electron Microscopy on our films that allows observing locally their overall quality and the presence of defects created to relax part of the stress. A typical image of an STO/Si template and a LSMO film grown by PLD on such template is shown in -Fig 1-.
- The temperature dependence of X-Ray Diffraction on different films, that allows to study the mechanical link between them, and to explain the changes that can take place

during a heat treatment. A study of the temperature dependence of the lattice parameters of an LSMO film grown on Si will presente in this work.

Keywords: Functional oxides, MEMS, TEM, PLD, MBE, XRD, integration functional oxides on silicon, microfabrication.



Figure 1: TEM images for a) STO/Si film, b) LSMO/STO/Si film.

- RE. Cohen, "Origin of ferroelectricity in perovskite oxides," Nature vol 358, pages 136-138 (1992).
- N. Reyren,S. Thiel, A. D. Caviglia, L. Fitting Kourkoutis, G. Hammerl, C. Richter, C. W. Schneider, T. Kopp, A.-S. Rüetschi, D. Jaccard, M. Gabay, D. A. Muller, J.-M. Triscone, J. Mannhart. "," Science. 31;317(5842):1196-9 (2007).
- L. Meda, L. Kennon, C. Bacaltchuk, H. Garmestani and K. H. Dahmen, "Effects of thermal annealing on the texture of La0.67Sr0.33MnO3 thin films," Journal of Material Research, 16(7), pages 1887-1889 (2001).
- 4. Aline Fluri1 and all, "In situ stress observation in oxide films and how tensile stress influences oxygen ion conduction," Nature 7:10692 (2016).

Challenges for High Performance of Polyaniline / Nanocomposite as Super Hydrophobic Coatings via Electrochemical Polymerization Technique

Z. Abdel Hamid^{*1}, M. Hasan Gomaa¹, S. S. Abd El Rehim², M.Abdel Hamid¹, A.Ibrahim³

1. Corrosion control & surface protection department, central metallurgical research and development institute, Cairo, Egypt

Chemical department, Faculty of science, Ain shams university, Caoiro, Egypt
 Farmingdale State University, USA

Abstract:

Superhydrophobicity is one of the research hotspots in surface science that has recently drawn a great deal of attention from both fundamental and practical application. In this study superhydrophobic polyaniline (PANI)/nano composite thin films were synthesized via electrochemical polymerization technique. Cyclic Voltammetry (CV) was the used method to synthesis PANI from strongly acidic medium (0.5M H₂SO₄). The effect of different deposition cycles on morphology, thickness, color, and properties of electrodeposited PANI thin films was investigated. The effect of the addition different contents of nano materials such as oxide and graphene on the morphology and contact angle (CA) of the formed coat was investigated. To investigate the morphological structure, field emission scanning electron microscopy (FE-SEM) and high resolution transmission electron microscopy (HR-TEM) were conducted. Characterization of the surface composition of the formed film has been performed using X-ray photoelectron spectroscopy (XPS). The results reveal that, the water contact angle of the prepared coat reaches to 150°. A granular morphology of PANI with a moderate amount of nanoparticles was obtained. XPS confirmed the incorporation of the oxides nanoparticles and graphene in the polymer matrix.

Keywords: Superhydrophobic; Nanostructures; Conducting polymers; electrochemical polymerization.



Figure: FE-SEM images of Polyaniline/TiO₂ composites deposited on ITO in the presence of different ratios of TiO₂ where, (a) 0.03g/L, (b) 0.4 g/L, respectively at 30th cycles.

- 1. Seong H. Kim ,"Fabrication of Superhydrophobic Surfaces". Journal of Adhesion Science and Technology, 22:3-4, 235-250
- Adel M.A. Mohamed, Aboubakr M. Abdullah, Nathalie A. Younan. "Corrosion behavior of superhydrophobic surfaces, A review". Arabian Journal of Chemistry, (2014).

^{*}Corresponding author: Corrosion Control & Surface Protection Lab., Central Metallurgical Research & Development Institute (CMRDI) P.O.8 7, Helwan, Cairo, Egypt. Tel.:+201223405792; Fax: +20 25010639. E-mail address: forzeinab@yahoo.com (Z. Abdel Hamid).

Nanotech ME 2020 Session II Nanomaterials for Energy and Environment / Nano Electronics

Application of Graphene Oxide Derivatives in Industrial Pharmaceutical Wastewater Treatment

T. Ibrahim 1, Mustafa Khamis2 and A. Zaka1

Department of Chemical Engineering, American University of Sharjah, Sharjah, UAE 2 Department of Biology, Chemistry and Environmental Sciences, American University of Sharjah, Sharjah, UAE

Abstract:

