EuroSciCon

DAY 1

Scientific Tracks & Abstracts

17th Edition of International Conference on

Emerging Trends in Materials Science and Nanotechnology

April 26-27, 2018 | Rome, Italy

DAY 1

April 26, 2018

Sessions

Advanced Nano Materials | Nano Electronics Nanotechnology For Clean Energy and Environment | Nano Applications and Others

Session Chair
Ping Furlan
U.S. Merchant Marine Academy, USA

Session Chair
Haruhisa Kato
AIST, Japan

Session Introduction

Title: **Bimetallic Acetate Complexes Derived La(III)-Doped TiO2 Nanofibers For Claus Catalysts**
Ruohong Sui, University of Calgary, Canada

Title: **Spin-orbit interaction and topological phase in atom-thin layers**
Junji Haruyama, University of Tokyo, Japan

Title: **Facile preparation of oxidation resistant magnetite-based nanocomposites for water treatments**
Ping Furlan, U.S. Merchant Marine Academy, USA

Title: **Morphological instability of thin films deposited on substrates**
Jerome Colin, University of Poitiers, France

Title: **The Use of Electron Spin Resonance in Studying the Synergy Be-tween Organic and Inorganic Component in Hybrid Elastomer Based Composites**
Aleksandra Ivanoska-Dacikj, Macedonian Academy of Sciences and Arts, Macedonia

Title: **Characterization of nanomaterials using filed-flow fractionation**
Haruhisa Kato, AIST, Japan

Title: **Crystallization of 1,2,4,5 tetrabromobenzene under nanoscale confinement**
Abdullah Khalil, New York University, Abu Dhabi

Title: **Tuning Ferroelectricity in [BaTiO3]m/[BaZrO3]n superlattices: an ab initio study**
Nadia Iles, Oran University, ESGEE, Algeria

Title: **Bio-based nanomaterials for diversified applications**
Md Iftekhar Shams, Khulna University, Bangladesh

Title: **Synthesis & Characterization of Cobalt –Graphene Nano Composite by Mechanical Milling and Sonicated Exfoliation**
Upender Pandel, Malaviya National Institute of Technology Jaipur, India

Title: **Synthesis & Characterization of Nickel nanocrystal –Graphene Composite by Mechanical Milling and Sonicated Exfoliation**
Krishna Kumar, Malaviya National Institute of Technology Jaipur, India

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Ruohong Sui et al., Nano Res Appl, Volume:4
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BIMETALLIC ACETATE COMPLEXES DERIVED LA(III)-DOPED TIO_2 NANOFIBERS FOR CLAUS CATALYSTS

Ruohong Sui, Christopher B Lavery, Nancy Chou and **Robert A Marriott**
University of Calgary, Canada

Modified Titania is of great interest for industrial catalysts and photocatalysts with applications in environmental engineering. In this research, La(III) was incorporated into titanium oxoacetate complexes via a one pot sol-gel process of metal alkoxides reacting with acetic acid, evidenced by electrospray ionization mass spectrometry analysis. The resulting well-defined nanofibers were calcined to obtain 1-dimensional La-doped TiO_2 materials. For comparison, lanthanum was also deposited on the surface of TiO_2 nanofibers by an impregnation method. X-ray photoelectron spectroscopy analysis shows that the oxygen defect in the La-doped sample was more significant than that in the La-deposited TiO_2. In addition, more interaction of lanthanum with the TiO_2 matrix was observed in the nanofibers synthesized via the sol-gel method. These features of doped TiO_2 nanofibers are anticipated to play a role in higher catalytic activity. In addition, both the La-doped and deposited TiO_2 nanofibrous materials exhibited excellent thermal stability. The N_2-physisorption and powder x-ray diffraction characterizations show that both anatase crystallites and surface areas in the lanthanum-modified TiO_2 were maintained better than the unmodified counterparts at temperatures up to 900°C. As a cleaner energy resource, natural gas provides about 30% energy consumption and more than 27% electricity generation in North America. However, many natural gas reservoirs contain H_2S, which needs to be removed by amine scrubbing followed by a Claus process. With pending stricter emission policies and lower commodity prices, it is urgent for natural gas producers to seek more efficient Claus catalysts. In this context, lanthanum-modified TiO_2 was tested as a Claus catalyst and a better performance was observed than the unmodified TiO_2. We attributed the promoted catalytic activity of La-modified TiO_2 to the M^{3+} cations, which causes oxygen defects in TiO_2 and thereby increases SO_2 adsorption capacity. A higher SO_2 adsorption on the catalytic surface enhances both H_2S and CS_2 conversion. In addition, sulfate concentrations in the used catalysts were studied to explain the catalytic activities.

