Global Advanced Materials and Surfaces – GAMS 2015
Conference Program

December 7, 2015
Session I: Advanced Materials Fabrication, Characterization and Tools / Properties

Al-Safa 1&2 Conference Room

Session Chairs: Prof Taleb Ibrahim - UAE / Prof Daniel Choi - UAE

08:00-09:30	**Registration**	
09:30-10:15	Recent Advances in Silica Aerogel Synthesis and Processing **K. Saoud**	**Prof Khaled. Saoud**, Virginia Commonwealth University in Qatar, **Qatar.**
10:15-10:45	**Coffee Break / Posters Session**	
10:45-11:30	Nanocrystals as Tunable Platforms for Chemical Reactions, Sensing and Imaging **H. Mattoussi**	**Prof Hedi Mattoussi**, Florida State University, **USA**
11:30- 11:45	Synthesis and Characterization of Hybrid Material based on Ionic Liquid and Amorphous Porous Silicon **M.R. Tchalala** and S .Chaieb	**Dr Mohamed R. Tchalala**, King Abdullah University of Science and Technology-Thuwal, **Saudi Arabia**
11:45-12:00	Effect of Repetitive Thermomechanical Processing on Grain Boundary Characteristics in alpha---phase brass **K.Al-Fadhalah**	**Dr. Khaled Al-Fadhalah,** Kuwait University, **Kuwait**
12:00-12:15	Ion Beam Induced Aluminum-doped Zinc Oxide-Bumps Aligning Liquid Crystals with the Tunable Surface Wettability for High Performance LCD **Y. Liu** and D-S. Seo	**Mr Yang Liu**, Yonsei University, **Republic of Korea.**
12:30-14:00	**Lunch Break / Posters Session**	

Session Chairs: Dr. Matteo Chiesa - UAE / Prof Khaled Saoud - Qatar

14:00-14:30	Functionalized Polyelectrolytes as Versatile Building Blocks **L.C.P.M. de Smet**	**Dr. Louis de Smet**, Delft University of Technology, **The Netherlands**
14:30-15:00	Quantifying grain refinement of twin-roll-cast AZ31B by friction stir processing A. H. Ammouri, G. Ayoub, B. Mansoor and **R. F. Hamade**	**Prof Ramsey Hamade**, American University of Beirut, **Lebanon**
15:00-15:15	Electrospinning of silica-polymer composite fibres by solution electrospinning **L. Christiansen** and P. Fojan	**Mr Lasse Christiansen**, Aalborg University, **Denmark**
15:15-15:30	Magnetic Exitation in Chiral Graphene Model Yu.P.Rybakov, M.Iskandar and **A.B.Ahmed**	**Mr. Abdullahi Bappah Ahmed**, Gombe State University, **Russian Federation**
15:30-15:45	Modification of metallic surfaces by duplex treatments involving severe shot peening, pulsed electron beams and nitriding **Y. Samih**, T. Grosdidier, S. Z. Hao and C. Dong	**Dr. Youssef Samih**, Lorraine University, **France**
15:45-16:00	Fabrication of Metal/Metal oxide/Reduced graphene oxide nanocomposites for anode in Li-ion batteries **H. Abuhimd**	**Dr Hatem Abuhimd**, King Abdulaziz City for Science and Technology, **Saudi Arabia**
16:00-16:30	**Coffee Break / Posters Session**	
16:30-17:00	Modern Ab-Initio Calculations Based on Thomas-Fermi-Dirac Theory in High-Temperatures and High-Pressures Environment **S. Seriy** and U. Kabaldin	**Dr. Sergey Seriy**, Komsomolsk-on-Amur State Technical University, **Russian Federation**
17:00-17:15	The Canonical Method of Nonholonomic Constraints **K.I. Nawafleh**	**Prof Khaled I. Nawafleh**, Mu'tah University, **Jordan**
17:15- 17:30	The effect of Starch Modification on Biodegradation of Nanocomposite Films reinforced with Lignin and Nanofiber extracted from Bamboo **A. Tawakaltu**, E.C. Evans and O. Prince	**Mrs. Tawakaltu Abdul Rasheed-Adeleke**, Federal University of Technology Minna, **Nigeria**

December 8, 2015
Session II: Advanced Materials/ surfaces for Energy and Environment

Al-Safa 1&2 Conference Room

Session Chairs: Prof Khaled Saoud - Qatar / Prof Taleb Ibrahim - UAE

09:00-9:45	Novel nanofabrication for constructing 3-dimensional composite structure with carbon-based nanomaterials for energy applications **D. Choi**	**Prof Daniel Choi**, Masdar Institute, **UAE**
09:45-10:30	Artificial Leaves for solar hydrogen **E. Sudhölter**	**Prof. Ernst J.R. Sudhölter**, Delft University of Technology, **The Netherlands**
10:30-11:00	**Coffee Break / Posters Session**	
11:00-11:30	Durability Improvement of Solid Oxide Fuel Cells M.Z. Khan, **R-H. Song**, S-B. Lee, J-W. Lee, T-H. Lim and S-J Park	**Prof Rak-Hyun Song**, Korea Institute of Energy Research, **Republic of Korea**
11:30-11:45	Assessment of microstructural, thermal, electrical and optical properties of Fe-Cu metastable compound **A.H. Alami**, J. Abed, M. Almheiri and A. Alket	**Dr. Abdul Hai Alami**, University of Sharjah, **United Arab Emirates**
11:45-12:00	Application of the exact muffin-tin orbitals method to the Bain path of metals: the overlapping potential sphere wells and the hard spheres **N. Al-Zoubi**	**Dr Noura Al-Zoubi**, Tafila Technical University, **Jordan**
12:00-12:15	Polytriazole-co-Polyoxadiazole Copolymers as a New Class of Membrane Material for Osmotically Driven Processes **P. H.H. Duong**, S. Chisca, P. Y.Hong, H. Cheng, S. P. Nunes, and T. S. Chung	**Dr. Duong Phuoc**, King Abdullah University of Science and Technology, **Saudi Arabia**
12:15-12:30	Silicon Nanoparticles for Room-Temperature Catalytic Dehy-drogenation of Secondary Alcohols into Ketones and Hydrogen **J. El-Demellawi**, Christopher R. Holt, Edy Abou-Hamad, Zeyad A. Al-Talla, Youssef Saih and Sahraoui Chaieb	**Mr. Jehad El-Demellawi**, King Abdullah University of Science and Technology, **Saudi Arabia**
12:30-14:00	**Lunch Break / Posters Session**	

Session chairs: Prof Daniel Choi, UAE

14:00-14:45	Green Corrosion Inhibitors for Metals **T.Ibrahim**	**Prof Taleb Ibrahim**, American University of Sharjah, **UAE**
14:45-15:15	Hybrid Pectin-Based Biosorbents for Zinc Removal **A. Jakóbik-Kolon**, J. Bok-Badura, K. Karoń and K. Mitko	**Dr. Agata Jakóbik-Kolon**, Silesian University of Technology, **Poland**
15:15-15:30	The use of optical fibers for environmental decontamination **S. Teixeira**, S. Y. Ryu, V. Sencadas, S. Lanceros-Méndez, K. Kühn, M. Hoffmann and G. Cuniberti	**Ms. Sara Teixeira**, Technische Universität Dresden, **Germany**
15:30-15:45	C5H11NO2S Effect on Concrete Steel-Reinforcement Corrosion in Industrial/Microbial Simulating Environment **J.O. Okeniyi**, A.O. Abioye, Z.C. Adikpewun, A.A. Otesanya, D.M. Eleshin, O.O. Gabriel and O. Adeoye	**Dr. Joshua Okeniyi**, Covenant University Ota, **Nigeria**
15:45-16:00	Biochemical Characterization of Cymbopogon citratus: Prospects on Environmentally-Friendly Corrosion-Protection of Concrete Steel-Reinforcement in Aggressive Environment J.O. Okeniyi, **E.T. Okeniyi**, O.O. Ogunlana, F.T. Owoeye and E.O. Ogunlana	**Mrs. Elizabeth Okeniyi**, Covenant University Ota, **Nigeria**
16:00-16:30	**Coffee Break / Posters Session**	
16:30-16:45	Performance of Cassia Fistula Leaf-extract on Stainless Steel Corrosion in 0.5 M HCl **O.A. Omotosho**, J.O. Okeniyi, A.S. Ogbiye, O.B. Ajibola and C.A. Loto	**Mr O.A. Omotosho**, Covenant University Ota, **Nigeria**
16:45-17:00	The Efficiency of Al2O3-water Nanofluid on a Flat-Plate Solar Collector **N. Budak,** H.L. Yucel, C. Yildiz and S.Tekalp	**Ms. Nese Budak**, Batman University- **Turkey.**
17:00-17:15	Nano Technology Application in Stablizing Expansive Soil: Irbid Clay **A. A. Sharo** and A.S. Alawneh	**Dr Abdulla A. Sharo**, Jordan University of Science and Technology- **Jordan**

December 9, 2015
Session III: Advanced Materials / surfaces for biomedical / Life Science

Al-Safa 1&2 Conference Room

Session chairs: Prof Khaled Saoud - Qatar

009:00-9:45	State-of-the-Art in Powder Metallurgy Materials with Atomic/Nano scale Microstructures **K. Kondoh**	**Prof Katsuyoshi Kondoh**, Professor, Osaka University, **Japan**
09:45-10:15	Immuno-nanotheronostics approach to detect and eliminate cancer cells **Ahmad Fawzi Hussain**, Harald Rune Krüger, Dirk Bauerschlag, Nicolai Maass, Marcelo Calderón and Stefan Barth	**Dr. Ahmad Hussain**, University Hospital Aachen, **Germany**.
10:15-10:45	**Coffee Break**	
10:45-11:00	Naproxen and Ibuprofen Molecular Liquids — A high yield su-percritical CO2 process platform **S.K. Sharma**, Abiy D Woldetsadik, Mazin Magzoub and R. Jagannathan	**Dr Sudhir Sharma**, New York University Abu Dhabi, **United Arab Emirates**
11:00-11:15	Mussel inspired nanointerface for an efficient biomolecular delivery into cells **B.G Naira** and Y.Ito	**Dr. Baiju Govindan Nair**, RIKEN Centre for Emergent Matter Science- Saitama, **Japan**
11:15-11:30	Synthesis, Charectrerization and applications of Iron oxide Nanoparticles in Cosmetics **Seema R Pathak**, M Nidhin, **V Monika** and K J Sreeram	**Dr Monika Vats**, Amity University, **India**
11:30-11:45	Mechanical Properties of Silver Coated Electro-Spun composite Scaffolds for Antibacterial Applications **P. Kalakonda** , M. A. Zaheri, S. Chaieb and A. Memic	**Dr. Parvathalu Kalakonda**, King Abdullah University of Science and Technology (KAUST), **Saudi Arabia**
11:45-12:00	Preparation and characterization of cross-linked β-cyclodextrin-graffted chitosan nanoparticles coated with hyaluronic acid **A. Ben Mihoub**, Y. Bal and B. Saidat	**Ms Amina Ben Mihoub**, University Amar Telidji of Laghouat, **Algeria**.
12:00-12:30	**Awards and Closing Ceremony**	
12:30-14:00	**Lunch**	