The consumption of water in pharmaceutical industries is not very high compared to other chemical industries. However, the produced wastewater generated by these industries is highly polluted and unsafe to the environment due to the presence of stable, persistent and biologically active organic component. Moreover, other direct or indirect sources such as hospital waste, treatment plant effluents and improper manufacturer's disposal have the potential to contaminate different water bodies. The presence of these pharmaceuticals in wastewater has led to a serious concern over their effect on human and animals because of their bioaccumulation in the food chain. Therefore, serious efforts are being made in the recent years to remove these contaminations from wastewater in order to reduce their effect on environment. The rising problem of pharmaceutical contamination in different water bodies calls for a swift action in the treatment and removal of these emerging pollutants from water using advance methods. Adsorption is employed as a primary treatment method for treating water containing Diclofenac sodium, Aspirin and Paracetamol (Acetaminophen). Two graphene oxide-based adsorbents namely, reduced graphene oxide magnetite (RGOM) and graphene oxide nickel ferrite (GONF) were used for the adsorption process. Batch experiments were conducted to find the optimum conditions such as contact time, adsorption dosage, pH of temperature and the solution, initial concentration. These optimum values were then used to perform number of experiments in order to fit isotherm models such as Langmuir, Freundlich and Temkin model. Pseudo-first and pseudo-second order kinetic models were also used to fit the kinetic data. Thermodynamic properties such as change in Gibbs free energy, enthalpy and entropy were then calculated to get further insight of the adsorption process. RGOM showed better results with the removal

efficiency of more than 90% for the abovementioned pharmaceuticals.

The removal efficiency of GONF to remove Diclofenac sodium, Aspirin and Paracetamol was around 20%, 40% and 65 % respectively. Reusability of both RGOM and GONF was studied for economic aspects of their applicability. Based on better performance, RGOM was also used to study continuous fixedbed adsorption of all three pharmaceuticals and the effect of flow rate of contaminated water and the bed depth of adsorbent in the column was studied. The adsorption data was fitted using different continuous adsorption models to obtain adsorption parameters.

Keywords: Pharmaceutical, Adsorption, wastewater treatment, graphene oxide, nanocomposites.

Modified graphene oxides as efficient electrode for Capacitive deionization

Khalil Abdelrazek khalili, *, Nasser A. M. Barakat2, Moaeed Motlak3 and Fahad S. Al-Mubaddel4

Department of Mechanical & Nuclear Engineering, College of Engineering, University of Sharjah, P.O. Box 27272, Sharjah, UAE 2Chemical Engineering Department, Minia University, El-Minia 61519, Egypt

nemical Engineering Department, Minia University, El-Minia 61519, Egypt

³Department of Physics, College of Science, University of Anbar, Anbar, Iraq. ⁴ Chemical Engineering Department, College of Engineering, King Saud University, Riyadh 11421,

Saudi Arabia

Abstract:

Here we developed N-doped & TiO₂ decorated graphene oxides as efficient non-precious electrodes for capacitive deionization. The activity of this new material has been evaluated insitu and in-vivo. The performance of the synthesized material was measured in different saline solutions (0.1, 0.5 and 1.0 M NaCl) electrolyte. The results showed that the new material shows very good value (157 F/g at 5 mV/s and 1.0 M NaCl compared to 19.5 F/g for the graphene oxide). In desalination test, which was performed in batch mode, the salt removal efficiency and the electrosorption capacity are 98 % and 9.2 mg/g, respectively. To check the stability, the desalination test has been repeated several times, no change in the performance was observed. Results show evidence that the new synthesized material provides a potential electrode material for CDI water desalination with a satisfactory salt removal.

Keywords: Capacitive deionization, TiO2&N-doped graphene oxides, Water desalination

Surface Deposited Copper Particles on Composite Nonwovens

J. Militký,1* M. Venkataraman1, J. Večerník2, M. Petrů,3

1 Technical University of Liberec, Textile Faculty, Department of Material Science, Liberec, Czech

Republic

2, Večerník s.r.o., Alšovice, Czech Republic

3 Technical University of Liberec, CxI, Department of Machine Constructions, Liberec, Czech

Republic

Abstract:

Textile structures with surface deposited metals have plenty of benefits as low cost, low weight and thickness, flexibility, durability comfort and porosity (air permeability). They can be applied for technical purposes as sensors, energy harvesting devices, field-effect transistors, electromagnetic interference (EMI) shieldings, antennas and ohmic heating. They can be integrated into fabrics forming wearable flexible devices for detecting human motion, monitoring and reporting health conditions of patients, preparation of textiles with reflection of body heat or sun rays (control of FIR radiation), antibacterial layers etc.

Main aim of this contribution is description of procedure for textiles surface deposition of dense nanoparticles layer based on the surface activation followed by surface metallization in strong alkali bath containing metallic salts at ambient temperatures.

Most fibrous polymers are hydrophobic, have a low surface free energy, which greatly hinder metal surface adhesion. A necessary step is modification of their surface creating chemical and/or physical changes to in order to improve the adhesion strength of the deposited metals.

As appropriate type of metal, copper was selected. The most important properties of pure copper are high thermal and electrical conductivity. Copper is a redox-active metal and has the ability to donate and accept electrons to shift between reduced (Cu_+) and oxidized (Cu_{2+}) states.