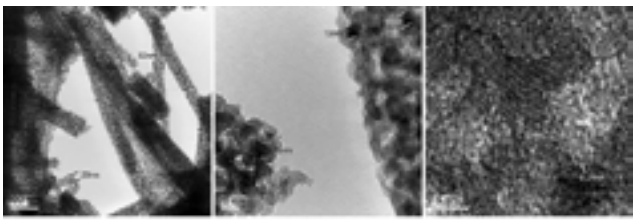

Figure 3. TEM images of La(III)/TiO_2 calcined at 500 °C with increased magnifications from left to right. Left panel: nanofibers with diameters ca. 30 nm. Middle panel: the nanofibers are composed of nanocrystallites less than 18 nm. Right panel: the signature anatase lattice fringe patterns.

Recent Publications

1. Sui R, Marriott R, et al. (2017) Organo sulfur adsorbents by self-assembly of titania based ternary metal oxide nanofibers. Journal of Materials Chemistry 5:9561-9571.
2. Sui R, Marriott R, et al. (2016) Selective adsorption of thiols using gold nanoparticles supported on metal oxides. Langmuir 32:9197-9205.
3. Clark P, Sui R, et al. (2013) Oxidation of CO in the presence of SO_2 using gold supported on La_2O_3/TiO_2 nanofibers. Catalysis Today 207:212-219.
4. Sui R and Charpentier P (2012) Synthesis of metal oxide nanostructures by direct sol–gel chemistry in supercritical fluids. Chemical Reviews 112:3057-3082.
5. Sui R, Berlinguette C, et al. (2008) Simple protocol for generating TiO_2 nanofibers in organic media. Chemistry of Materials 20:7022-7030

Biography

Ruohong Sui has his expertise in making metal oxide nanomaterials using a sol-gel process. He is interested in self-assembly of metal-ligand complexes to make 1- and 2-dimensional nanomaterials in non-aqueous media, and using the resulting materials for clean energy applications.

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SPIN-ORBIT INTERACTION AND TOPOLOGICAL PHASE IN ATOM-THIN LAYERS

J Haruyama[1, 2]

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[2]Institute for Solid State Physics - University of Tokyo, Japan

Three dimensional (3D) topological insulating (TI) state, in which the bulk is insulator with an energy band gap while the surface is gapless conductor, has been reported in some materials and attracted significant attention. On the other hand, 2D TI states have been experimentally reported only in few materials, such as quantum wells of HgTe/CdTe or InAs/GaSb. In 2D TI state, quantum SHE (QSHE) is observed with a bulk energy gap but gapless helical edge states protected by time reversal symmetry, in which opposite spin states forming a Kramers doublet counter propagate. Although 2D TI states are theoretically predicted for graphene, atomically thin 2D carbon layer, experimental observation is rare. On the other hand, atom-thin transition metal dichalcogenide (TMDC) layers are attracting significant attention from various viewpoints. It has been recently predicted that 1T'-phase of such layers can be within 2D TI states due to the band inversion. Thus, it is indispensable to realize 2D and 1D TI states in various atom-thin materials. For the creation of TI states, introduction of spin-orbit interactions (SOIs) is crucial. Recently, challenge of introduction of SOI into graphene has been experimentally reported by some methods [e.g., surface decoration by (1) right-mass adatoms or (2) heavy nanoparticles, and (3) using heavy substrates]. In the talk, I will present (1) and (2) using small-amount of hydrogen atoms and Pt or Bi_2Te_3 nanoparticles, respectively, which result in introduction of large SOI gaps and subsequent emergence of the 2D TI states. Moreover, I will present that 1T' phase of MoS_2, one of TMDC family, which is created by laser beam irradiation, can be within the 2D TI states. These observation must open doors to 2D topological phases of graphene and atom-thin TMDCs and those application to low-power and voltage-controlled spintronics devices.

Biography

J Haruyama is a Professor of Aoyama Gakuin University, Tokyo, and a Visiting Professor of The University of Tokyo, Institute for Solid State Physics. He graduated from Waseda University, Tokyo, Japan, in 1985. Then, he joined Quantum Device Laboratory, NEC Corporation, Japan and worked until 1994. He received his PhD in Physics from Waseda University in 1996. During 1995–1997, he worked with The University of Toronto, Canada, and also Ontario Laser and Lightwave Research Center, Canada as a Visiting Scientist. Since 1997, he has been working at Aoyama Gakuin University. He was also a Visiting Professor at NTT Basic Research Laboratories, Japan, and a Researcher for Zero-emission Energy Center grant, Kyoto University, Japan.

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FACILE PREPARATION OF OXIDATION RESISTANT MAGNETITE-BASED NANOCOMPOSITES FOR WATER TREATMENTS

Ping Furlan, Adam Fisher, Alexander Furlan, Monica Keeley, Michael Melcer, David Shinn and **John Warren**
United States Merchant Marine Academy, USA

Magnetite nanoparticles (MNPs) - based nanocomposites are promising for drinking water and ballast water treatments due to their easy synthesis and magnetic recyclability. The bifunctional nanocomposite we recently prepared by incorporating both MNPs and silver nanoparticles into activated carbon matrix has demonstrated recoverability and reusability with high antimicrobial efficiency for water disinfection. However, prolonged exposure of MNPs to the dissolved oxygen in water converts iron (II) ions to iron (III) ions, weakening the magnetic responsiveness and reducing the recovery rates for the nanocomposites. In this work, we explore various strategies inhibiting the access of oxygen to the MNPs and preventing them from being oxidized in water. This includes capping the MNPs with inorganic, organic, and surfactant agents. The effectiveness is evaluated based on their oxidation resistance in water. The nanocomposites with protected MNPs are evaluated for their recoverability and ability to remove water pollutants and/or disinfect water.