Posters Session
December 7 and 8, 2015

N.	Title	Author/Affiliation/Country
1	Molecular dynamics simulation of functionalized graphene – a study of the mechanical properties of graphene and the interac-tion between graphene and epoxy **Liliana Sofia Melro**, Ryszard Pyrz and Lars Rosgaard Jensen	**Ms Liliana Melro**, Department of Mechanical and Manufacturing Engineering, Aalborg University, **Denmark**
2	Characterization of an EDTA-based Gemini Surfactant at the Air-Liquid Interface **H. Younesi Araghi** , J. Rehman, B. Dessert and M.F. Paige	**Dr Hessamaddin Younesi Araghi**, University of Saskatchewan, **Canada**
3	Temperature Dependence Control of Birefringence of Zero-Birefringence Polymers for LCDs **M. Shikanai**, A. Tagaya and Y. Koike	**Ms. Mio Shikanai**, Keio University-Kanagawa, **Japan**
4	A method for determination of metals contained in carbon nanotubes **J. Bok-Badura**, A. Jakóbik-Kolon, M. Turek, K. Karoń and A. Łamacz	**Mrs. Joanna Bok-Badura,** Silesian University of Technology, **Poland**
5	The effects of temperature and pH on swelling of stimuli-sensitive hydrogels **C.-G. Sanporean**, A.D. Drozdov and J. de C. Christiansen	**Dr. Catalina-Gabriela Sanporean**, Department of Mechanical and Manufacturing Engineering, Aalborg University, **Denmark**
6	Experimental Studies for the Impact of SiO2 Particle onto a Planar Surface at Different Temperatures **M. Dong**, L. Bai, J. Xie and S. Li	**Dr Ming Dong**, Dalian University of Technology, **China**
7	WO3-Nanowire@Graphene Nanocomposite for Efficient Visible Light Induced Photodegradation and Photocapacitance Performance **M.E.Khan**, M.M. Khan and M. Hwan Cho	**Mr. Mohammad Ehtisham Khan**, Yeungnam University- Gyeongsan, **Republic of Korea**
8	Modeling anticorrosive and adsorption mechanism of Rhizophora mangle L leaf-extract admixture in steel-reinforced concrete immersed in saline/marine simulating-environment J.O. Okeniyi, C.A. Loto,A.P.I. Popoola and **O.A. Omotosho**	**Mr. Olugbenga Omotosho,** Covenant University Ota**, Nigeria**
9	Modeling of the optical fiber using the VHDL-AMS language **F.Baouche**, F. Hobar and Y. Hervé	**Dr. Baouche Fatima Zohra**, Khemis Miliana University, **Algeria**
10	Zinc Sorption on Modified Waste PMMA **A. Milewski**, D. Zdybał and A. Jakóbik-Kolon	**Mr. Andrzej Milewski**, Silesian University of Technology, **Poland**
11	Removal of textile dyes by composite based on chitosan **S.Kara Slimane** and A.Benosman	**Dr. Sofia Kara Slimane**, University Abou Bekr Belkaid-Tlemcen, **Algeria.**
12	Electrical transport properties of an isolated single walled carbon nanotube aligned on an ST-cut quartz substrate **E. S. Sadki**	**Dr. El-Hadi Sadki,** United Arab Emirates University- Ain, **United Arab Emirates**
13	Study of Interaction between the Molecule 2-Mercaptobenzimidazole and Metal Atom Substrate for Self-Assembled Monolayers **O. Mahmoudi**, T. Bordjiba and M.-A. Affoune	**Ms Ourida Mahmoudi**, 08th May 1945 University-Guelma, **Algeria**
14	Effects of Alkali Metal Doping on the Graphene/Ni(111) Surface **J. W. Park** and M. H. Kang	**Dr. Jaewhan Park**, Pohang University of Science and Technology, **Korea**

Session I
Advanced Materials Fabrication, Characterization and Tools / Properties

Recent Advances in Silica Aerogel Synthesis and Processing

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Abstract
Lightweight materials with adequate mechanical properties are highly desired for various structural applications. The unique physical properties of aerogels make them attractive for many applications ranging from environmental remediation to space dust collection;1–4. However, aerogel production is slow and takes days. Starting from Wet gels, Aerogel can be rapidly synthesized by well-known procedures,5,6. Drying step is time-consuming due to capillary forces and solvent evaporation can caused cracking and shrinking of the monolith. Several methods have been developed to overcome the capillary forces. Supercritical CO2- and ambient pressure-drying are the most established methods. Using the supercritical CO2 drying is the most common method were solvent inside the Aerogel can be exchanged with liquid CO2 in an autoclave when heated to the supercritical point of CO2. While the ambient pressure drying uses silane such as trimethylchlorosilane which diffused through aquogels and attached to the pore walls and derivatizes them with a hydrophobic moiety which reduces surface energy and capillary stresses.8–11. As mentioned above, solvent exchange step is the processing limiting and time-consuming step because it is controlled by diffusion time of the solvent through the gel.

Recently, we reported one pot synthesis of native and cross-linked aerogel monoliths that can be fabricated and dried supercritically without solvent exchange step. Our technique is based on the use of ethanol–water azeotrope mixture as a gelation solvent, which contains 4.4% water by volume. The small water content allows for drying at temperatures close to the supercritical temperature of the drying solvent, where reactions such as silica dissolution and polymer degradation are negligible. As a result, native oxide and cross-linked aerogels can be fabricated in few hours. These results represent a breakthrough since they dramatically shorten fabrication times of native and, most importantly, cross-linked aerogel monoliths. 12.

Recent breakthrough is the development of a new method for rapid fabrication of polymer cross-linked silica aerogel using visible light and low cost laser induced photogelation. In this method, a solution of an alkoxysilane (tetraorthosilicate, TEOS), a monomer (hexanedioldiacrylate, HDDA), a visible-light freeradical photoinitiator (Eosin Y) and a tertiary amine (as co-initiator and pH modifier), was prepared in ethanol solvent. The solution then irradiated with a laser beam, and the energy liberated by the polymerization reactions induced gelation in a matter of seconds.13. The potential of this method enables mold-free and rapid fabrication of bulk or thin film aerogel structures using this method to open new avenues for their application in areas such as 3D printing since in the near future every structure, simple or complex, will be fabricated using 3D printing technology. Here, we demonstrate that instantaneous gelation leading to mechanically strong and ultra-lightweight silica aerogels offer a new direction for 3D industry to fabricate lightweight 3D structures with complex geometries using a visible light emitting low power laser.

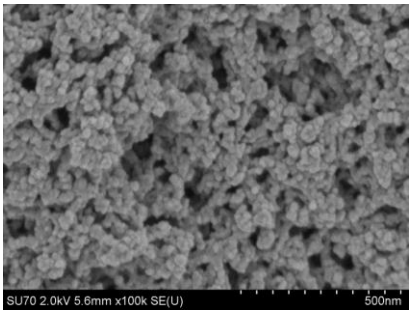

Figure 1: SEM Micrograph of synthesized Aerogel

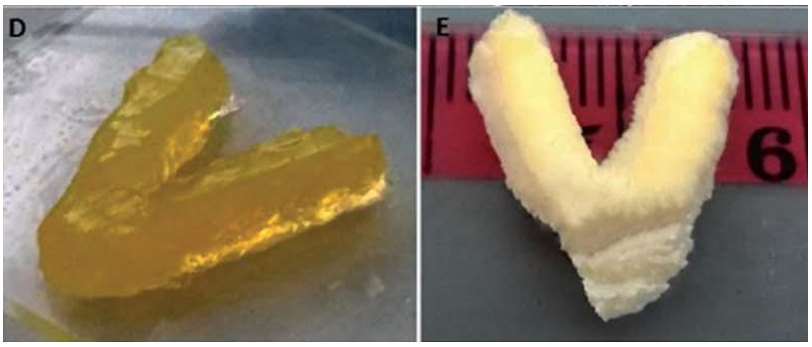

Figure 2: Shows letter “V” printed on substrate and without substrate.

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14. Saeed, Shaukat, Rola M. Al-Sobaihi, Massimo F. Bertino, Lauren S. White, and Khaled M. Saoud. "Laser induced instantaneous gelation: aerogels for 3D printing." Journal of Materials Chemistry A 3, no. 34 (2015): 17606-17611.

Nanocrystals as Tunable Platforms for Chemical Reactions, Sensing and Imaging

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Abstract:

Colloidal nanocrystals made of semiconductor, metal and meal oxide cores exhibit unique optical and physical properties that are not shared by their bulk parent materials. For instance semiconductor nanocrystals (quantum dots, QDs) exhibit size-, composition- and shape-dependent absorption and emission properties, while gold nanostructures exhibit size- and shape-dependent surface plasmon peaks. These nanoscale colloids have large surface to volume ratios, and can provide platforms for arraying various functional molecules ranging from proteins to redox active complexes. The emission of luminescent of QDs can be highly sensitive to potential interactions with proximal dyes and metal complexes. We have developed a phase transfer approach, based on ligand exchange, along with covalent coupling and non-covalent self-assembly to conjugate various biomolecules to CdSe-ZnS QDs and Au nanoparticles (AuNPs). These nanocrystals were rendered water-soluble using multi-coordinating and multifunctional ligands (molecular scale as well as polymeric) relying on the lipoic acid (LA) and/or imidazole motifs.

In this presentation, we will start with a description of the ligand design, characterization and a phase transfer strategy. This strategy exploits the photochemical transformation of lipoic acid groups followed by coordination onto the nanocrystals. We then provide a few examples of hybrid bioconjugates and the use of those conjugates for sensor design, based on charge or energy transfer interactions, and for imaging live cells and blood capillaries. We will conclude by discussing the utility of these photochemically-modified ligands to grow luminescent gold clusters.

Keywords: inorganic nanostructures, quantum dots, gold nanoaprticles, ligands, polymers, phase transfer, conjgation, potochemistry, sensing, imaging, biomedical applications.

Synthesis and Characterization of Hybrid Material based on Ionic Liquid and Amorphous Porous Silicon

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Abstract:
Ionic liquids are salts that are liquids over a wide range of temperature (Suarez et al., 1998). Because they can be designed by a choice of a cation and anion, they are called "designer solvents." (Eik et al., 2003) they are gaining huge momentum as new solvents for nanoparticles synthesis, or for batteries as well in heat storage for solar-thermal. They have potential applications in gas handling, pharmaceuticals, nuclear fuel processing and many other industrial processes such as separation or paper industry. In contrast to organic solvents, ionic liquid have a large liquid range, high thermal stability, polarity and volatility. They are non-flammable and are miscible with a variety of solvents. Their physico-chemical properties can be designed by judicious choice of cation/anion combinations, which makes them the most diverse solvent around.

Although IL has been studied as suitable solvents for nanoparticles synthesis as well as for catalysis their interactions with substrates as well as nanoparticle have been largely ignored. In the current study we report for the first time the behavior of various ILs when mixed with silicon nanoparticles for eventual applications in batteries or solar cells. While fluorine based IL behave as good solvent to the nanoparticles, the thiocyanate complexes with traces of iron ions(khare et al., 2010) that were used as a catalysis during the nanoparticles synthesis. This complexation stabilizes the dispersion. Several spectroscopic studies were used to investigate the interactions between the silicon nanoparticles and the ILs. We suggest that, contrary to the common belief, not all ILs are good solvents for silicon nanoparticles because of many limiting factors.

Keywords: ionic liquids, cation/anion combinations, silicon nanoparticles, hybrid material,complexation, stabilization, potential applications.

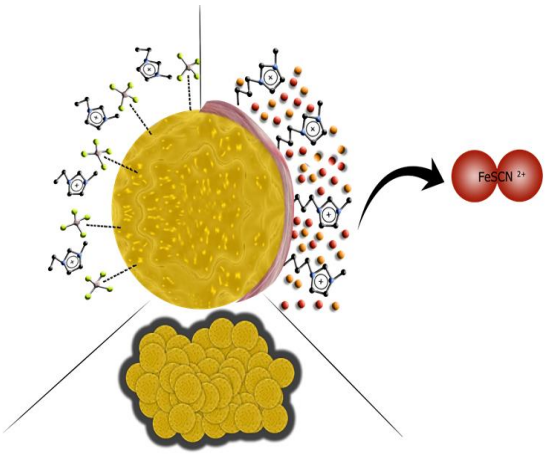

Figure 1: Schematic representation of nonstructural organization in binary amorphous porous silicon/ionic liquids mixtures

References:

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Eike, D. M., Brennecke, J. F., Maginn,E. J., (2003)Predicting Melting Points of Quaternary Ammonium Ionic Liquids.Green Chem.,5, 323-328.

Khare, V., Kraupner, A.,Mantion, A., Jelicić, A., Thünemann, A. F., Giordano, C.,Taubert, A. (2010) Stable Iron Carbide Nanoparticle Dispersions in [Emim][SCN] and [Emim][N(CN)2] Ionic Liquids.Langmuir,26,10600-10605.