For copper deposition the composite nonwovens MILIFE (product of JX Nippon ANCI Corp.) from cross-over layers of PET monofilaments (combination of machine direction and cross direction oriented nonwoven layers) from poly (ethylene terephthalate/ isophthalate) copolymer with very low thickness, excellent shape stability and mechanical properties was selected. Copper coating have been realized by using of autocatalytic deposition where, Cu₂₊ ions contained in the depositon bath were reduced in the presence of a catalyst. MILIFE with surface deposited copper (abbreviation MIC) is shown in fig. 1.



Figure 1: Surface deposited copper (different magnifications)

Measured planar mass of MIC was equal to 42.13 [g m-2], thickness was 0.112 [mm] and volume porosity 72.35 [%]. By EDX elemental analysis the surface deposition of Cu 54.8 % was found. The reflectivity transmissivity and emissivity of MIC were evaluated from IR measurements. The IR reflectance at 10 µm was 79.74 % and at 1 µm it was was 69.2 %. The effectivity of electromagnetic shielding was measured from 30 MHz up to 1.5 GHz (according to ASTM D 4935-10) - mean value 62.71 dB was found. MIC is extraordinary in electrical properties. Specific volume resistivity $rv = 0.816 [\Omega m]$ was evaluated according to EN 1149-2. The surface resistivity was rs = 1.466 [Ω /sq]. Measured air permeability was 1341 [l /m2/s]. The main applications of MIC are discussed in ref. [1].

ACKNOWLEDGEMENT

This work was supported by project "Modular platform for autonomous chassis of specialized electric vehicles for freight and equipment transportation", Reg. No.

CZ.02.1.01/0.0/0.0/16_025/0007293.

References:

1. Militký J. et al, chap. 8 in book Křemenáková D., et al. eds.: *Advances in Fibrous Material Science*, OPS Kanina Publ. House, Pilzen 2015

Keywords: deposition of copper nanoparticles, multifunctional effects, electrical conductivity, EMI shielding, thermal reflection.

Nanotech ME 2020 Session III Nanomaterials for Energy and Environment

Optimized wet graphene transfer on SiO₂/Si substrate using chemical surface treatment for potential solar cell application

A.F. Abdelaal,1 B. Salhi,2 T. Laoui,3,*

King Fahd University of Petroleum and Minerals, Department of Mechanical Engineering, Dhahran, Saudi Arabia

² King Fahd University of Petroleum and Minerals, Centre of Research Excellence in Renewable Energy, Dhahran 131261, Saudi Arabia

³ University of Sharjah, Department of Mechanical and Nuclear Engineering, Sharjah, United Arab Emirates

Abstract:

Graphene is the thinnest, strongest and stiffest material with exceptional properties such as thermal conductivity and electron mobility. Therefore, it is widely considered for solar cells applications and electronic devices. These unique properties allow graphene to be explored in many technologies such as gas detection sensors, flexible touch screens and solar cells. However, the main challenge is to transfer graphene layer, from the growth substrate (typically copper, Cu) to the target substrate to produce a large-area, low or almost defect-free graphene, which plays an important role in the performance of the graphene/substrate. Chemical vapor deposition (CVD) is a common method for growing graphene on a metal surface (e.g. Cu) used as a catalyst for graphene nucleation. This induces a transfer step by etching the metal substrate and then transferring the graphene layer onto a desired target substrate. Interfacing between graphene layer and the target substrate surface is a critical challenge in preserving its promising high mobility. This has initiated the motivation for studying the effect of intermediate interfaces imposed by transfer processes. The present work has investigated the effect of cleaning SiO2/Si substrate using hydrofluoric acid (HF), piranha solution, and plasma on the wettability of the substrate surface towards enhancing the transfer process and reducing the typical defects (wrinkles, tears, and cracks) obtained on the transferred graphene layer. It is found that HF has resulted in the highest hydrophilicity of the SiO₂/Si substrate. The surface cleaning using HF for 80 sec has decreased the water contact angle to the lowest value of ~ 30, yielding a minimal amount of wrinkles and cracks on the transferred graphene, as shown in Figure 1. Moreover, this cleaning method has greatly improved the transparency and electrical conductivity of the considered substrate, these being important properties for potential solar cells application.

Keywords: Graphene, graphene transfer, SiO₂/Si substrate, surface cleaning, hydrophilicity, chemical vapor deposition



Figure 1: Graphene transferred on (a) bare SiO₂/Si substrate (b) SiO₂/Si substrate after treatment with HF for 80 seconds.

- Mahmoudi, T., Wang, Y. & Hahn, Y.-B.
 B. Graphene and its derivatives for solar cells application. *Nano Energy* 47, 51–65 (2018).
- 2. Macucci, M., Betti, A. & Marconcini, P. Graphene as a material for nanoelectronics. *Adv. Mater. Sci.* **15**, 67 (2015).
- Kalita, G., Matsushima, M., Uchida, H., Wakita, K. & Umeno, M. Graphene constructed carbon thin films as transparent electrodes for solar cell applications. *J. Mater. Chem.* 20, 9713– 9717 (2010).
- 4. Yuan, W. & Shi, G. Graphene-based gas sensors. J. Mater. Chem. A 1, 10078 (2013).