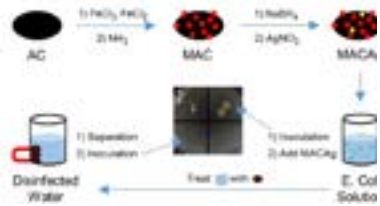

Figure 1: Magnetically recyclable and reusable antimicrobial nanocomposite based on activated carbon, magnetite nanoparticles, and silver nanoparticles for water disinfection

Recent Publications

1. **P Y Furlan, A J Fisher, A Y Furlan, M E Melcer, D W Shinn and J B Warren (2017) Magnetically recoverable and reusable antimicrobial nanocomposite based on activated carbon, magnetite nanoparticles, and silver nanoparticles for water disinfection. Inventions doi: 10.3390/inventions2020010.**
2. **P Y Furlan, A J Fisher, M E Melcer, A Y Furlan and J B Warren (2017) Preparing and testing a magnetic antimicrobial silver nanocomposite for water disinfection to gain experience at the nanochemistry-microbiology interface. Journal of Chemical Education 94(4):488-493.**
3. **P Y Furlan, Brian Ackerman, Mike Melcer and Sergio Perez (2016) Reusable magnetic nanocomposite sponges for removing oil from water discharges. Journal of Ship Production and Design DOI: https://doi.org/10.5957/JSPD.32.4.160017.**
4. **S Perez, P Furlan, S Ellenberger, P Banker (2016) Estimating diluted bitumen entrained by suspended sediments in river rapids using O_2 absorption rate. Int. J. Environ. Sci. Technol. 13(2):403-412.**
5. **P Y Furlan and M Melcer (2014) Removal of organic water pollutant surrogate by recyclable magnetite-activated carbon nanocomposite: an experiment for general chemistry. Journal of Chemical Education 91(11):1966-1970.**

Biography

Ping Furlan is a Professor in Chemistry with 21 years of academic experience at the U.S. Merchant Marine Academy since 2011 and in the University of Pittsburgh during 1997-2011. She is an Active member of American Chemical Society (ACS) and leader of various ACS major science outreach programs and 2016 Middle Atlantic Regional Meeting. She has done her research with numerous publications, grants and invited presentations in the areas of developing nanomaterials for marine pollution prevention; nanoscience and technology curriculum materials; and chemistry in maritime industry curriculum materials. Her recent ACS recognitions include 2017 Middle Atlantic Regional Partners for Progress and Prosperity Award, 2016 Outreach Volunteer of the Year Award, 2016 National ChemiLuminary Award Finalist, 2015 E. Ann Nalley Middle Atlantic Regional Award, and 2014 New York Section Distinguished Service Award for Leading National Chemistry Week.

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MORPHOLOGICAL INSTABILITY OF THIN FILMS DEPOSITED ON SUBSTRATES

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[2]ENSMA, France

The main topic of this presentation is concerned with the study of the coupling between the mechanical properties of thin films on substrates and their morphologies. In a first part, the aging of the buckling patterns experimentally observed at the mesoscopic scale onto the surface of metallic thin films deposited on substrates is studied by means of finite element simulations (FEM). The conditions for the transition from straight-sided wrinkles to telephone-cords or circular blisters are first discussed. The problem of the shape instability of multilayered hyperelastic solids has been then considered and the in-phase and out-of-phase configuration for a thin layer embedded in a heterogeneous matrix has been discussed versus the elastic coefficients of the different neo-hookean materials. In a second part, the evolution of the vicinal surface of gold single crystals deformed by external uniaxial compression tests and *in situ* observed by UHV scanning tunneling microscopy is investigated (see figure 2). It is demonstrated that the slip traces resulting from the emergence of moving dislocations at the free surface highly modify the organization of the vicinal steps. A model based on energetic considerations is proposed and discussed to explain the observed phenomenon.