Effect of Repetitive Thermomechanical Processing on Grain Boundary Characteristics in alpha-phase brass

K. J. Al-Fadhalah
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Abstract:
Commercial (70Cu–30Zn) brass alloy of alpha-phase was thermomechanically processed to enhance the special coincidence site lattice (CSL) boundaries. Four cycles of thermomechanically processing (TMP) were applied, with each cycle consisting of uniaxial compression (strain of 0.15) and annealing (670ºC/10 min). Also, three different compression temperatures (25ºC, 250ºC and -100 ºC) were used. Microstructure evaluation by electron backscattered diffraction (EBSD) indicates that the use of high compression temperature of 250ºC after one cycle promoted the largest formation of Σ3 boundaries (frequency of 57%), associated with the formation of annealing twins. It was also found that the use of 4 cycles of TMP was necessary to stabilize the grain boundary characteristics and to further increase the frequency of Σ3 boundaries to about 62%. In addition, the formation of annealing twins was accompanied by partial randomization of the compression texture.

Keywords: brass, thermomechanical processing, annealing twins, microstructure, texture.

Ion Beam Induced Aluminum-doped Zinc Oxide-Bumps Aligning Liquid Crystals with the Tunable Surface Wettability for High Performance LCD

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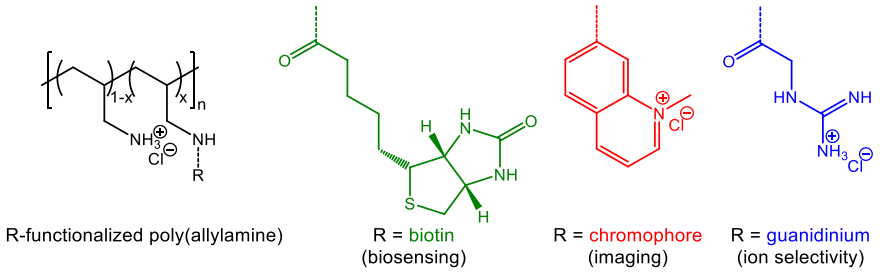
Abstract:
Alignment of liquid crystals (LC) in general optic devices without complicated pre-treatment of alignment layers is necessary when LC are working as light shutter as LC electrical sensitivity. Here an ion beam (IB) spurted aluminum-doped zinc oxide (AZO) bumps thin layer working as alignment layer homogeneously aligning LC is presented. AZO-bumps were observed after an IB spurting process, and these bumps were identified via XPS spectra, in which the feature O 1s signal, Zn 2p1 signal and Zn 2p3 signal transform was observed; and the morphology change of IB spurted AZO thin layers were investigated via field-emission scanning electron microscopy and atomic force microscopy. With 0.6-keV IB spurting, only non-uniform wrinkles were observed; however, since when 1.2-keV IB spurting was adopted to spurt thin layer, AZO bumps were observed, and AZO bumps were found covering the surface in a thin layer with columnar morphology, several nano-meters in diameter only after a 1.8-keV IB spurting. The Wettability change of AZO thin layers was detected from the observation of corresponding contact angles, and 1.8-keV IB irradiated AZO bumps thin layer was found exist the highest wettability due to the bumps covering the surface. AZO-bumps thin layer based liquid crystal displays (LCD) presented super electro-optic performances compared with conventional rubbed PI alignment layer cell, and the slightly residual direct current voltage. These obtained excellent electro-optic performances could be due to the intrinsic high conductivity of AZO thin layer, which induced the electric field effect for a low-power fast operation of LC switching, and the super-fast release of the accumulated ion charges in AZO alignment layers. These results indicate that AZO-bumps thin layer is one of most promising candidates to aligning LC for LCD with excellent electro-optic performances.

Keywords: liquid crystals, alignment, ion beam irradiation, aluminum-doped zinc oxide, bump, thin layer, surface wettability.

Functionalized Polyelectrolytes as Versatile Building Blocks

L.C.P.M. de Smet
Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands

Abstract
Polyelectrolytes (PEs) form an interesting class of water-soluble polymers that are used in a wide variety of applications. They exist in a large chemical diversity, which may not only explain their high abundance in soft matter systems, but it also enables tunable chemical modification to add specific functionalities. In this presentation, three examples of functionalized polyallylamine hydrochloride (PAH) will be given to utlize them in the fields of biosensing, fluorescent labelling, and ion selectivity, respectively (see Figure).



First, PAH was chemically modified with biotin to ensure binding sites for antibodies via a streptavidin-biotin binding scheme [1]. The biotinylated PAH was used as a building block to form PE multilayers onto sensor platforms. Second, PAH was functionalized with a chromophore for the visualization of latent fingerprints [2]. Exposing fingerprints to pH neutral, dilute aqueous solutions of this polymer results in bright green fluorescent images, which are clearly visible to the naked eye. Third, PAH was chemically functionalized with a guanidinium (Gu) moiety [3], which is known to bind oxoanions. Addition of the Gu functionality affected the structural properties of the PE multilayers, including their thickness, rigidity and pH stability. Morover, the Gu-containing multilayers were found to have a high binding affinity for $H_2PO_4^-$.

Keywords: polyelectrolytes, chemical modification, functionalization, interfaces, surface engineering, thin films, coatings

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Quantifying grain refinement of twin-roll-cast AZ31B by friction stir processing

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Abstract:

Zener-Hollomon parameter (Z-parameter) may be defined as "temperature compensated strain rate" and has been related to resulting grain size due to dynamic recrystallization (DRX) in metals. This study aims to quantify the values of Z-parameter (from estimated values of generated values of strain rate and temperature) generated in the FSP-processed material to process parameters (here, spindle speed and tool feed). From the estimated values of Z-parameter, grain size estimates of the processed material are developed in the form of simple formulae that relate grain size to process parameters.

In order to accomplish this aim, a numerical (FEM) based-model was developed for predicting the values of such salient state variables as strain, strain rate, and temperature in the material during friction stir processing of AZ31B (supplied by POSCO, 892 Daechi4-dong, Gangam-gu, Seoul, 135-777 and has the chemical composition by weight percentage: Mg 95.4%, Al 3.32%, Zn 0.803%, Mn 0.304%, and Si 0.147%). To model the flow of the magnesium metal, utilized in FEM is a HCP specific Zerilli-Armstrong (ZA) constitutive relation, based on thermally activated dislocation mechanics. The procedure for calculating the Z-parameter depends on the history of strain rate and temperature of 9 moving observation points placed in the FEM model. The estimated temperature and strain rate values for each test case were estimated from the FEA model and were used in the calculation of the Z-parameter.

For verifiying the results of FEM simulations, an experimental test matrix comprised of different ranges of FSP process parameters of spindle speed and feed rate was run. Experimental single pass FSP was performed on a HAAS VF6 vertical machining center which was retrofitted with external hardware. The FSP tool is machined from SVERKER 21 (AISI-D2) tool steel supplied by Uddeholms AB (SE-683 85 Hagfors, Sweden). The tool has a shoulder diameter of 19 mm, with a 6.4 mm pin diameter (2.7 mm high). The resulting grain size (d) of the processed material was measured using optical microscopy. The samples were cut, ground, polished, and etched using Acetic-Picral solution according to the ASM Specialty Handbook of Magnesium and Magnesium Alloys. Microstructure images were taken using a B41 Olympus microscope equipped with an Olympus XC50 digital camera. Grain size measurements is characterized according to ASTM E112-10.

The experimental grain size measurements confirmed the rsults of the FEM simulations thus verifying the found formulae relating grain size to process parameters. Such an equation can be used in controlling the desired grain size during friction stir processing by varying the process parameters.

Keywords: friction stir processing, process parameters, Zener-Hollomon parameter, twin-roll-cast, AZ31B, grain size, dynamic recrystallization.

Electrospinning of silica-polymer composite fibres by solution electrospinning

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Abstract:
Electrospinning is a fast way to produce polymer and composite fibres from solutions or melts.In the past it has mainly been used to produce fibres for textile, membrane and filtration purposes (Tan et al.). Nowadays this technique has been expanded to create fibre structures for, scaffolds (Li et al.) and shells for more brittle materials, such as fumed silica (Li et al.).Due to their high porosity as well as high insulation properties, fumed silica particles have proven to be useful in insulation as well as filtration applications. Their lack of mechanical stability has so far been their main limitation, which can be overcome by embedding them into a a polymer fibre scaffold. Solution electrospinning of silica-polymer fibres have been investigated, and the optimal silica concentration in the solutions are evaluated. The mechanical and thermal properties of the resulting fibre mats and the influence of the polymer- and silica properties are evaluated and discussed.
In order to obtain stable fibres, the process of preparing the solution for electrospinning is important. With propper solution preparation, stable fibres with a fumed silica content of 90% can be obtained. At higher concentrations, the mechanical properties of the material was too low to withstand the turbulent forces in the electrospinning process, and a composite with equal mechanical properties to fumed silica was obtained.

Keywords: polymer, silica, aerogel, fumed, fibres, composite, electrospinning, solution, PEO, thermal conductivity, mechanical properties, characterization

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Magnetic Exitation in Chiral Graphene Model

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Abstract

The s- and p- hybridization effect for the valence electrons of carbon atoms appears to the main property of the electron in mono-atomic carbon layers of graphene. For realizing this effect the chiral model of graphene was suggested, the unitary $SU(2)$ matrix $V = a_0\tau_0 + i(\vec{a}\vec{\tau})$ being considered as an order parameter. Here $\tau_0, \vec{\tau}$ denote the unit matrix and the Pauli matrices respectively, scalar and vector fields $a_0, \vec{a}; a_0^2 + \vec{a^2} = 1$, describing s- and p-states of the free valence electron. For the description of spin and quasi-spin excitation in graphene, the latter ones corresponding to independent excitation modes of the two triangular sub-lattices of graphene, we introduce the two Dirac spinors ψ_1, ψ_2 and consider the combined spinor field $\Psi = \xi \otimes (\psi_1 \oplus \psi_2)$as a new order parameter, where ξ stands for the first column of V.

keyword: chiral model of graphene, dirac spinors

Modification of metallic surfaces by duplex treatments involving severe shot peening, pulsed electron beams and nitriding

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Abstract:
Long term surface peening, such as the Surface Mechanical Attrition Treatment (SMAT), was developed to upgrade directly the mechanical properties of the materials as well as a surface activator prior to chemical treatments such as Plasma Nitriding. The High Current Pulsed Electron Beam (HCPEB) technique is also a recent technique that has been proved to increase surface hardness as well as wear and corrosion resistances. These techniques create a deformed graded surface for which the grain size reduction, the increased grain boundary density and the introduction of structural defects improves directly the properties. It was also suggested that they promote the diffusion of nitrogen and thereby, the reductions in the nitriding temperature and/or duration, leading to avoid the formation of nitrides which affect the corrosion behavior.

In the present work, the surface of the AISI 316L steel was treated by SMAT or HCPEB under different processing conditions then subjected to Plasma Nitriding (350 °C for 8 hours). The evolutions of the nitrided depths and hardness of the processed surfaces are analyzed and their evolutions discussed depending on the processing conditions at the light of quantitative analysis of the deformed state using a recently developed procedure. This new procedure -based on the analysis of Geometrically Necessary Dislocation (GND) and grain size determination obtained from EBSD measurments-is here extended to the analysis of duplex treatments involving plastic deformation and nitriding.

Keywords: SMAT, HCPEB, nitriding, Duplex treatments, stainless steels.

Fabrication of Metal/Metal oxide/Reduced graphene oxide nanocomposites for anode in Li-ion batteries

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Abstract

Graphene based materials have attracted much attention as promising electrode materials for electrochemical energy storage devices, such as Li-ion batteries, and supercapacitors, due to their high surface area and superior electronic conductivity. In this work, nanocomposites of metal/metal oxide/reduced graphene oxide (RGO) were prepared from the graphite oxide (GO) with different degrees of oxidation and furthermore their structural, morphological, optical characteristics and electrochemical properties as anode materials for Li-ion batteries were investigated. These nanocomposites were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), ultra violet visible (UV-Vis) spectroscopy, and Raman measurements. The detailed characterization studies confirmed that the metal and metal oxides with good crystalline structure are well distributed onto the RGO sheets. These prepared nanocomposites persist specific high surface area and demonstrated high reversible capacity mainly in the way of lithium absorption, where the specific surface area was the key structural parameter. This fascinating electrochemical performance can be ascribed to their specific area, providing numerous active sites for Li^+ insertion, reduced effective diffusion distance for the Li^+ ions, high electrical conductivity, low charge-transfer resistance across the electrolyte–electrode interface, and improved structural stability against the local volume change during Li^+ insertion–extraction. Such electrodes are envisioned to be mass scalable with relatively simple and low-cost fabrication procedures, thereby providing a clear pathway toward commercialization.