Electric field hotspots of all-inorganic APbX $_3$ (A = Cs, Rb and X = Cl, Br, I) perovskite quantum dots

Junais Habeeb Mokkath

Quantum Nanophotonics Simulations Lab, Department of Physics, Kuwait College of Science And Technology, Doha Area, 7th Ring Road, P.O. Box 27235, Kuwait

Abstract:

Fully-inorganic perovskite quantum dots (QDs) have emerged as an exciting family of semiconductor materials with outstanding opto-electronic properties. Here, using state-of-the-art time dependent density functional theory calculations, we present a comprehensive study of the absorption crosssections and the electric field enhancements of fully-inorganic APbX $_3$ (A = Rb, Cs and X = Cl, Br, I) perovskite QDs. We show that the type of halide element is a key parameter in determining the QD optical features. Specifically, we demonstrate the dramatic variations in the electric field enhancements and the significant modifications in the hotspot regions with respect to the halide element, confirming the excellent photo-catalytic activity of perovskite QDs reported by the recent experiments. Fully-inorganic perovskite quantum dots (QDs) have emerged as an exciting family of semiconductor materials with outstanding opto-electronic properties. Here, using state-of-the-art time dependent density functional theory calculations, we present a comprehensive study of the absorption cross-sections and the electric field enhancements of fully-inorganic APbX $_3$ (A = Rb, Cs and X = Cl, Br, I) perovskite ODs. We show that the type of halide element is a key parameter in determining the QD optical features. Specifically, we demonstrate the dramatic variations in the electric field enhancements and the significant modifications in the hotspot regions with respect to the halide element, confirming the excellent photo-catalytic activity of perovskite QDs reported by the recent experiments.

Keywords: TD-DFT, perovskite quantum dots, electric field modulations

Polymer and Nanoparticles as a New Method for Chemical Enhanced Oil Recovery

P. Druetta (p.d.druetta@rug.nl)*, F. Picchioni,

Department of Chemical Engineering, ENTEG, University of Groningen, Nijenborgh 4, 9747AG, Groningen, The Netherlands.

Abstract:

Enhanced Oil Recovery (EOR) is one of the most relevant topics in oil industry. It is well the use of numerical simulation known techniques to improve production and drilling strategies as well as the design of new products to increase the recovery in mature oil fields. Furthermore, during the last years nanotechnology was considered as a way to boost these methods. Several research lines have been developed, not only in EOR but also in exploration, drilling and refining. This work is based in previous ones published by the authors (see Appl Math Model 2017; 47: 141-159, doi: 10.1016/j.apm.2017.03.017, Applied Sciences 2018; 8: 2596, doi: 10.3390/app8122596 and Energies 2018; 11: 2280, doi: 10.3390/en11092280), dealing with the numerical simulation of chemical EOR processes and review of nanotechnology in EOR.

The aim is to present a novel simulator, proposing a new combined EOR flooding method comprising polymers and nanoparticles and considering several characteristics which, to our best understanding, have never been published in the open literature. With this respect, we have developed a two-phase, fivecomponent reservoir simulator, adopting the compositional approach, using a fully secondorder discretization scheme with TVD flux limiters in the mass conservation equation. This renders a highly non-linear system of equations that are solved using the IMPEC (Implicit in Pressure, Explicit in Concentration) scheme. The polymer behavior is modeled considering all the physical phenomena mentioned in the including a degradation module literature. considering the scission of the polymer's backbone and the influence of the (macro)molecules' architecture on the rheological properties. On the other hand, the nanoparticles are considered to affect several parameters in the rock formation and phases, namely: interfacial tension, viscosity, adsorption, wettability alteration, porosity and

permeability. This also includes the aggregation of nanoparticles, affecting the rheology and adsorption rates. With respect to the synergy between polymer and nanoparticles, the combined presence has an influence on the particles' diffusion coefficient and on the adsorption process, phenomena which have never been reported in the literature in reservoir simulation. The results evidenced the potential in combining the effects of polymers with nanoparticles as a mean to increase the recovery efficiency in low- and medium viscosity oilfields (see Figure 1).

Keywords: Enhances Oil Recovery, reservoir simulation, polymer, nanotechnology, polymer architecture, Total Variation Diminishing.



Figure 1: EOR using different techniques. The secondary recovery (black) is compared to a standard polymer flooding (red) and a process combining nanoparticles with polymers (green).

Antioxidant Gold nanoconjugates for the treatment of neurodegenerative diseases

Maria Elena Piersimoni1,3, Tony Cass2,3, Liming Ying1

Faculty of Medicine, National Heart and Lung Institute, Imperial College London, United Kingdom
 Faculty of Natural Sciences, Department of Chemistry, Imperial College London, United Kingdom
 Bio Nano Consulting, London, United Kingdom

Abstract

Gold nanoparticles (GNPs) have emerged as promising carriers in drug delivery, sensing and imaging applications because of their ability to internalize within cells and their physicochemical properties. Furthermore, GNPs have been increasingly used in biomedical applications and have shown great potential as drug delivery systems for the treatment of Parkinson's (PD) and Alzheimer's (AD) disease1,2.