Figure 1: Ni thin film on polycarbonate substrate

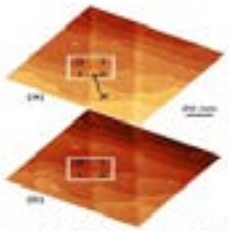

Figure 2: STM observation of gold

Recent Publications

1. **Coupeau C, Camara O, Drouet M, Durinck J, Bonneville J, Colin J and Grilhé J (2016) Slip trace-induced vicinal step destabilization. Physical Review B 93:041405.**
2. **Hamade S, Durinck J, Parry G, Coupeau C, Cimetière A, Grilhé J and Colin J (2001) Effect of plasticity and atmospheric pressure on the formation of donut and croissant-like buckles. Physical Review E 91:012410.**
3. **Ruffini A, Finel A, Colin J and Durinck J (2016) Effect of interface plasticity on circular blisters. Scripta Materialia 113:222-225.**
4. **Coupeau C, Durinck J, Drouet M, Douat B, Bonneville J, Colin J and Grilhé J (2015) Atomic reconstruction of niobium (111) surfaces. Surface Science 632:60-63.**
5. **Colin J, Coupeau C, Durinck J, Cimetière A and Grilhé J (2014) Re-deposition of a straight-sided buckle under pressure. Physical Review E 89:032410.**

Biography

Jérôme Colin works in the field of the Mechanics of Materials and Materials Science. He is involved in modeling of the mechanical properties of nano-structured materials, thin films on substrates and coatings. More precisely, he has developed models in the framework of the elasticity and thermodynamics theories, to characterize the morphological evolution of layers under strain, the formation of atomic defects such as dislocations in strained nanostructures or the delamination and buckling of thin films on substrates.

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THE USE OF ELECTRON SPIN RESONANCE IN STUDYING THE SYNERGY BETWEEN ORGANIC AND INORGANIC COMPONENT IN HYBRID ELASTOMER BASED COMPOSITES

Aleksandra Ivanoska Dacikj[1], Gordana Bogoeva Gaceva[2] and **Srečko Valić[3]**
[1]Macedonian Academy of Sciences and Arts, Macedonia
[2]Ss. Cyril and Methodius University, Macedonia
[3]University of Rijeka, Croatia

Recently an increasing interest is becoming evident for incorporation of hybrid systems based on different fillers in elastomeric matrices. This leads to already confirmed benefits, regarding the properties of the nanocomposites, but jet some new aspects and methods are needed to reveal and understand the origin of the synergism between the nanofillers and its influence on the macroscopic properties. In this study electron spin resonance (ESR) investigations on hybrid natural rubber based nanocomposites loaded with 2 phr of multi-walled carbon nanotubes (MWCNT) and various amounts of expanded organically modified montmorillonite (EOMt) (0; 8 and 16 phr) were reported. The temperature dependence of resonance line parameters in the range 160–353 K was analyzed. From the obtained results it was evident that the presence of the EOMt influenced the appearance of the ESR spectra. The shape of the spectral lines was changed from Lorentzian one for the sample that does not contain EOMt to a Dysonian line for the sample that contains the highest amount of EOMt. This was in good correlation with the argument that the type of the ESR spectra line is closely connected to the state of dispersion of the CNT in the matrix. Also the values of the g-factor were shifted, from the values close to that of the free electron for the sample that does not contain EOMt to higher values with the increase of EOMt content. The observed behavior of the double integral of the resonance spectra was not temperature invariant, suggesting that it does not obey a simple Pauli law behavior. Therefore, it was assumed that the observed ESR signal originated not only from the metallic but also from the intrinsic conduction electrons in MWCNT and defects with an odd number of vacant carbon sites in the honeycomb configuration that can also introduce spins.

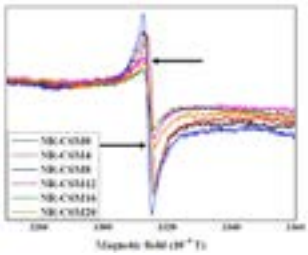

Figure 1: The ESR spectra of 6 phr MWCNT in NR-based nanocomposites containing different quantities of EOMt, at room temperature. Lorentzian shapes of the resonance spectra prove the good dispersion of the nanotubes within the NR matrix, regardless of the presence of EOMt.

Recent Publications

1. **Ivanoska-Dacikj A, Bogoeva-Gaceva G and Buzarovska A (2015) Clay improved dispersion of carbon nanotubes in different solvents. Contributions, Section of Natural, Mathematical and Biotechnical Sciences 36(1):5-10.**
2. **Ivanoska-Dacikj A, Bogoeva-Gaceva G, Rooj S, Heinrich G and Wießner S (2015) Fine tuning of the dynamic mechanical properties of natural rubber/carbon nanotube nanocomposites by organically modified montmorillonite: A first step in obtaining high-performance damping material suitable for seismic application. Applied Clay Science 118:99-106.**
3. **Ivanoska-Dacikj A, Bogoeva-Gaceva G, Wießner S and Heinrich G (2016) Rheometric and dynamic mechanical analysis of complex natural rubber based composites. Contributions, Section of Natural, Mathematical and Biotechnical Sciences 37:5-14.**

4. Ivanoska-Dacikj A, Bogoeva-Gaceva G, Jurk R, Wießner S and Heinrich G (2017) Assessment of the dynamic behavior of a new generation of complex natural rubber based systems intended for seismic base isolation. Journal of Elastomers and Plastics 49:595-608.
5. Ivanoska-Dacikj A, Bogoeva-Gaceva G, Valić S, Wießner S and Heinrich G (2017) Benefits of hybrid nano-filler networking between organically modified montmorillonite and carbon nanotubes in natural rubber: experiments and theoretical interpretations. Applied Clay Science 136:192-1198.