Modern Ab-Initio Calculations Based on Thomas-Fermi-Dirac Theory in High-Temperatures and High-Pressures Environment

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Abstract:
Thomas-Fermi theory (TFT) is an approximate method, which is widely used to describe the properties of matter at various hierarchical levels (atomic nucleus , atom, molecule , solid , etc.). Special development achieved using THF to the theory of extreme states of matter appearing under high pressures, high temperatures or strong external fields. Relevant sections of physics and related sciences (astrophysics, quantum chemistry, a number of applied sciences) and determine the scope of TFT. Popularity TFT is related to its relative simplicity, clarity and versatility.
The latter means that result of the calculation by TFT applies immediately to all chemical elements: the transition from element to element is as simple scale transformation. These features make it highly convenient tool for qualitative and, in many cases, and quantitative analysis. TFT was originally proposed by Thomas and Fermi to describe the electron shell of a heavy atom, which is characterized by a relatively uniform distribution of the electron density. TFT is the semi-classical (WKB) limit in relation to self-consistent Hartree field equations, and therefore modification of this model are associated with a more detailed account of the correlation, exchange, quantum and multi-shell effects.

Keywords: “ab-initio” quantum-mechanics, mathematical modeling, computational material science, density functional theory, Thomas-Fermi-Dirac theory.

The Canonical Method of Nonholonomic Constraints

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Abstract
We discuss an extension of the Hamilton-Jacobi theory to nonholonomic mechanics with a particular interest in its application to exactly integrating the equations of motion. The major advantage of our result is that it provides us with a method of integrating the equations of motion just as the unconstrained Hamilton-Jacobi theory does.

Keywords*:* Hamilton-Jacobi equation, Nonholonomic constraints

The effect of Starch Modification on Biodegradation of Nanocomposite Films reinforced with Lignin and Nanofiber extracted from Bamboo

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Abstract:
The effect of starch modification on biodegradation of Nanocomposite films reinforced with Lignin and Nanofiber extracted from Bamboo was determined. Biodegradation was based on the determinations of water absorption, weight loss (soil burial test and enzyme studies) and reducing sugars. When studied within 6 hours, great variations in enzyme susceptibilities were observed with thermoplastic starch (TPS) having the highest glucose equivalent followed by unmodified starch and the modified starches. Modification led to decrease in weight loss and water uptake thus, degradation was well pronounced when the percentage water absorption capacity was high.

Keywords: nanocomposites, biodegradation, water absorption, reducing sugar, modification, starch, lignin, bamboo, TPS.

Session II
Advanced Materials/ surfaces for Energy and Environment

Artificial leaves for solar hydrogen

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Abstract:

There is today a strong need for an energy transition to reduce our energy needs by performing our processes more energy efficient, and at the same time we have to search for economically feasible and renewable energy sources, like wind energy and solar energy.

This contribution focusses on the use of solar irradiation to split water into hydrogen and oxygen, mimicking in an artificial system the natural photosynthesis process. Hydrogen is seen as a highly promising near future energy carrier. Water can be split via photo-electrochemical cells and also by an integration of photo-voltaic cells and electrolyser. Both systems will be compared and our favourite integrated system well be discussed in more details, including energy payback time and life cycle assessment.

Durability Improvement of Solid Oxide Fuel Cells

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Abstract:

Durability is an important requirement for the commercialization of solid oxide fuel cell (SOFC) technology. The study highlights the degradation investigation and improvement of SOFC anode, cathode and metallic interconnects which have been studied in our group. The effect of gadolinium-doped ceria (GDC) interlayer on the SOFC cathode degradation under accelerated current cycling was investigated (ref 1, Khan *et al.,* 2014). The SOFC half cells were tested under rapid current load cycles and area specific resistance (ASR) was measured. The half-cells with GDC interlayer showed less ASR increase in comparison to those without GDC interlayer due to smaller elemental diffusion across GDC interlayer. The effects of various sintering inhibitors (SiC, SiN, Al_2O_3, AlN, CeO_2 and GDC) on the long-term performance of nickel-yttria stabilized zirconia (Ni-YSZ) for SOFC anodes were studied (Khan *et al.,* 2015). During the long-term performance test, ASR was measured and triple phase boundary (TPB) density was calculated by image analysis techniques before and after test. Among various inhibitors, CeO_2 and GDC exhibited best performance in terms of lowest ASR and TPB density change rates. Finally high temperature oxidation kinetics, ASR and interfacial microstructure of metallic interconnects in air atmosphere were studied (ref.3, Pyo *et al.,* 2011). An efficient conductive layer of $(La_{0.8}Sr_{0.2})_{0.98}MnO_3$ (LSM) was coated on SOFC interconnects (Crofer22APU) by wet spray coating method. The adhesive strength of coated layer/metal substrate interface increased with increased surface roughness of interconnects. SOFC interconnect treated at 1100°C in N_2 with 10 vol.% H_2 showed long-term stability and a lower ASR value than the other samples, heat-treated at 800°C and 900°C. The results showed that the coated oxide layer prevents the formation and growth of scale, and enhances the long-term stability and electrical performance of metallic interconnects used for SOFCs.

Keywords: durability, SOFC, degradation, cathode, anode, interconnect, area specific resistance, triple phase boundry, GDC interlayer, long-term stability, current cycling, electrical performance.

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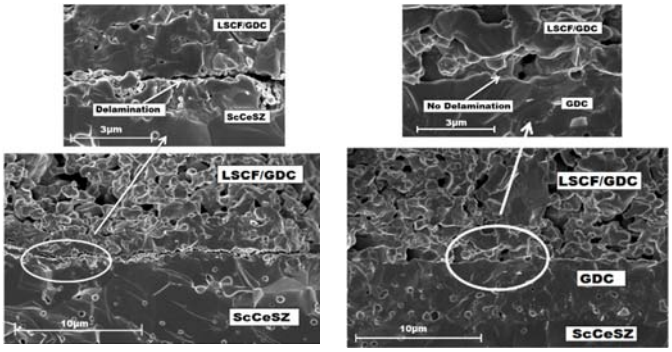

(a) **(b)**

Figure 1: Figure illustrating the microstructures of the SOFC half-cells after current load cycling (a) without GDC interlayer, showing interface delamination (b) with GDC interlayer, showing no interface delamination[ref.1].

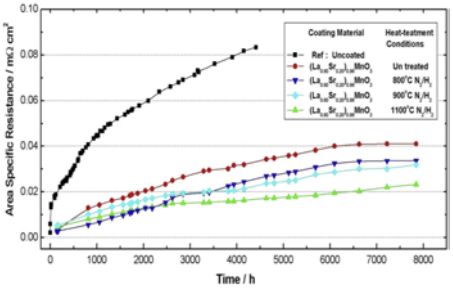

Figure 2: Change of ASR of non-coated and LSM coated SOFC interconnect (Crofer22APU) specimens with holding time in air at 800°C[ref.3].

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Assessment of microstructural, thermal, electrical and optical properties of Fe-Cu metastable compound

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Abstract:
This paper investigates the synthesis, microstructural characterization, electrical and optical and thermal testing of Fe-Cu metastable alloy system for selective solar absorption applications. The system is produced by mechanical alloying (MA) using high energy ball milling while monitoring its crystallographic morphology via X-ray diffraction (XRD) from the initial as-is mixture up to the one produced after 8 h milling time. The resulting homogeneous, metastable microstructure is examined by scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS) to verify the sought result of efficient inter-diffusion of elements. Optical spectroscopy results exhibit enhanced absorption in the UV-Vis-NIR wavelength range with increased milling time, while the trends of absorptivity curves had clear correlations with microstructural evolution. The impedance measurement of the resulting compound shows an increase in the resistance to up to 120 ohm, compared with zero for the as-is starting mixture, which is a useful observation for many applications.

Keywords: Metastable alloys; Fe-Cu systems; selective solar absorbers; mechanical alloying

Application of the exact muffin-tin orbitals method to the Bain path of metals: the overlapping potential sphere wells and the hard spheres

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Abstract:

We present the optimized overlapping muffin-tin approximation (OOMT) using the exact muffin-tin approximation (EMTO) formalism. Within the OOMT approximation, the potential is spherically symmetric around the atomic site and constant in the interstitial region and can be overlaps depending on the size of the potential sphere. To investigate the size of the potential sphere, total energy calculations are carried out along the Bain path that connects the body-centered cubic (bcc) and face-centered cubic (fcc) structures for set of simple and transition metals. We demonstrate that for potential sphere radius S =1.10w (where the radial overlap around 30%) yields accurate results and small S give worse results. The hard sphere radius (b) is also discussed. It is shown that when large hard spheres are taken into account (b = 0.7w and 0.8w), the total energy results are consistent ($E_{0.7w} \sim E_{0.8w}$), but for small hard sphere (b = 0.6w), the results are not good. We ascribe this slow convergence of the total energy in case of small hard spheres to the delocalization of the screened spherical waves. Our total energy results along the Bain path are in good agreement with previous theoretical calculations.

Keywords: The Bain Path, transition metals, first-principles calculations, simple metals, structural properties.

Polytriazole-co-Polyoxadiazole Copolymers as a New Class of Membrane Material for Osmotically Driven Processes

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Abstract:
Global scarcity of freshwater and environmental impacts of wastewater are becoming of great concern around the world. Hence, separations of freshwater from other contaminants by membrane–based processes have been intensively developed. Here in, a new type of thin-film composite (TFC) forward osmosis (FO) membranes using highly thermal stable, chemical resistant and anti-organic/biological fouling hydroxyl functionalized polytriazole-co-polyoxadiazole (PTA–POD) copolymers as porous substrates. The roles of PTA/POD ratios in the membrane substrates and TFC layers formation and FO membrane performance have been investigated. The results show that substrate fabricated from the copolymer containing 40 mol % PTA is optimal for the TFC-FO membranes. In addition, the PTA/POD–TFC membrane with 40 mol % PTA support shows better FO performance and enhanced anti-fouling properties compared to a polysulfone (PSU)-TFC membrane under the similar fabricated conditions. The 40 mol % PTA supported TFC-FO membrane exhibits high water fluxes of 37.5 LMH (FO mode)/78.4 LMH (PRO mode). Hence, hydroxyl functionalized polytriazole-co-polyoxadiazole copolymers may be potentially used as a new class of material for FO processes.

Keywords: polytriazole, membrane, water treatment, forward osmosis.

Silicon Nanoparticles for Room-Temperature Catalytic Dehydrogenation of Secondary Alcohols into Ketones and Hydrogen

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Abstract:

Because of their high surface-to-volume ratio, nanoparticles are used in a plethora of applications such as chemical sensors, optical devices, energy harvesting as well as flexible devices and many more. One of their most extensive usages is in chemical synthesis and in particular their catalytic properties. In particular, silicon nanoparticles dispersed in solvents are used in several applications ranging from biosensing to hydrogen production, yet their reactivity and their catalytic properties remain still uncharted. In this work, we have been using an inexpensive method, through colloidal stain etching, to fabricate silicon nanocrystals. We discovered that, because of their surface structures and mechanical strain, crystalline silicon nanoparticles have a strong reactivity with their solvents and may act as catalysts for the dehydrogenation of secondary alcohols into ketones and hydrogen. Although the production of ketones is a well-known industrial process, but it usually occurs with the usage of toxic heavy metals and at relatively high temperature, which is not cost-effective when done at large scales. Thus, there is an incentive to develop new replacement catalysts, which are non-toxic and which could be used at standard conditions of temperature and pressure. We want to disclose here that we were able to attain a catalytic production of ketones at room-temperature and low pressure.