PD and AD are progressive and degenerative disorders of the central nervous system (CNS). Although there are a variety of pathological features in PD and AD, including the loss of dopamine signals from the *subsantia nigra* and the loss of synapse and selective neuronal death, respectively, the accumulation of Reactive Oxygen Species (ROS) has an established role in both diseases₃. The lack of an effective therapy as well as the increased number of PD and AD patients raise a huge and unmet need for the development of a promising and proper treatment. Herein we present the synthesis of GNPs, their functionalization with lipoic acid (LA) and α-synuclein via thiol-gold bond self assembly and electrostatic adsorption respectively. We then monitor the interactions between the two type of nanoparticles and SH-SY5Y neuroblastoma living cells in real-time, employing a variety of microscopy techniques. Since Lipoic Acid is known to be able to reduce the endogenous ROS level and to act as an antinflammatory agent₄, an in-depth understanding of GNPs-LA interaction within living neuroblastoma cells is expected to result in a more targeted application of the antioxidant GNPs-LA system for alleviating PD and AD severity triggered by ROS.

Furthermore, recent findings, having demonstrated that LA also prevents α -synuclein accumulation⁵, GNPs-LA may serve as an anti-oxidative agent towards the generated ROS by α -synuclein as well as a down-regulated agent of the protein accumulation



Figure 1. A Transmission electron microscopy of GNPs (scale bar= 50μ m). B Zeta-potential measurements of GNPs (black), GNPs-LA (orange) and GNPs- α -syn (green) (mean \pm SD, n =3). C Intracellular uptake and distribution of GNPs-LA (red, Cy5.5 label) and GNPs- α -synuclein (green, AlexaFluor label). Live SH-SY5Y cells were exposed to GNPs-LA and GNPs- α -synuclein 12 h prior to imaging by confocal microscopy. The nucleus is visualized in blue (Hoechst 33342). Scale bar = 10μ m.

- 1. V. Amendola, R. Pilot, Frasconi M., Maragò OM, Iati MA, vol. 29, p. 203002, 2017.
- 2. J. Ruff, S. Hüwel, M. J. Kogan, U. Simon, and H. Galla, vol. 13, pp. 1645–1652, 2017.
- 3. D. Hadavi and A. A. Poot, vol. 4, n. June ,2016.
- 4. H. Moini, L. Packer, N. E. L. Saris, vol. 182, pp. 84–90, 2002.
- 5. Y. Ge, K. Xu, pp. 1-7, 16:86, 2016.

Shape-Stabilized Phase Change Materials for Solar Energy Storage: MgO doped CaCO₃ mixed with Polyethylene Glycol

Salem Khaled Saeed Basamad 2, Md. Hasan Zahir 1,*, Mohammad M. Hossain 2

¹ Center of Research Excellence in Renewable Energy (CoRE-RE), Research Institute, King Fahd University of Petroleum & Minerals, (KFUPM), Dhahran 31261, Saudi Arabia, 1Researcher at K.A.CARE Energy Research & Innovation Center at Dhahran,

² Department of Chemical Engineering, King Fahd University of Petroleum & Minerals, (KFUPM), Dhahran 31261, Saudi Arabia

Abstract:

Non-renewable resources such as fossil fuels have many drawbacks, including their limited availability and the emission of harmful gasses upon use. The world is switching to new renewable energy sources as a result. Latent heat storage through phase change materials (PCMs) is one of the most promising techniques employed in this area. Due to their extremely small variation in temperature, isothermal operating conditions, and high density of energy storage, PCMs have turned out to be a hotspot of research in the fields of air-conditioning systems, solar heating systems, thermal regulation and insulation, energy conservation of buildings, recovery of waste heat, etc.[1-2] In this study nanosize porous powders of MgO containing phase pure CaCO₃ were successfully synthesized hydrothermally and impregnated with polyethylene glycol-6000 (PEG) to form a shape-stabilized PCM (ss-PCM). The micro-structure and composition of the supporting materials were characterized using XRD, FT-IR spectra, Raman spectra, FE-EM, EDS, XPS, TGA, and BET surface area determination. About 69% of PEG was impregnated into the 10 mol% MgO doped-CaCO₃ (10MgCaCO₃) supporting matrix. A considerably high latent heat of fusion of 152.5 J/g was obtained for the PEG/10MgCaCO3 PCM. The 10MgCaCO₃ powders possess two types of pore formations, i.e., sharp mesopores and a broad type mixed mesopore and macropore distribution. They may play a crucial role in retaining a large amount of PEG, resulting in a high latent heat. Additionally, TGA analysis indicates that PEG/10MgCaCO3 PCM also possess excellent thermal properties. In addition, the supporting materials enhance the thermal conductivity of PEG, which overcomes the low-thermal conductivity of the organic PCM. The supercooling effect of pure PEG is reduced by 23.5% when PEG is impregnated into 10MgCaCO₃. After several thermal heating and cooling cycles, PEG/10MgCaCO₃ PCM retains the ability of storing and releasing energy without a significant change. {Fig. 1]

Keywords: solar thermal energy storage, phase change materials, MgO doped-CaCO₃ porous support, hydrothermal



Fig. 1. Melting–freezing DSC cycling curves of PEG/10MgCaCO₃ PCM samples, repeated 10 times.