Biography

She has three years of working research experience at the Research Centre for Environment and Materials in Macedonian Academy of Sciences and Arts in Skopje. She is specialized in Elastomeric Nanocomposites. She has published six research papers in scientific journals and one book chapter.

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CHARACTERIZATION OF NANOMATERIALS USING FIELD-FLOW FRACTIONATION

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Size and size distribution are significant physicochemical properties of bio and functional materials since it determines many of the functional properties of these materials. Methods for the accurate determination of the size and the size distribution of materials are therefore one of the key to the development of nano and biotechnologies. In the past few decades, dynamic light scattering (DLS) and particle tracking analysis (PTA) have been widely used for determining the sizes of Brownian nanoparticles in nano and submicron scale biocolloidal suspensions. Because of the convenience and usability of DLS, a large number of commercial instruments and analytical methods based on various principles underlying the DLS method are available. In DLS and PTA analysis, the diffusion coefficients of nanomaterials are determined first, after which the averaged diameters of the particles are calculated from the diffusion coefficients by using the Stokes–Einstein relationship. However, the apparent diameters of nanoparticles over a wide size distribution as determined using such diffusion based analysis method depends on the particular analytical algorism. Electron microscope is an effective method to obtain the primary particle information visually, however; it requires counting a large number of materials for ensemble characterization. Additionally, the European Commission has declared that a nanomaterial is a natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50% or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm–100 nm. According to this definition, not only the size but also the size distribution of nanomaterials in is an important factor for nanomaterial industrial field. Fractionation methods such as field-flow fractionation (FFF) and microfluidic/nanofluidic technological separation have recently been focused upon as methods for the determination of accurate size distribution. FFF is elution techniques wherein nanoparticles, microparticles, and macromolecules are separated by their physicochemical properties. In nano and micro technology, various FFF methods are attractive techniques for separating materials in colloidal dispersions by means of flow, centrifugal, magnetic, and thermal field control. Different fields enable nanoparticle separation based on various criteria: diffusion coefficient (i.e. hydrodynamic size) by flow FFF, thermal diffusion coefficient, density, mass, and so forth. The most general applicable FFF methods are flow FFF and centrifugal FFF because of their practicality and the robust theoretical foundation established for separation of nano and micro materials in many areas. Herein, we performed FFF assessments of various materials combined with DLS and EM methods to characterize more accurate size and size distribution of materials than the results by single sizing method such as DLS. This study plays an important role in producing a new application of nano and biotechnology.

Recent Publications

1. H Kato, et al. (2018) Separation of different-sized silica nanoparticles using asymmetric flow field-flow fractionation by control of the Debye length of the particles with the addition of electrolyte molecules. Colloids and Surfaces A: Physicochemical and Engineering Aspects 538:678-685.
2. H Kato, et al. (2017) Simultaneous measurement of size and density of spherical particles using two-dimensional particle tracking analysis method. Powder Technology 315:68-72.
3. Y Matsuura, et al. (2017) Accurate size determination of polystyrene latex nanoparticles in aqueous media using a particle tracking analysis method. Colloids and Surfaces A: Physicochemical and Engineering Aspects 525:7-12.
4. H Kato, et al. (2017) Determination of bimodal size distribution using dynamic light scattering methods in the submicrometer size range. Material Express 6:175-182.
5. H Kato, et.al (2014) Separation of nano and micro sized materials by hyphenated flow and centrifugal field-flow fractionation. Analytical Methods 6:3215-3218.

Biography

Haruhisa Kato has his expertise in characterization of polymer and nano-materials. He has been investigating novel characterization instruments and methods. Various nanomaterial standards (certified reference materials) are also produced by his laboratory and he also concerned with the International standardization work in ISO/TC24, TC229, and TC256.

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CRYSTALLIZATION OF 1, 2, 4, 5-TETRABROMOBENZENE UNDER NANOSCALE CONFINEMENT

Abdullah Khalil[1], Chunhua Tony Hu[2] and **Panče Naumov[1]**
[1]New York University Abu Dhabi, UAE
[2]New York University, USA