The simplest model reaction chosen was the dehydrogenation of isopropanol to acetone and hydrogen. The "dissociative chemisorption" of isopropanol occurs on the Si nanocrystals to produce an Si−H and an Si-isopropoxy radical.. This discovery provides a new grasp of the role played by silicon nanocrystals in their reactivity with solvents in general, as well as being good candidates for catalytic applications. This catalytic reactivity was scrutinized by extensive gas chromatography, FT-IR, pH measurements and solid-state NMR.

Keywords: Silicon Nanocrystals; Heterogenous Catalysis; NMR; Mass Spectroscopy; Hydrogen Production

Green Corrosion Inhibitors for Carbon Steel

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Abstract

Corrosion is recognized as one of the most serious problems in our modern societies and is the culprit of billions of US dollars losses each year. Corrosion occurs in corrosive environments such as humidity, contaminated soil, acid rain, and other factors. Failure of process entities such as equipment, pipes, fittings, and valves could cause major shut downs to plants, emission of hazardous chemicals to the environment, injury to employees, material contamination, and in some cases could cause catastrophic failures. Carbon steel is used in a wide range of industries due to its cheap cost and easy availability. The main setback for this metal is its tendency to corrode easily in an acidic and brine environment. Inorganic acids like HCl and H_2SO_4 are used for drilling operations in oil exploration, descaling operations and in many industrial applications. Carbon dioxide (CO_2) is injected into oil wells to reduce the oil viscosity and enhance its production. CO_2 has the tendency to dissolve in water and form carbonic acid which is more aggressive than hydrochloric acid. Wet acidic gases such as CO_2, H_2S and weak acetic and formic acids cause significant amount of corrosion for steel pipelines and storage processing facilities used in the oil and gas production networks. Since these acidic environments cause corrosion of steel, several protective measures are taken, one of them being the use of corrosion organic inhibitors. But, most of the synthetic organic inhibitors are unfavorable environmentally due to various levels of their toxicity, bioaccumulation and/or biodegradability and this has led to the need of natural products which are eco-friendly and harmless. The green inhibitors extracted from plant leaves and vegetable skins were investigated as potential corrosion inhibitors for steel under relevant brine solution saturated with CO_2 and HCl at different temperature. The research work is devoted to investigate the corrosion inhibition efficiencies of aqueous extracts such as Fig, Calotropis Procera leaves, and Eggplant and Potato Peels. The inhibition process was evaluated using various electrochemical techniques including linear polarization resistance (LPR), potentiodynamic scans, and electrochemical impedance spectroscopy (EIS) at various temperatures in 2M HCl and 3.5wt% NaCl saturated with CO_2. The adsorption isotherms as well the surface coverage of steel by the inhibitors are also investigated. Further mechanistic information at the molecular level of the active sites, reactivity and adsorption of selected major aqueous extracts constituents on Fe (110) crystal surface were obtained using a combination of quantum chemical approach and molecular dynamics simulations. Research in this direction of bringing out novel, viable and cost effective corrosion inhibitors will help in a long way to maintain lower cost of operation and reduce potential economic losses.

Hybrid Pectin-Based Biosorbents for Zinc Removal

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Abstract:
Biosorbents are commonly used in removal of heavy metals, such as zinc, which is an important element for the living organisms. Zinc takes part in the metabolism of peptides and nucleic acids, stimulates the activity of various enzymes and controls the work of immunological system; however, its daily dosage above 100 mg can seriously damage the liver, kidneys and pancreas. Widespread zinc usage in anti-corrosive coatings, batteries, paints and cosmetics, as well as its presence in the mine waters, allows the element to accumulate in the environment and makes zinc removal from waste waters an important issue. Therefore, new, cheap and effective zinc biosorbents are demanded.
In this paper, a set of hybrid biosorbents made of pectin with various secondary polysaccharide additives (inulin, agar-agar, gum arabic, gum gellan, gum tragacanth, gum karaya) was investigated. Hybrid pectin-based biosorbents were prepared by introduction of additives during the gellation of pectin by Ca^{2+} ions. The additives not only have sorption capabilities on their own, but also may influence the sorption capacity of pectin biosorbent, e.g. due to the change in swelling ratio, or decrease the biosorbent price. The maximum possible amount of studied gums immobilized in pectin biosorbent was determined. The immobilization of the polysaccharides was proved by Raman spectroscopy. The influence of the additive type on biosorbent swelling ratio was also investigated. All of the obtained hybrid materials had similar Zn sorption capacity, up to 20 mg/g at pH = 5 and zinc concentration of 20 mg/dm^3. The results show that the hybrid pectin-based biosorbents are a promising method for zinc removal from aqueous solutions.

Keywords: pectin, biosorbents, polysaccharides, hybrid materials, zinc removal.

The use of optical fibers for environmental decontamination

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Abstract:
Environmental pollution by pharmaceuticals is an increasingly important public health issue, specially for water contamination because of its scarcicity. Pharmaceuticals are mostly introduced in the sewage system through excretion of unmetabolized compounds after use or inappropriate disposal and then transported into the wastewater treatment plants (WWTPs). However, conventional WWTPs are not designed to treat water polluted with pollutants present at trace levels and therefore, the applied treatments are ineffective. Consequently, they reach the aquatic system and can be found in surface and ground water, soil, and even in tap water. Their presence can negatively affect human and animal health and aquatic ecosystems. From these pharmaceuticals, antibiotics represent a serious problem since they may lead to the development of antibiotic resistance in microorganism. Diverse efforts have been made to remove pharmaceuticals from wastewater. Photocatalysis has become an attractive method to remediate environmental microcontamination due to its high photocatalytic activity, non-toxicity and photostability. These photocatalysts can be employed either in a colloidal or in an immobilized form. However, whenever the particles are dispersed in the aqueous phase the depth of penetration of radiation is limited due to absorption or scattering by the catalyst particles and dissolved organic species. Therefore, optical fiber are used both as a photocatalyst support and as a light transmission tool. This approach avoids light loss due to scattering of the light by the medium because the light reaches directly the photocatalyst coated on the optical fiber surface without passing through the liquid, avoids the costly and extra final filtration process since the catalyst is immobilized on the surface of the fiber, and allows its reusability which is of highly importance to reduce the costs associated with this process. Immobilized photocatalytic systems are thus an advantage for the treatment of contaminated water, because they are ecofriendly, cost-effective and allow reusability.

Keywords: antibiotics, immobilization, pharmaceuticals, photocatalyst, sunlight.

$C_5H_{11}NO_2S$ Effect on Concrete Steel-Reinforcement Corrosion in Industrial/Microbial Simulating Environment

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Abstract:
This paper investigates effect of $C_5H_{11}NO_2S$ (Methionine) on steel-reinforcement corrosion in concrete immersed in 0.5 M H_2SO_4, simulating industrial/microbial environment. For this, corrosion rate test-data were obtained by linear polarization resistance instrument from duplicates of steel-reinforced concrete samples immersed in the corrosive medium for eighty-four days experimental period and the obtained test data subjected to statistical distribution analyses as per ASTM G16-95 R04. While the analysed results obtained showed that there is no statistically significant difference from test-data obtained between the duplicated concrete samples, the different admixtures of $C_5H_{11}NO_2S$ employed in the study reduced corrosion rate in their admixed concrete compared to the control specimen without admixture. By this, 0.25% $C_5H_{11}NO_2S$ admixture (per weight of concrete mixing cement) was identified as exhibiting optimal inhibition efficiency of 87.95±7.64 on the corrosion reinforcing steel embedments in concrete studied in the paper.

Keywords: Methionine admixture, steel-rebar corrosion, industrial/microbial simulating-environment, statistical tests of significance, corrosion inhibition efficency.

Biochemical Characterization of *Cymbopogon citratus*: Prospects on Environmentally-Friendly Corrosion-Protection of Concrete Steel-Reinforcement in Aggressive Environment

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Abstract:
Biochemical characterization of inorganic and organic constituents of the leaf of *Cymbopogon citratus* was investigated in this paper. For this, methods of atomic absorption spectroscopy (AAS), Fourier transform infrared spectroscopy (FT-IR) and phytochemical screening analyses were employed. Results showed that the leaf of *Cymbopogon citratus* exhibited inorganic constituents including iron, Fe = 4,641.025 μg/g, manganese, Mn = 849.5069 μg/g, copper, Cu = 171.045 μg/g, lead, Pb = 13.2938 μg/g, nickel, Ni = μg/g, cadmium, Cd = 4.9310 μg/g, and chromium, Cr = 0.0 μg/g, from the AAS method. The FT-IR detailing indicates organic constituents from *Cymbopogon citratus* leaf-extract includes S-, N-, O- containing heteroatoms and aromatic compounds that are rich in π-electrons and which are known to exhibit coordinate affinity with the iron-containing reinforcing steel metal. Analyses of phytochemical screening of *Cymbopogon citratus* leaf-extract showed it is constituted of tannins, phlobatannins, saponins, steroids, terpenoids and glycosides. Further tests on corrosion protection ability showed that this natural plant reduced total corrosion, analyzed as per ASTM G109-99a, in steel-reinforced concrete samples immersed in 0.5 M H_2SO_4 environment. These suggests implications of positive prospects of *Cymbopogon citratus* as an environmentally-friendly inhibitor of reinforcing steel corrosion in concretes having acidic medium as service-environment.

Keywords: *Cymbopogon citratus* leaf, environmentally-friendly natural plant material, reinforcing steel in concrete, total-corrosion analyses, inorganic and organic characterization, phytochemical screening, sulphuric acid environment

Performance of *Cassia Fistula* Leaf-extract on Stainless Steel Corrosion in 0.5 M HCl

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Abstract:
In this study performance *Cassia fistula* leaf-extract on stainless steel corrosion in 0.5 M HCl medium was investigated. For this, different concentrations of *Cassia fistula* leaf-extract was employed in the acidic medium in which stainless steel specimens were immersed and corrosion rate was obtained through linear sweep voltametry instrumentation, at the ambient temperature of 28°C. Results showed that inhibition effectiveness of *Cassia fistula* leaf-extract on stainless steel corrosion in the test-environment, tends to increased with increasing concentration of the natural plant extract. By this, 10 g/L *Cassia fistula* leaf-extract, which is the highest concentration of the leaf-extract employed in the study, exhibited optimal inhibition efficiency η = 88.46% on stainless steel corrosion in 0.5 M HCl.

Keywords: Linear sweep voltametry, corrosion rate, *Cassia fistula* leaf-extract, stainless steel, inhibition efficiency, acidic medium,

The Efficiency of Al_2O_3-water Nanofluid on a Flat-Plate Solar Collector

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Abstract:
The perceived shortage of fossil fuels as well as environmental considerations will constrain the use of fossil fuels in the future. Therefore, researchers are motivated to find alternative sources of energy. Of all the renewable sources of energy available, solar thermal energy is the most abundant one and is available in both direct as well as indirect forms. It is also used in different applications including solar electricity, air conditioning, cooker and water heater (Thirugnanasambandam et al.; 2010). Solar collectors are particular kind of heat exchangers that transform solar radiation energy into internal energy of the transport medium. One of the most effective methods is replacing the working fluid (water, ethleyene glycol, engine oil…) by developing a new class of fluids with a higher thermal conductivity for thermal systems. Applying nanotechnology to thermal engineering, the novel concept of 'nanofluid' which was coined by (Choi; 1995) has been proposed to meet cooling challenges. In the present work the effect of Al_2O_3-water, as working fluid, on the efficiency of a flat plate solar collector is investigated experimentally. The mass flow rate of nanofluid is 150 Lit/h. The volume fraction of the nanoparticles is 0.2 % , 0.4 % and 0.8 % respectively (Figure 1). The results reveal the impact and importance of each of these parameters. Experimental results reveal that utilizing the nanofluid increases the collector efficiency in comparison to water as an absorbing medium.

Keywords: nanofluid, flat-plate solar collector, efficiency.