- Mohamed, S.A., F. A. Al-Sulaiman, A., Ibrahim, N.I., Zahir, M.H., Al-Ahmed, Saidur, A.R.,Yılbaş, B.S. (2016), Sahin, A.Z. A Review on Current Status and Challenges of Inorganic Phase Change Materials for Thermal Energy Storage Systems, *Renew. Sustain. Energy Rev.* 70, 1078-1089.
- Zahir, M.H., Mohamed, S.A., R. Saidur, R., Al-Sulaiman, F. Supercooling of phasechange materials and the techniques used to mitigate the phenomenon (2019) A. *Appl. Energy* 240, 793-817.

Nanotech ME 2020 Posters Session

Effect of the Concentration of Graphene Nanoplatelets in the Photo-oxidation of the Polypropylene

F.P. La Mantia,1,2,* L. Botta1,2, M.C. Mistretta1, M. Ceraulo1,2

¹ Department of Engineering, University of Palermo, Palermo, Italy ² INSTM, Firenze, Italy

Abstract:

The photo-oxidation behaviour of polymer nanocomposites depends, of course, on the photo-oxidation behaviour of the matrix, but also on the concentration, on the physical and geometrical characteristics of the nanoparticles and on the possible interactions between the two phases. In the case of nanocomposites with carbon nanotunes or graphene nanoparticles, the polymer matrix is photo-stabilized because of the absorption of the UV energy from the carbon nanoparticles. In this work we effect investigated the of different concentrations of graphene nanoplatelets (GnP) on the photo-oxidation kinetics of the polypropylene. The photo-oxidation kinetics of the polypropylene is remarkably reduced in presence of graphene nanoplatelets and this effect increases with the graphene content. The time at which the elongation at break reaches one half of its initial value, indeed increases from 16.5 hr for the pure matrix to 50 hr for the sample with 1% GnP and to 60 hr for nanocomposite with 2% of GnP. This feature is common to all the other carbonaceous substances like carbon black and carbon nanotubes and due to the absorption of the ultraviolet energy that is no more available for the formation of radicals and for the consequent propagation of the oxidation reactions. However, the increase of this time is not linear with the GnP content, but it increases less than linearly when the GnP content is larger than 1%. This behaviour, then, cannot be correlated only with the higher content of GnP. Moreover, this result cannot be correlated also with the dimensions of the graphene nanoplatelets. Indeed, it has been demonstrated that the particle size of the nanocomposite with 2% of GnP is slightly larger than that of the less concentrated nanocomposites due to some aggregation of the nanoparticles with increasing the GnP content. This effect has been interpreted in terms of larger exposed surface of the sample with 2% of GnP with respect to the

other samples with lower GnP content which show smaller dimensions of the GNP, but also lower exposed surface.

Keywords: photo-oxidation, photostabilization, polypropylene, graphene, exposed surface, particle size.

References:

M.C. Mistretta, L. Botta, A.D. Vinci, M. Ceraulo, F.P. La Mantia "Photo-oxidation of polypropylene/graphene nanoplatelets" Polym. Deg. Stab., 160, 35-42 (2019)

Sub-millimeter-scale synthesis of chromium doped CdS nanosheets and their temperature-dependent excitonic emission

D. J. Lee,1,* D. Y. Kim,1,2

1 Quantum-Functional Semiconductor Research Center, Dongguk University, Seoul, Korea 2 Department of Semiconductor Science, Dongguk University, Seoul, Korea

Abstract:

Recent nanoscale science requires the development of smaller and more functional materials. However, as the size becomes smaller, the device utilization is not easy. Therefore, one solution for device utilization of nanomaterials may be to increase aspect ratio by making large areas with nanoscale thicknesses. We grew submillimeter scale chromium doped cadmium sulfide (CdCrS) nanosheets by a simple catalystfree vapor phase epitaxy (VPE) process and investigated the photoluminescence spectra of CdCrS nanosheets with temperature change.

The CdCrS nanosheets exhibited a clear luminescence peak from the neutral acceptorbound exciton (AoX), which persisted near room temperature. Compared to the undoped CdS nanosheets, the inhomogeneous thermalbroadening of the excitonic-emission line-width in CdCrS nanosheets is dominant at lower temperatures. This is attributed to the increase of ionized impurity scattering from Cr ions and results in the increase of exciton-phonon coupling strength. We have evaluated it through fitting of the Bose-Einstein approximation. As a consequence, Cr dopant can lead to low excitonic emission efficiency of CdS nanosheets.

Keywords: cadmium sulfide, nanosheets, photoluminescence, sub-millimeter scale.