Thermosalient (TS) crystals are an emerging class of organic materials that undergo macroscopic motion when taken over their phase transition. The visually observable motion occurs over distances that are several times greater compared to the size of the crystals. Such efficient conversion of heat into mechanical work favors these crystals for application as thermomechanical actuators. Recent reports have shown that crystalline organic compounds exhibit unusual polymorphism and preferred orientation when confined within nanospaces. Inspired by such behavior and in an attempt to observe the TS effect at the nanoscale, 1, 2, 4, 5-tetrabromobenzene (TBB) was selected as a model material that undergoes TS phase transition from β to γ phase at about 40°C. To that end, TBB was crystallized within the 20-200 nm-wide channels of anodic aluminum oxide (AAO) templates, and its structure was studied using two-dimensional x-ray microdiffraction (2D-μXRD) and powder x-ray diffraction (PXRD) analyses. Whereas bulk TBB crystallizes in the β phase at room temperature, the analysis revealed that when confined within the anodized aluminum oxide (AAO) nanopores, TBB crystallizes in the metastable γ phase with preferred orientation at room temperature. Figure 1a shows the 100 nm pores of AAO templates filled with TBB, whereas Figure 1b shows TBB crystals released after dissolving the AAO templates. The 2D-μXRD pattern of the TBB filled AAO template in Figure 1c shows discrete spots, revealing preferred growth of the TBB nanocrystals. The PXRD pattern of TBB-filled AAO template, shown in Figure 1d, is identical to that of bulk γ phase TBB, confirming that TBB grows in the γ phase within the nanopores. We also found that these TBB nanocrystals remain indefinitely stable in the γ phase from cryogenic temperatures up to nearly 80°C, where they sublime. These findings uncover fundamental differences between nanosized organic TS crystals and their bulk counterparts.

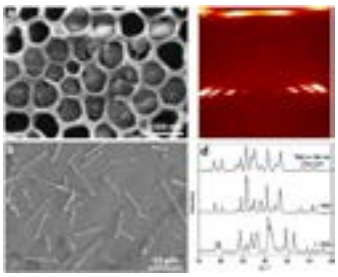

Figure 1: (a,b) SEM images of TBB-filled AAO template (a) and TBB nanocrystals obtained after dissolving the AAO template (b)&(c) 2D-μXRD pattern of TBB filled AAO template. (d) PXRD pattern of crushed TBB-filled AAO template shown together with PXRD pattern of bulk β and γ phase of TBB crystals.

Recent Publications

1. **N K Nath, M K Panda, S C Sahoo and P Naumov (2014) Thermally induced and photoinduced mechanical effects in molecular single crystals - a revival. CrystEngComm 16(10):1850-1858.**
2. **P Naumov, S Chizhik, M K Panda, N K Nath and E Boldyreva (2015) Mechanically responsive molecular crystals. Chemical Reviews 115(22):12440-12490.**
3. **C L Jackson and G B McKenna (1996) Vitrification and crystallization of organic liquids confined to nanoscale pores. Chemistry of Materials 8(8):2128-2137.**
4. **H F Lieberman, R J Davey and D M T Newsham (2000) Br···Br and Br···H interactions in action: polymorphism, hopping, and twinning in 1,2,4,5-tetrabromobenzene. Chemistry of Materials 12(2):490–494.**
5. **Khalil C, T Hu and P Naumov (2018) Nanoscale crystallization and thermal behaviour of 1,2,4,5-tetrabromobenzene. CrystEngComm 20:636-642.**

Biography

Abdullah Khalil is currently a Postdoctoral Associate at New York University, Abu Dhabi since July 2016. He obtained his PhD degree in May 2016 while working at the Advanced Fibers and Biofuel Laboratory at Masdar Institute of Science & Technology in the United Arab Emirates where he investigated the microstructure evolution and applications of electrospun metal oxide nanofibers. His research interests include synthesis of various organic and inorganic nanostructures with controlled microstructure and chemistry for functional applications. He has also contributed to studies of the microstructure and chemistry of nanomaterials by using microscopic and spectroscopic techniques. He is also experienced with using transmission electron microscopy in which he uses to study microstructure evolution in nanostructured materials.

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TUNING FERROELECTRICITY IN [BATIO$_3$]M/[BAZRO$_3$]N SUPERLATTICES: AN AB INITIO STUDY

Nadia Iles, Ilham Kara and **Kouider Driss Khodja**
University of Oran, ESGEE, Algeria

The ABO3 perovskites are nowadays considered as the best candidates for highly reliable electronic devices thanks to their multifunctional properties. Most of the time, these ternary oxides can combine at least two different physical properties. Barium Titanate ($BaTiO_3$) is a typical ferroelectric in its tetragonal phase with a spontaneous polarization at the bulk scale. Barium Zirconate ($BaZrO_3$) is stable in a cubic structure and is widely used as substrate for other perovskites. The lattice mismatch is an important parameter for stacking two different perovskites. For $BaTiO_3$/$BaZrO_3$ superlattices, the lattice mismatch of induced important structural and electronic modifications at nanoscopic scale. Few experimental works were conducted on $[BaTiO_3]_m$/$[BaZrO_3]_n$ superlattices with modulation period Λ=(n+m)ã = 3.2 , 4.8 , 6.4 et 8 nm (ã is the mean lattice parameter in the transverse direction to the substrate). Hysteresis loops measurements show that the out of plane polarization increases with the modulation period (Λ). However these experimental studies were restricted to high modulation period and no results were available on very short modulation period of these superlattices. In this theoretical study, we investigated [$BaTiO_3$]m/[$BaZrO_3$]n systems with n and m varying from 1 to 3 to predict their structural and electronic modifications with respect to n/m and different symmetries (*P4mmm, P4mm, Pmm2, Pm, P1*). For this purpose, ABINIT code based on density functional theory (DFT) and plane waves (PW) basis is used for our *ab initio* calculations. Our results show that the P1 symmetry with three dimensional polarizations is the most stable for all the studied modulation periods. Our finding can be useful for tuning ferroelectric devices.