Figure 1: Prepared Al_2O_3- water nanofluids

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Nano Technology Application in Stablizing Expansive Soil: Irbid Clay

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Abstract:
Recently, there has been a great deal of interest for the application of nanotechnology in geotechnical engineering. Soil stabilization is one of the fertile areas for the use of nanotechnology in the field of geotechnics. According to Kolias *et al*. (2005) soil stabilisation is a customary strategy used to enhance soils to accomplish the specifications of different projects. Due to the swelling behavior, expansive soils, like eastern Irbid clayey soil, is increasing in its volume once exposed to water. This increase in volume will produce uplift pressure under the footing of the structure resting on it. Unless this type of soil is treated to lower its expansive amount, a severe damage may cause to the structure. Soil treatment, stabilization, by additives is a well know method in this field. As a new technique, the addition of finer particles such as nanomaterials, even at low doses, could enhance the expansive soil properties (Taha, 2009). In this study, a systematic investigation for the effects of the addition of nanomaterials on the expansive soil strength's characteristics, mainly compaction and unconfined compressive strength, was carried out. The improvement attained is dependent on the type of nanomaterials. Nano clay, Fig. 1, was used in this study as an additive material.

Keywords: expansive soil, soil stabilization, nano clay, uplift pressure, compaction, unconfined compressive strength.

Session III
Advanced Materials/ surfaces for biomedical / Life Science

State-of-the-Art in Powder Metallurgy Materials with Atomic/Nano scale Microstructures

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Abstract

Advanced light metals such as aluminum, titanium, magnesium and their alloys, with atomic/nano-scale microstructures are fabricated by solid-state powder metallurgy (PM) process. Carbon nanotubes (CNTs) are promising useful reinforcements for the metal matrix composites, and their uniform coating process on metal powder surfaces has been established by using the wet or dry process. PM pure Al nano-composites reinforced with CNTs showed 350-400 MPa tensile strength, which was much higher than that of the monolithic pure Al with no CNT having 120 MPa UTS. Regarding the strengthening behavior of pure Ti material with no rare metal element, the ubiquitous elements such as oxygen, nitrogen, hydrogen, silicon and iron, were employed for solid-solution strengthening of PM Ti materials. For example, the solid-solution of 0.7 wt% oxygen atoms into α-Ti successfully improved UTS of 1050 MPa while its elongation was over 25 % at room temperature. These atomic/nano-scale materials design was effective by using PM process in solid state, not by the conventional casting ingot metallurgy process.

Immuno-nanotheronostics approach to detect and eliminate cancer cells

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Abstract:

Theranostics approach holds great promise for improving cancer prognosis and management and represents a new paradigm in medicine especially for cancer treatment. It is widely believed that theranostics approach will have a great chance in fine-tuning cancer care by providing the right patient with the right dose of the right drug at the right time.

Currently, the majority of theranostics agents in the clinical development are nanoparticle-based reagents. Although, the development of theranostics nanoparticles (TNPs) progress rapidly, systemic or cellular toxicity and off target accumulation set a countless challenges preventing TNPs from a breakthrough in the clinic.

Immuno-nanotheranostics approaches are expected to target specific cells and therefore reduce the toxicity and off targeting effects of nanotheranostics agents. This system combines the highly potent therapeutic activity and powerful imaging properties of TNP with the specificity of monoclonal antibodies (mAbs) or their fragments to detect and selectively eliminate tumor cells. However, complexity and high production cost of immuno-nanotheranostics agents generate substantial challenges that limits the success of developing immuno-nanotheranostics agents. To overcome these limitations, we have used SNAP tag technology to synthesized an epidermal growth factor receptor (EGFR)-targeted dendritic polyglycerol theranostics agent, and investigate whether it could be used for cancer cell imaging and therapy in different cancer entities. This immune-nanotheranostics agent is provided with a dendritic core as a multifunctional anchoring point, doxorubicin (Doxo) coupled through a pH-sensitive linker, a fluorescence marker, poly(ethylene glycol), as solubilizing and shielding moiety and a specific antibody fragments conjugated through the SNAP-Tag technology. This agent shows powerful imaging properties and highly potent therapeutic activity in different cancer cells that expressing different levels of EGFR.

Keywords: Immuno-nanotheranostics, anti-EGFR antibody fragment (scFv-425), dendritic polyglycerol, doxorubicin, SNAP-tag, targeted delivery, antibody drug conjugate.

Naproxen and Ibuprofen Molecular Liquids — A high yield supercritical CO_2 process platform

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Abstract:
One of the major unsolved problems in pharmaceutical drug development is the poor water solubility of many active pharmaceutical ingredients (APIs) and hence reduced bioavailability. Researchers have attempted to minimize the problem by reducing the drug particle size. While, many of these platforms bring unique advantages to the field of drug delivery, an ideal solution would be to remove the problem of solubility entirely, by reducing the API size to clusters of a few molecules, bound by weak, van der Waal's forces that would readily dissociate into molecules, during enteral or parenteral drug delivery process. In order to have commercial impact, such molecular clusters should also be produced in sufficiently high yield. In our research, we have successfully addressed both these challenges.
We have precipitated molecular clusters of two drug molecules, Ibuprofen and Naproxen, respectively, via supersonic jet expansion of the supercritical CO_2 drug formulation into a collection vessel cooled to liquid N_2 temperatures and capturing the clusters instantaneously in "dry ice" with up to 80% yield. Slowly warming the "dry ice" in water, at room temperature, resulted in the solubilization of the clusters in water, creating a stable solution. Drop casting and ambient drying of the solution on a substrate (e.g. silicon) resulted in a stable, viscous liquid film, which we refer to as a nanostructured molecular liquid. This is a significant observation, considering the fact that, normally, Ibuprofen and Naproxen are solid powders at room temperature and pressure, with melting points of 76^o C and 154^o C, respectively. *In vitro* cancer cell viability studies of water-solubilized Ibuprofen and Naproxen exhibit similar cytotoxicity to that of the original raw materials, thus retaining their potency. Besides its scientific importance, this invention is expected to open up new drug delivery platforms.

Keywords: **:** poor water solubility, pharmaceutical drug development, nonsteroidal anti-inflammatory drugs (NSAIDs), supercritical CO_2, RESS Process and cell viability, biomedical applications.

Mussel inspired nanointerface for an efficient biomolecular delivery into cells

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Abstract:
The mussel-adhesion phenomena inspired dopamine treatment has been highlighted as a versatile agent for surface modification through simple polymerization using solution oxidation process under alkaline conditions. Emerging nano- and microfabrication techniques are fostering the development of novel materials as functional nano- and microstructures, with improved capability for overcoming the challenges associated with complex biological applications. For instance, high aspect ratio nanomaterials such as nanotubes, nanowires, nanopillars, and nanoneedles are shown to have excellent mechanical, optical, and electrical properties for various intracellular applications. We have already reported the ability of polydopamine for siRNA immobilization on steel surfaces and RNA interference caused by high surface concentration of siRNA. This study looks into the dopmaime based nanowire interfaces for intracellular transfer of biomolecules.
Keywords: siRNA, polydopamine, nanowires, RNA interference, nanointerfaces.

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Synthesis, Charectrerization and applications of Iron oxide Nanoparticles in Cosmetics

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Abstract:
Iron oxide nanoparticles are well known for their excellent biocompatibility, chemical stability and less toxicity. The nanoparticles of iron oxides are commonly used in various fields such as targeted drug delivery, contrast agents in MRI and magnetic storage materials. In this work we have used iron oxide nanoparticles in cosmetics where the nanoparticles can fine tune the SPF value and also it is preventing the skin from harmful UV rays . The iron oxide nanoparticles were synthesized through biotemplates and the characterization of nanoparticles were carried out using TEM , SEM, TGA, and DLS. The synthesized iron oxide nanoparticles were used in various cosmetics products such as nano-suncream, talcum powder, nanolipstic etc. These nanoparticles provide uniform color, higher SPF value and excellent UV protection to the cosmetic products.

Keywords: Templates, nanocosmetics, Transmission Electron Microscope, Dynamic Light Scattering.

Mechanical Properties of Silver Coated Electro-Spun composite Scaffolds for Antibacterial Applications

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Abstract:

A biocompatible, and biodegradable electrospun composite scaffold of poly(glycerol sebacate)–poly(ε-caprolactone) (PGS–PCL) has generated greatest interest as composite scaffold materials due to desirable thermal and mechanical properties. In this work, we fabricated the microfibrous scaffold from a composite of PGS/PCL fibers using a standard electro-spinning method and then coated with silver (Ag) on the surface of the pristine fibrous scaffold. The Ag coating makes lower the pore size and higher the diameter of fiber scaffold in a resulted higher thermal and mechanical properties. We further compared the mechanical properties of the composite fibrous scaffold with different Ag coating scaffolds. The composite fibrous scaffold with Ag coating showed higher tensile modulus (E), ultimate tensile strength (UTS) and lower tensile strain. Lastly, the antibacterial activity of Ag coating on composite fibrous scaffold materials was greatest interest against Band-Aid and tissue engineering applications.

Keywords: Fibrous Scaffold, electro-spinning, antibacterial activity, biomaterials

Preparation and characterization of cross-linked β-cyclodextrin-graffted chitosan nanoparticles coated with hyaluronic acid

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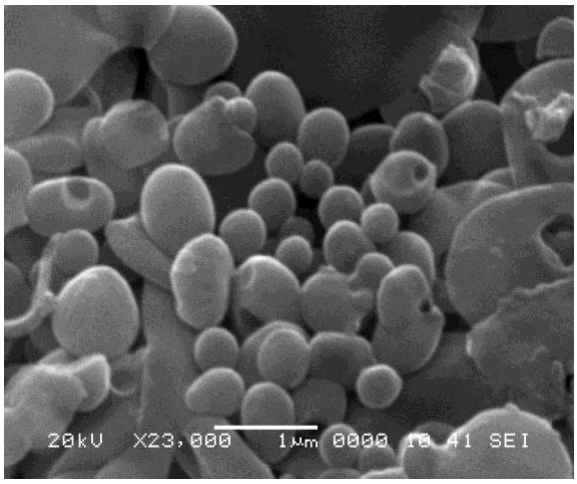
Abstract: We report in this study a new strat-egy for the preparation of biodegradable chitosan- β-cyclodextrin nanoparticles that would be used as potential drug carrying and delivery systems. The nanoparticles obtained by dialysis and lyophilization could be prepared only within a range of appropriate chito-san and sodium tripolyphosphate concentrations at pH 5 according to the ionotropic gelation method (Jingou J *et al.*;2011). Chitosan and β-CD grafted chitosan nanoparticles were coated with hyaluronic acid (HA) as a new procedure to prevent proteins adsorption (op-sonisation). SEM (Figure 1) and TEM microscopies examination showed that the obtained nanoparticles had more spherical shape and smooth surface. The chitosan and β-CD grafted chitosan nanoparticles have a mean particle diameter of approximately 120 and 220 nm (light scattering (DLS)) and a zeta potential +35 to +30 mV, respectively. The treatment of these compounds with hyaluronic acid led to an increase of the size of the nanoparticles (235 and 330 nm), with significant modification of their zeta potentials (-25 and -20 mV). According to the data obtained, CS-β-CD nanoparticles coated with hyaluronic acid opens new and interesting perspectives and may be considered as beneficial drug nanocarriers.



Keywords: Nanoparticles; Chitosan; β-Cyclodextrin; Hyaluronic acid; Ionic gelation technique.

Figure 1: Figure illustrating the SEM image of lyophilized nanomaterial of HA-β-CD-g-CS

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Posters Session

Molecular dynamics simulation of functionalized graphene – a study of the mechanical properties of graphene and the interaction between graphene and epoxy

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Abstract:
Carbon fibres are common and efficient fillers providing composites with high strength and stiffness. Because this is a structurally graphitized material, commercial carbon fibres undergo post treatment in order to improve their handeability and promote a good adhesion to the polymer. Their surface is normally oxidized followed by sizing treatment by introducing functional groups such as hydroxyl, carbonyl, and carboxyl. A good adhesion leads to improved load transfer from the matrix to the fibres resulting in greater composite stiffness and strength. On the other hand a weak fibre/matrix interface results in lower composite strength but higher toughness.
In this study, molecular dynamics simulations are carried out to investigate the influence of functional groups on the mechanical properties of carbon fibres. For the sake of simplicity these fibres are modelled as graphene. Both sized and pristine graphene models are taken into account. As mentioned previously, only hydroxyl, carbonyl, and carboxyl functional groups are considered for the functionalized models given the very little influence of other chemical species. The effects of the functional groups on the carbon network that form the graphene layer will be assessed through the determination of the elastic properties of each model system and through visual inspection of the bonding structure.
Furthermore, the interaction between functionalized graphene sheets and partially cured epoxy, TETA hardener and DGEBA epoxy resin, respectively.