Figure 1: Figure shows temperature-dependent photoluminescence spectra of sub-millimeter – scale CdCrS nanosheets at 10-300K. Inset shows the emission energy of A_0X as a function of temperature.

- Mullaugh, K. M., Luther, G. W., (2010) Spectroscopic determination of the size of cadmium sulfide nanoparticles formed under environmentally relevant conditions, *J. Environ. Monit.*, 12, 890-897.
- 2. Bie, C., Fu, J., Cheng, B., Zhang, L. (2018), Ultrathin CdS nanosheets with tunable thickness and efficient photocatalytic hydrogen generation, *Appl. Surf. Sci.*, 462, 606-614.

Activation Energy of Hydrogen Evolution Reaction on Strontium modified TiO₂ nanotubes

Khadijah M. Emran

Chemistry Department, College of Science, Taibah University, Al-Madinah Al-Monawarah, Saudi Arabia. (*E-mail: kabdalsamad@taibahu.edcu.sa)

Abstract:

A highly active electrochemical catalyst of Strontium/titanium dioxide nanotube composite (Sr-TNTs) has been developed for the hydrogen evolution reaction (HER). The TNT and Sr-TNTs were synthesized by the method of direct hydrothermal synthesis. The morphology of the final product was characterized by SEM, EDX, X-ray diffraction and Raman Pattern. The enriched Sr-TNT/Pd modified catalyst on Au electrode with highly dispersed nanowires and uniform Sr nano crystallites provides an efficient electrocatalysis, leading to their superior HER activity with lower Activation Energy (5.56 kJ/mol) and optimum current densities (1.393 mA/cm₂) in 0.1 mol L-1 H₂SO₄ solution. The reaction mechanism is identified according to Volmer-Tafel mechanism. The TNT/ Pd and Sr-TNT/ Pd modified Au electrode demonstrated affords faster electron transfer during electrochemical experiments. The exceptional performance of the Pd@Sr-TNTs cathodes is assigned to the unique semiconducting properties of the threedimensional, interactive TNTs supporting structures that, on the one hand, provide abundance of Pd active sites with optimized atomic hydrogen binding energy in acidic media for the hydrogen production and on the other hand, Sr metal that increase the conductivity. A mechanism for hydrogen evolution reaction on Sr-TNT/ Pd has been proposed where both hybrid metal and support metal are involved in the charge transfer process.

Keywords:	Electrocatalysts;	Strontium
nanotubes;	Hydrothermal;	Hydrogen
generation;Ac	tivating energy.	



Figure 1: Mechanism of electrocatalysts and charge separation of Au/Sr-TNT/Pd.

- 1. Su, E., Huang, B., Wey M.(2016), Enhanced optical and electronic properties of a solar light-responsive photocatalyst for efficient hydrogen evolution by SrTiO₃/TiO₂ nanotube combination, *Solar Energy*, 134, 52–63.
- Zhao, Q., Zhang, Q., Du, C., Sun, S., Steinkrug er, J.D., Zhou, C., Yang, S. (2019), Synergistic Effect of Dual Particle-Size AuNPs on TiO₂ for Efficient Photocatalytic Hydrogen Evolution, *Nanomaterials*, 9(4), 499.

Efficient hydrogen production electrocatalytic using hydrothermal Synthesized Sn-TNT nanotubes

Khadijah M. Emran*, Rawan M. A. Alsahli

Department of Chemistry, College of Science, Taibah University, Madinah 30002, KSA. Corresponding author: Khadijah M. Emran, E-mail: kabdalsamad@taibahu.edu.sa, Tel: +699-551-6360035

Abstract:

Advanced nanomaterials for electrocatalytic water splitting are central to the area of renewable energy. Here, we developed for the first time a hydrothermal synthesis of Sn-TNT nanotubes selectively on GC electrode in acid solution. XRD, SEM, EDX and Raman spectra characterizations on TNT and doped Sn-TNT were carried out and suggested successful incorporation of Sn in tubular structure of TiO2. The catalytic activity toward hydrogen evolution reaction (HER) of TNT and doped Sn-TNT with electrodeposited of Pd and/or Pt nanoparticle was investigated using CV and Tafel polarization. The activation energy (E_a) , and reaction mechanism have been determined using Tafel polarization. The Sn-TNT/Pt-Pd modified catalyst showed up to 58 times more efficiency with low Ea (2.78)kJ/mol) towards electrocatalytic production of hydrogen than Sn-TNT where no activity has been shown with TNT. Adsorption of hydrogen on the catalyst controlled the overall reaction rate. The TNT/Pt-Pd and Sn-TNT/Pt-Pd modified GC electrode demonstrated highly stability and affords faster transfer during electrochemical electron experiments. This study opens a new perspective for the development of highly active TNT electrocatalysts for hydrogen production from water splitting.

Keywords: Titanium Dioxide Nanotubes, Hydrogen evolution reaction, Water electrolysis, Tin-doped, electrocatalytics. Temperature electrode, Activation energy, Catalyst support.



Figure 1: Cyclic voltammograms of bare GCE and the TNTs annealed at $459 \circ C \text{ in } 0.1 \text{ M H}_2SO_4$ solution at scan rate of 100 mV/s.