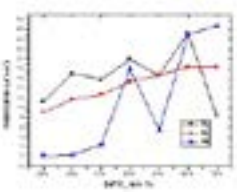

Figure 1: In-place (Px and Py) and out of plane Pz Polarizations for the most stable P1 symmetry of [$BaTiO_3$]m/[$BaZrO_3$]n superlattices.

Recent Publications

1. **N Iles, A Kellou, K Driss Khodja, B Amrani, F Lemoigno, D Bourbi and H Aourag (2007) Atomistic study of structural, elastic, electronic and thermal properties of perovskites Ba(Ti,Zr,Nb)O_3. Computational Materials Science 39:896-902.**
2. **T Belaroussi, B Amrani, T Benmessabih, N Iles and F Hamdache (2008) Structural and thermodynamic properties of antiperovskite $SbNMg_3$. Computational Materials Science 43:938-942.**
3. **N Iles, F Finocchi and K Driss Khodja (2010) A systematic study of ideal and double layer reconstructions of ABO3 (001) surfaces (A=Sr, Ba and B=Ti, Zr). Journal of Physics: Condensed Matter 22(30):305001.**
4. **N Iles, K Driss Khodja, A Kellou and P Aubert (2014) Surface structure and polarization of cubic and tetragonal $BaTiO_3$: An *ab initio* study. Computational Materials Science 87:123-128.**
5. **Imène Cherair, Nadia Iles, Lyacine Rabahi and Abdelhafid Kellou (2017) Effects of Fe substitution by Nb on physical properties of BaFeO3: A DFT+U study. Computational Materials Science 126:491–502.**

Biography

Nadia Iles has finished her PhD studies in 2010, devoted at the same time to teaching and research at Oran 1 University and Oran's High School of Electrical Engineering and Energetics. She is interested in computing physics of low dimensional systems based on perovskites materials. She has published more than seven international and national research papers. She has participated in oral and poster presentations in more than 16 international, national conferences and in seminars. She is supervising more than five Master's and Doctoral thesis. She is a Member of numerous national and international projects such as PHC TASSILI (CMEP) with European funding, CNEPU and PNR with national funding.

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Md. Iftekhar Shams et al., Nano Res Appl, Volume:4
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BIO-BASED NANOMATERIALS FOR DIVERSIFIED APPLICATIONS

Md. Iftekhar Shams[1] and **Hiroyuki Yano**[2]
[1]Khulna University, Bangladesh
[2]Research Institute for Sustainable Humanosphere - Kyoto University, Japan

This study demonstrates the preparation of chitin nanofibers from shrimp and crab wastes using different mechanical treatments such as high speed blender and ultrasonic homogenizer. FE-SEM image and microscopic image showed that uniform fibrillated nanofibers having diameter of 30-50 nm can be obtained. The obtained chitin nanofibers were small enough to retain the transparency of the neat acrylic resin. Chitin acrylic resin films exhibited much higher transparency than cellulose acrylic resin films. The incorporation of chitin nanofibers contributes to the significant improvement of the thermal expansion and mechanical properties of the neat acrylic resin. Furthermore, by reinforcing chitin powder with acrylic resin, optically transparent composites were developed, since particles substantially larger than the optical wavelength do not cause light scattering if the particles are composed of nano-elements such as nanofibers and have nanoporous space so that matrix resin impregnation is possible. Encouraged by these findings, we developed low thermally expanded transparent film by exploiting wood fibers that can be considered to be nanostructured fibers in which individual nanofibers do not significantly agglomerate and are orientated parallel to the fiber direction in S2 layer which accounts for 70-80% of wood fibers. In addition, three dimensional moldable optically transparent nanocomposites with low thermal expansion through emulsification process were developed. Emulsions of chitin nanofibers and acrylic resin are stabilized by the hydrophilic and high specific surface area chitin nanofiber networks preventing the coalescence of tiny emulsion resin droplets. The properties of high light transmittance and low thermal expansion make chitin nanocomposites promising candidates for the substrate in a continuous roll-to-roll process in the manufacturing of various optoelectronic devices such as flat panel displays, bendable displays, and solar cells. We are presently working on deacetylated chitin nanofibers film which are embedded by chitosan and could be suitable for bio-medical applications.