Keywords: functional groups, graphene, interaction analysis, mechanical properties, molecular dynamics.

Characterization of an EDTA-based Gemini Surfactant at the Air-Liquid Interface

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Abstract :
The surface-active properties of an EDTA-based gemini surfactant are studied at the air-liquid interface in order to determine the association constants and ion binding ratios as well as rationalize the functions of the compound through its structure. Compression isotherms of monolayer films were taken for various concentrations of sodium and calcium containing subphases at both pH 6 and pH 10. These isotherms were compiled into association behaviour plots through the use of a simple ion-binding model. This process led to the relationship between ion valence, pH and ion-binding ratio. The effect of both pH and valence on the association constant is also documented and rationalized. Qualitative studies were performed using Brewster Angle Microscopy (BAM) which allowed for visualization of surfactant behaviour at the air-liquid interface. Non-ordered structures are observed for ion-containing subphases, indicating strong influence by the ions on the formation of a structured monolayer.

Keywords: Gemini surfactant, Compression Isotherm, Brewster Angle Microscopy, Air-Liquid Interface, Langmuir.

Temperature Dependence Control of Birefringence of Zero-Birefringence Polymers for LCDs

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Abstract:

Optical polymer films are now widely used such as in liquid crystal displays (LCDs). However, birefringence of optical polymer films can degrade the contrast ratio of LCDs. Therefore a film that does not show any birefringence is required. Generally, birefringence is categorized into two types depending on how it is generated (Iwata *et al.*, 1997). One is orientational birefringence and the other is photoelastic birefringence. In the previous research of our group, zero–zero-birefringence polymer (ZZBP) which exhibits neither orientaional birefringence nor photoelastic birefringence was successfully prepared in a ternary copolymerization system (Tagaya *et al.*, 2006). But recently, we observed little temperature dependence in orientational birefringence. Because polymer films are used under the condition where the temperature changes, optical polymer films with no temperature dependence of orientational birefringence is needed.

In this research, we first clarified what the main cause of temperature dependence of orientational birefringence is by focusing on poly(methyl methacrylate) (PMMA). Temperature dependnence of retardation *Re* of PMMA was measured, which is the function or orientaitonal birefringence and film thickness as shown in equation (1).

$$Re = d \cdot \Delta n_{or} = f \cdot \Delta n^0 \cdot d \qquad (1)$$

Here, d, Δn_{or}, f are film thickness, orientational birefringence and degree of orientation. By considering the temperature change of the three parameters on the right hand side of the equation, it was indicated that temperature dependence of intrinsic birefringence due to the change in conformation is the main cause of the temperature dependnence of orientational birefringence.

Next we clarified temperature coefficient of intrinsic birefringence $d\Delta n^0/dT$ of various polymers, such as PMMA, poly(2,2,2-trifluoro ethyl methacrylate) (PTFEMA), poly(benzyl methacrylate) (PBzMA) and poly(phenyl methacrylate) (PPhMA). The results showed that there are both polymers which shows negative and positive signs of temperature coefficient of intrinsic birefringence. It also showed that as the side-chain got bulkier, the absolute value of temperature coefficient of intrinsic birefringence got smaller (Table 1).

Orientational birefringence itself can be adjusted to zero by copolymerizing monomers with different signs of intrinsic birefringence in a certain composition. Since there were polymers that shows opposite signs of temperature coefficient of intrinsic birefringence, we suggested a method to control the temperature dependnence of orientational birefringence by copolymerizing monomers with different signs of temperature coefficient of intrinsic birefringence. By using this process, we designed and synthesized polymer that shows no temperature dependence of orientational birefringence and also no orientational birefringence (Figure 1 ◇).

Keywords: optical polymer film, birefringence, temperature dependence, retardation, bulk polymerization, liquid crystal displays.

Table 1: Birefringence properties of each polymer.

	PMMA	PTFEMA	PBzMA	PPhMA
Δn^0 ($\times 10^{-3}$)	-5.6	3.5	17.3	-10.9
$d\Delta n^0/dT$ ($\times 10^{-5}$ °C^{-1})	3.3	2.6	-1.0	-2.4

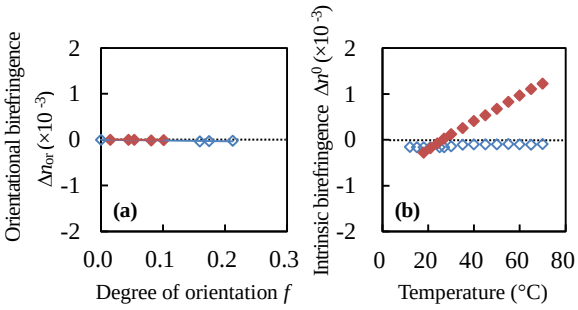

Figure 1: Relationships between (a) orientational birefringence Δn_{or} and degree of orientation f, (b) intrinsic birefringence Δn^0 and temperature of P(MMA/BzMA/PhMA) (◇) and P(MMA/TFEMA/BzMA) (ZZBP) (◆).

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A metod for determination of metals contained in carbon nanotubes

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Abstract:
Carbon nanotubes (CNTs), due to their particular structure and unique properties (optical, electrical, magnetic and mechanical) are still one of the most interesting materials for scientists. They have been used or they may be in the future used in the fields of power and materials engineering, electronics, medicine, and biotechnology. Recently carbon nanotubes were proposed as a new type of catalyst carbon support. Pt, Fe, Ni, Co, and other metals anchored to CNTs are used in various reactions. Due to the fact that production processes are unpredictable and the total amount of metal deposited on the CNTs can only be estimated, the methods for examining the properties, structure, and the chemical composition are necessary. Methods proposed so far have certain limitations, e.g. they are only surface-sensitive, not always can distinguish between the elements, they are insufficiently sensitive to determine trace amounts of metals. In some studies, ICP-AES or ICP-MS were used for quantitative analysis of metal impurities or metal modifiers. However, they require digestion of CNTs, which is extremely difficult and constitute the most problematic step in whole analysis. In this study, hybrid CNT-based material with $CeZrO_2$, Ni and Ni-$CeZrO_2$ particles, were analyzed by direct, fast and simple ICP-AES analysis with slurry sample introduction. Slurries of hybrid catalysts were prepared in Triton X-100 solution, ultrasonicated and directly measured by ICP-AES. The impact of slurry concentration, plasma RF power on analytical signal was investigated. Obtained results proved that this method can be applied for determination of Ce, Zr and Ni in CNT-based materials. Moreover, this method can also find an application in other fields, where the knowledge of total amount of metals contained in CNTs is crucial.

Keywords: carbon nanotubes, metal impurities, metal catalyst, ICP-AES analysis, slurry sampling

The effects of temperature and pH on swelling of stimuli-sensitive hydrogels

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Abstract:
Multistimuli-sensitive gels have recently become a focus of attention as these materials demonstrate potential for a wide range of applications including (i) micro- and nano-carriers for targeted drug delivery, (ii) sensing systems for bio-analytes, (iii) soft actuators, (iv) antimicrobial packaging systems, and (v) devices for removal of organic contaminants from wasted water. This study deals with modeling of the elastic behavior of thermo- and pH-responsive copolymer gels by taking into account changes in (i) hydrophilicity of segments of a thermo-sensitive component and (ii) degree of ionization of a polyelectrolyte component. Adjustable parameters in the constitutive equations are found by fitting swelling diagrams on five gel systems with various molar fractions of ionic monomers. Results of simulation lead to the following conclusions: (i) the model ensures good agreement with observations when swelling tests are performed in water and aqueous solutions of salt, (ii) material parameters change consistently with concentration of ionic monomers, (iii) when these quantities are determined in one type of experiments, the model predicts correctly the response in another type of tests, (iv) the Flory-Huggins parameter determined in simulation belongs to a physically reasonable interval at various temperatures, pH, and molar fractions of ionic monomers, (v) observations on changes in shape of swelling diagrams with molar fraction of ionic monomers are in qualitative agreement with results of simulation, (vi) the model predicts adequately a strong decrease in degree of swelling and a pronounced weakening of the effect of pH on shift of the apparent volume phase transition temperature under constrained water uptake.

Keywords: stimuli-sensitive gels, hydrophobic-hydrophilic transitions, ionization of functional groups, modeling, simulation.

Experimental Studies for the Impact of SiO_2 Particle onto a Planar Surface at Different Temperatures

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Abstract:
The impact of micro-particle onto solid surfaces can find its wide applications in many engineering fields such as ash deposition (Wigley *et al*.; 1998), spray coating (Kawakita *et al*.; 2008), filtration (Li *et al*.; 2011) and agglomerates(Ning; 1995),etc. The impact process is mainly affected by the impact velocity and angle, the particle size and shape, and the material types. As the duration of a single impact is very short and large contact stress is generated in the vicinity of the contact area, the practical impact is usually inelastic. Experimental and theoretical studies have been reported to gain the rebounding characteristics of the impact process. The objective of this work presented here is to study the interaction between micron sized particles impacting a plane surface under different temperatures.This paper presents the results of a comprehensive program of experiments in which SiO_2 particles were impacted under controlled conditions against a planer steel surface. The overall aim of these experiments was to gain an understanding of the ash deposition process in a pulverized coal boiler system. A continuous nitrogen flow carrying particles was used to simulate the flue gas in boiler, and planer steel surface was used to simulate the heat transfer tube in boiler. The effect of particle incident velocity, particle temperature and planer surface temperature on the normal restitution coefficient was examined. The results show that the normal restitution coefficient increases firstly with increasing incident velocity, and then decreases with increasing incident velocity in the measurement range (ranging from 8m/s to 13m/s). The normal restitution coefficient decreases with increasing particle temperature and surface temperature, and with temperature difference between particle and surface. The damping coefficient firstly decreases and then increases with increasing incident velocity. The maximum contact displacement increases with the increasing temperature. The experiments are carried out in an atmospheric column, and individual impacts are recorded by a digital camera system(Figure 1).

Keywords: Normal restitution coefficient, impaction experiments, particle, rebound characteristics.

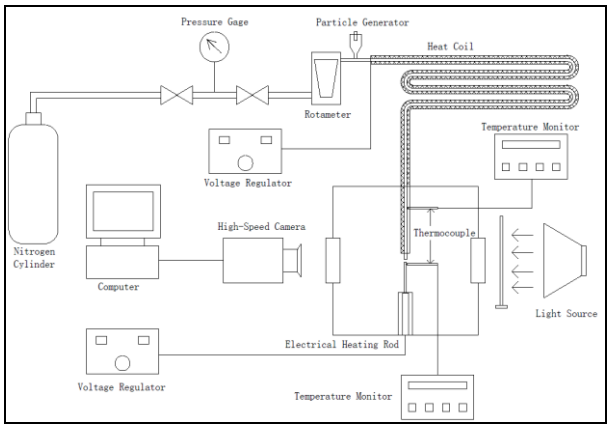

Figure 1: Figure illustrating the experimental system that primarily consisted of a nitrogen cylinder, a particle generator, a temperature controller and a target surface. In these experiments, nitrogen flow is the carrier which conveys the micro-particles to the target surface (providing a velocity range from 0.1m/s~30m/s). The target surface with the diameter of 2 millimeter was oriented normal (90 degree) with respect to the outlet of the particle. The heating equipment and temperature controller was used to make the particles' and the flat surface's temperatures range from 20-200℃.