- Yin, K., Cheng, Y., Jiang, B., Liao, F., Shao, M. (2018) Palladium – silicon nanocomposites as a stable electrocatalyst for hydrogen evolution reaction, J. Collo. & Interf. Sci.522, 242–248.
- Du, J., Wang, X., Li, C., Liu, X., Gu, L., Liang, H. (2018) Hollow Rh nanoparticles with nanoporous shell as efficient electrocatalyst for hydrogen evolution reaction, Electroch. Acta, 282, 853e859

Synthesis of quaternary chalcogenide CPSS (CuPbSbS₃) as a candidate absorber material for solar cells

Yasser T. Alharbi,1 and David J. Lewis 2*

School of Chemistry, University of Manchester, Oxford Road, Manchester, M13 9PL, UK 2 School of Materials, University of Manchester, Oxford Road, Manchester, M13 9PL, UK E-mail: david.lewis-4@manchester.ac.uk

Abstract:

The precursors bis(diethyldithiocarbamato) Copper(II), $Cu(S_2CNEt_2)_2$, bis(diethyldithiocarbamato) lead(II), Pb(S₂CNEt₂)₂ and bis(diethyldithiocarbamato) antimony (III), Sb(S2CNEt2)3 were prepared, characterized and employed for synthesis of the quaternary material CuPbSbS3 (CPSS) by two techniques of melt reaction and of spray pyrolysis. The polycrystalline material was characterized via p- XRD diffraction and Raman spectroscopy, and corresponded with the orthorhombic bournonite phase. The platy like morphology was investigated by using scanning electron microscopy. Further characterization with EDX and UV-Vis were confirmed the formation of CPSS. The optical band gap was measured 1.5 eV, which is a good candidate absorber material for solar cells.1 To the best of our knowledge this is the first report on the synthesis CuPbSbS3 (bournonite) from single source precursors by solvent-less melt and spray pyrolysis methods.

Keywords: precursors, diethyldithiocarbamato, melt reaction, spray pyrolysis, , circular dichroism spectroscopy, polycrystalline,



Figure 1: Figure illustrating the SEM images of quaternary material CuPbSbS₃ at 500 °C by melt method. **References:**

 S. K. Wallace, K. L. Svane, W. P. Huhn, T. Zhu, D. B. Mitzi, V. Blum and A. Walsh, Sustainable Energy & Fuels, 2017, 1, 1339– 1350.

Mechanical and electrical properties of GeSn nanowires and their application in NEM switches

R. Meija, 1 J. Kosmaca, 1 M. Antsov, 1 R. Sondors, 1 Justin D. Holmes, 2 D. Erts1,3

1 University of Latvia, Institute of Chemical Physics, Riga, Latvia

² University College Cork, School of Chemistry, ERI and the Tyndall National Institute, Cork, Ireland ³ University of Latvia, Faculty of Chemistry, Riga, Latvia

Abstract:

Germanium tin (GeSn) has been proposed as a promising material for optical and electronic applications due to the formation of a direct band-when a Sn content >7 at.% and its compatibility with Si. The ability to manipulate via synthesis properties of GeSn nanowires can enable realization of advanced mechanical devices. Here for the first time the mechanical properties of GeSn nanowires (7.1 – 9.7 at % Sn) are reported. Mechanical resonance and AFM bending tests to obtain Young's modulus and maximum bending strength of the nanowires were used.

and show their suitability for use in novel design nanoelectromechanical switches.

Furthermore, the ability to manipulate the properties of GeSn at the nanoscale will

further permit the realisation of advanced mechanical devices. Here we report for the first time the mechanical properties of Ge1-xSnx nanowires (7.1 - 9.7 at % Sn) and assess their suitability as nanoelectromechanical (NEM) switches . Electron microscopy analysis showed the nanowires to be single crystalline, with surfaces covered by a thin native amorphous oxide layer. Mechanical resonance and bending tests at different boundary conditions were used to obtain size-dependent Young's moduli and to relate the mechanical characteristics of the alloy nanowires to nanowire geometry and Sn incorporation. The mechanical properties of the GeSn alloy nanowires make them highly promising for applications in next generation NEM devices [1].

Keywords: Nanoelectromechanical systems, NEMS, nanowires, GeSn, Young modulus



Figure 1: (a) SEM and (b) AFM images for a GeSn nanowire suspended on a trench for threepoint bending tests (top view); (c) FEM simulation of the bending test (cut plane through centre axis of the nanowire and threedimensional model); (d) force–displacement curves obtained during nanowire bending (black dots) and from FEM simulation (red circles), used for determining the Young's modulus of the nanowire.

References:

 Kosmaca, J.; Meija, R.; Antsov, M.; Kunakova, G.; Sondors, R.; Iatsunskyi, I.; Coy, E.; Doherty, J.; Biswas, S.; Holmes, J. D.; et al. (2019) Investigating the Mechanical Properties of GeSn Nan-owires, *Nanocale* 11 (28), 13612-13619.