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WO_3-Nanowire@Graphene Nanocomposite for Efficient Visible Light Induced Photodegradation and Photocapacitance Performance

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Abstract:
Tungsten oxide (WO_3) nanowire was synthesized on to the surface of graphene (G) nanosheets by using a template-free and surfactant-less hydrothermal process at 200℃. The as-synthesized sample was found to be pure as confirmed by X-ray diffraction. The synthesis was further confirmed by UV-vis diffuse reflectance measurements, photoluminescence spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy and TEM. It revealed that WO_3 nanowire was well distributed on graphene nanosheets. The excellent photocatalytic activity of the WO_3@G nanocomposite was analyzed via photodegradation of organic dye under visible light irradiation. The photocapacitance performance of the prepared nanocomposite was investigated by cyclic voltammetry. The superior photocatalysis and photocapacitance performances of the WO_3@G nanocomposites could be attributed due to the synergistic effects of the combined WO_3 nanowire and G nanosheets. The sensitization of WO_3 by graphene enhances the visible light absorption property of WO_3@G nanocomposite. The robust nanocomposite structure and better conductivity, large surface area and good flexibility of WO_3@G nanocomposites seems responsible for enhances the performance. This methodology opens up a new way of obtaining photoactive WO_3@G as a semiconductor nanocomposite for visible light photocatalysis. Our results show the potential applications of WO_3@G nanocomposite such as enhanced photocatalysis and photcapacitive studies.

Keywords: WO_3 nanowire, WO_3@G nanocomposite, visible light, photodegradation, photocapacitance.

Modeling anticorrosive and adsorption mechanism of *Rhizophora mangle* L leaf-extract admixture in steel-reinforced concrete immersed in saline/marine simulating-environment

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Abstract:
Electrochemical test data, obtained from *Rhizophora mangle* L leaf-extract admixed steel-reinforced concrete samples immersed in saline/marine simulating medium, were employed in this paper for modeling anticorrosive adsorption mechanism of the natural plant admixture on the reinforcing steel metal. This entails noise resistance modeling from the ratio of standard deviation of corrosion potential, as per ASTM C876-91 R99, to the standard deviation of corrosion current, from zero resistance ammeter, before correlation of the leaf-extract admixture concentration and the modeled noise resistance with corrosion rate. Analyzed results showed that the corrosion rate from linear polarization resistance instrumentation exhibited very good correlation with the leaf-extract admixture concentration and the noise resistance model (R = 92.26%, Nash-Sutcliffe Efficiency = 85.11%) and ANOVA p-value = 0.0068. Evaluations from these indicated that concentrations of *Rhizophora mangle* L leaf-extract admixture exhibited anticorrosive effects ranging from good, η > 60%, to excellent, η > 90%, efficiencies on reinforcing steel and that the anticorrosion performance followed Langmuir adsorption isotherm model. The adsorption modeling indicated physisorption as the prevalent anticorrosive adsorption mechanism of the plant extract admixture on reinforcing steel metal in concrete immersed in the saline/marine simulating-environment.

Keywords: *Rhizophora mangle* L leaf-extract, concrete steel-reinforcement, noise resistance modeling, correlation analysis, adsorption isotherm model, saline/marine simulating-environment

Modeling of the optical fiber using the VHDL-AMS lunguage

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Abstract:
In this paper, we present the modeling results from a transmission block and a propagation channel of an optical transmission system. The transmitter section consists of a VCSEL laser diode which is responsible for converting electronic signals into optical power. This block is associated with an input circuit which provides the current for the laser diode. The propagation channel comprises the multi-mode optical fiber. The domains to be considered in our modeling are: electronics, optoelectronics, optical, and thermal. The models that we develop should meet the needs of designers and developers by enabling them to highlight the strengths and weaknesses of their electronic systems and manufacturing techniques. They must also be designed to be reused for developments in the next generation of optoelectronic components.

Keywords: VCSEL; VHDL-AMS; optical fiber, chromatic dispersion.

Zinc Sorption on Modified Waste PMMA

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Abstract:
Increasing demand for acrylic sorbents is related with waste-polymer production. Poly(methyl methacrylate) – PMMA –is being recycled to form of granulate with low wholesale price and properties stable enough to use this waste-PMMA as a base for chemical modification. High-molecular, atactic PMMA was considered as a hard to be hydrolysed polymer. Due to its steric hindrance and unpleasant solubility with the most of polar solvents, hydrolysis reaction usually proceeds slowly. This research presents a novel "one-flask" reaction of hydrolysis and synthesis polymeric sorbent based on waste poly(methyl methacrylate). In this synthesis method, diethylene glycol dimethyl ether (diglyme) was used as an extraordinary medium for basic hydrolysis of high molecular atactic poly(methyl methacrylate). Thus, considerable PMMA solubility in glymes has resulted in preparation of sorbents in the fast and simple procedure. The waste PMMA was modified at temperature between 110 to 140ºC, and solid sorbents were obtained in diglyme-polymer emulsion by fast cross-linked reaction with diols or amines. Structures of non-crosslinked sorbents were confirmed by means of ^{1}H and ^{13}C NMR spectroscopy. Zinc ion sorption capacity of the microcapsules and the plain modified PMMA beads was very high – up to 130 mg/g. The results indicate that hydrolysed waste PMMA is suitable as sorbent material for adsorption and recovery of the ions from aqueous solutions.

Keywords: Zn(II) ions removal, waste PMMA, poly(methacrylic acid), poly(methyl methacrylate), sorbents, polymeric materials, hydrolysis.

Removal of textile dyes by composite based on chitosan

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Abstract:
Transparent organic-inorganic nanoporous silica glasses obtained via the sol-gel method constitute the ideal sup With the development of textile, increasing amounts of wastewater that contains dyes are discharged into bodies of water, thereby pos-ing serious hazards because of the toxic and carcinogenic properties of most of these dyes. Therefore, the removal or decolorization of these dyes before their discharge into water systems is necessary. Several physical, chemical, and biological techniques have been employed to remove dyes from wastewater, among which are photochemical degradation, biological degradation, coagulation, chemical oxidation, and adsorption. Adsorption has been shown to be most promising for the removal of organic contaminants from wastewater.
Chitosan (CS), a derivative desacetylated of the chitin, has attracted remarkable attention because of its non-toxicity, biocompatibility, and biodegradability. it is widely used in dye adsorption from aqueous solutions.
In this work, we investigated the removal of acid dyes in aqueous solution: the red telon and the yellow irionyl by the modified chitosan: chitosan-benzylamine composite and nanoparticles of chitosan-MgO. We studied the influence of various parameters on the kinetics of biosorption as: contact time, initial concentration of the dye, the mass of biosorbent and the initial pH of the solution. The results showed that the removal of the dye depends on several factors such as pH and the contact time. The biosorption of red telon and yellow irionyl by chitosan-benzylamine composite and nanoparticles of chitosan-MgO showed better results for the removal of the dyes, the adsorbed quantities at equilibrium by chitosan-benzylamine composite and nanoparticles of chitosan-MgO are higher than those of the only chitosan.

Keywords:chitosan, biomaterial, composite, wastewater, nanoparticle, biosorption.

Elecrical transport properities of an isolated single walled carbon nanotube aligned on an ST-cut quartz substrate

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Abstract:
Highly aligned single walled carbon nanotubes (SWNTs) are synthesized by chemical vapor deposition (CVD) from a mixture of methane and hydrogen gases on ST-cut quartz substrates. We intdoduce a technique to conduct electrical measurements on an isolated nanotube. The temperature dependence of its electrical resistance is measured from room temperature down to few Kelvins. The results are compared the theoritical models on the electrical properites of carbon nanotubes.

Keywords: single walled carbon nanotubes, electrical transport properties, highly aligned on substrate, ST-cut Quartz,

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Study of Interaction between the Molecule 2-Mercaptobenzimidazole and Metal Atom Substrate for Self-Assembled Monolayers

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Abstract
Self-assembled monolayers (SAMs) have expected interest due to their durability and easy preparation. The potential application of SAMs consists of several fields such as sensor fabrication, molecular electronics, high-density memory storage devices and electrocatalytic studies. Self-assembled monolayers of aliphatic systems have widely studied in the past years, whereas more recently the attention has focused on SAMs of aromatics and hetero-aromatics thiols. Aromatic thiols SAMs are moreover attractive for the reason of highly delocalized electron density, strong intermolecular interactions and structural rigidity of the phenyl ring. Among the hetero-aromatics thiols, the 2-mercaptobenzimidazole (2MBI) molecule has a simple thiolfunctionnel group that may be expected acting as the main chemisorption center and allows the formation of self-assembled monolayers. The interaction between the molecule 2-mercaptobenzimidazole and metal atom substrate is unclear and it is still in debate.
We propose to study the adsorption of 2-mercaptobenzimidazole on three different atom gold, palladium and nickel with the intention to understand and estimate the interaction between this molecule and the abovementioned metallic atoms. We have used the density functional theory (DFT) methods to determine the quantum chemical parameters such as the Mulliken charges, the highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}) energies, the difference (ΔE) between E_{LUMO} and E_{HOMO} energy, chemical hardness (η), total energies and dipole moment (μ).
The complexation of 2MBI with Au, Pd and Ni atoms modifies the quantum chemical parameters of the organic molecule. This study reveals that gold bonds with 2MBI molecule via sulfur atom, however, the palladium and nickel atoms bond with 2MBI molecule via nitrogen atom.
The results of the present work give a new insight on self assembly of 2-Mercaptobenzimidazole molecules at metal surface.

Key words: 2-mercaptobenzimidazole, self-assembly, Adsorption, Density Functional Theory (DFT), Energy gap, chemical hardness η, Dipole moment, Theoretical calculation, Gold, Palladium, Nickel.

Effects of Alkali Metal Doping on the Graphene/Ni(111) Surface

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Abstract:
We use density functional theory calculations to investigate the atomic and electronic structure of the K doped graphene/Au/Ni(111) surface and the Na doped graphene/Ni(111) surface. An ARPES study [1] and DFT calculation [2] reported an interesting result that the graphene on Au/Ni(111) is quasi-freestanding. Manipulation by alkali-metal doping of the structural and electronic properties of such epitaxial graphenes is also an interesting issue.

A recent ARPES study reported that the K doped graphene/Au/Ni(111) surface has a large band gap of 0.6 eV [3], which is interesting in view that the graphene on Au/Ni(111) is quasi-freestanding and the K-doped freestanding graphene itself shows no band gap [2, 3]. Interestingly, however, our DFT study demonstrates that the K doped graphene/Au/Ni(111) surface still preserves the Dirac cone band shape only with a uniform shift of 0 ~ -1.1 eV depending on the K coverage [4]. The Dirac cone undergoes a weakening of the graphene π character due to the hybridization with Ni *d* bands. We suspect that this weakening of the π character may affect the ARPES intensity of the Dirac cone, which could be the origin of the experimental band gap estimation.

In the case of the Na doped graphene/Ni(111) surface, our DFT calculations demonstrate that the doped Na atoms prefer the interface intercalation to the surface adsorption: The intercalation is more stable than the adsorption at high coverages [5]. Whereas the complicated band structure of the chemisorbed graphene/Ni(111) surface is little affected by the Na adsorption, it is drastically changed by the Na intercalation, fully recovering the Dirac cone of ideal freestanding graphene with a uniform band shift of -0.4 ~ -1.4 eV depending on the Na coverage.

Keywords: graphene, Ni(111), alkali metal, density-functional theory

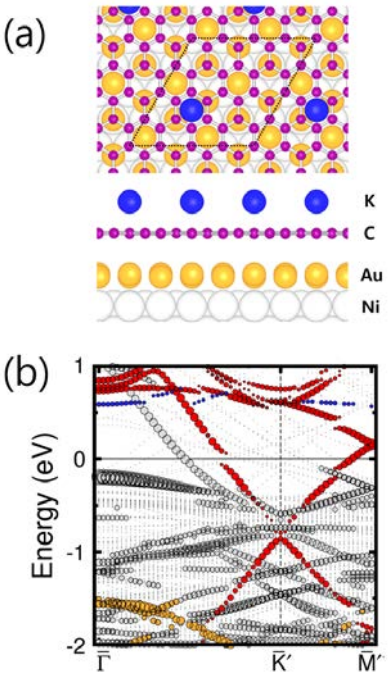

Figure 1: Atomic and electronic structure of the K-adsorbed graphene/Au/Ni(111) surface at 0.25 ML.

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