Recent Publications

1. **S K Biswas, H Sano, M I Shams and H Yano (2017) Three-dimensional-moldable nanofiber reinforced transparent composites with a hierarchically self-assembled "reverse" nacre-like architecture. ACS Applied Materials and Interfaces 9(35):30177-30184**
2. **M I Shams and H Yano (2015) Doubly curved nanofiber-reinforced optically transparent composites. Scientific Reports 5:16421**
3. **H Yano, S Sasaki, M I Shams, K Abe and T Date (2014) Wood pulp based optically transparent film: A Paradigm from nanofibers to nanostructured fibers. Advanced Optical Materials 2(3):231-234**
4. **M I Shams and H Yano (2013) Simplified fabrication of optically transparent composites reinforced with nanostructured chitin. Journal of Polymers and the Environment 21:937-943.**
5. **M I Shams, M Nogi, L Berglund and H Yano (2012) The transparent crab: preparation and nanostructural implications for bioinspired optically transparent nanocomposites. Soft Matter 8:1369-1373.**

Biography

Md. Iftekhar Shams has completed his MS and PhD in Wood Science and Technology from Kyoto University, Japan under Japanese Government Monbukagakushu scholarship. From 2008- 2010, he worked as JSPS Post-doctoral fellow and later in 2012-2014, he worked as Visiting Scientist in Kyoto University, Japan. He was also working as an invited Visiting Scientist in Royal Institute of Technology Sweden, Nanjing Forestry University, China and Kyoto University Japan. He holds two patents and has published more than 35 journal articles. For greater contribution in the field of Forest and Agricultural Science in Bangladesh, he was awarded 'UGC AWARD 2015' from University Grants Commission of Bangladesh. His research involves production of biocomposites and extraction of nanofibers from biomass resources and their utilization for optical and structural purposes. He also handled a good number of funded projects including World Bank sponsored, Japan Society for the Promotion of Science (JSPS), The World Academy of Sciences (TWAS) and so on. He is now working as a Professor of Forestry and Wood Technology Discipline, Khulna University, Bangladesh.

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Upender Pandel et al., Nano Res Appl, Volume:4
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SYNTHESIS AND CHARACTERIZATION OF COBALT-GRAPHENE NANO COMPOSITE BY MECHANICAL MILLING AND SONICATED EXFOLIATION

Upender Pandel, Krishna Kumar and **M K Banerjee**
Malaviya National Institute of Technology, India

A cobalt nanoparticle-graphene composite was synthesized by using mechanical milling and sonication assisted exfoliation. Graphite powder and cobalt metal powder in the ratio of 4:1 by weight was first mechanically milled for 60 hrs. in Toluene medium. The milled powder was then exfoliated by using sodium lauryl sulfate surfactant to produce cobalt-graphene nano composite. The composite have shown good magnetic property due to the presence of cobalt nanocrystals and this was confirmed by vibrating sample magnetometer (VSM). Due to the sonication-assisted exfoliation, few layers of graphene formed which were confirmed by Raman spectroscopy, x-ray photo electron spectroscope (XPS) and atomic force microscopy. Phase analysis and size of the cobalt-graphene nano composite was calculated with the help of x-ray diffraction pattern and transmission electron microscopy.

Biography

Upender Pandel is expertise in Nanomaterials, Engineering Materials, Corrosion and Surface Coatings. As a professions in MITI jaipur they has published many papers in national and international journals and conferences.

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Krishna Kumar, Nano Res Appl, Volume:4
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SYNTHESIS & CHARACTERIZATION OF NICKEL NANOCRYSTAL –GRAPHENE COMPOSITE BY MECHANICAL MILLING AND SONICATED EXFOLIATION

Krishna Kumar
Malaviya National Institute of Technology, India.

A Nickel nanocrystal – Graphene composite was synthesized by using mechanical milling and sonication assisted exfoliation. Graphite powder and Nickel metal powder in the ratio of 4:1 by weight was first mechanically milled for 60 hrs in Toluene medium. The milled powder was then exfoliated by using sodium lauryl sulfate surfactant to produce Nickel – Graphene nano composite. The composite have shown good magnetic property due to the presence of Nickel nanocrystals and this was confirmed by Vibrating Sample magnetometer (VSM). Due to the sonication-assisted exfoliation, few layers of Graphene formed which were confirmed by Raman Spectroscopy, X-ray Photo Electron Spectroscope (XPS) and Atomic Force Microscopy. The size, Phase identity and composition of the Nickel nanocrystal in the composite was calculated with the help of X-Ray Diffraction pattern and Transmission Electron Microscopy.

Biography

He is expertise in Nanomaterials, Engineering Materials, Corrosion and Surface Coatings. As a professions in MITI jaipur they has published many papers in national and international journals and conferences.

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DAY 2

Scientific Tracks & Abstracts

17th Edition of International Conference on

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DAY 2

April 27, 2018

Sessions

Bio Polymers And Bio Plastics | Advanced Materials Science | Nano Composites | Nano Technology In Materials Science and Others

Session Chair
Raffaella Signorini
University of Padova, Italy

Session Co-Chair
Ana-Maria Albu
Politehnica University, Romania

Session Introduction

Title: **Semiconductor Quantum Dots for Light Emitting Applications**
Raffaella Signorini, University of Padova, Italy

Title: **Design and potential cosmetic applications of multi-responsive microgels and self-assembled microgel films**
Garbine Aguirre, University of Pau & Pays Adour, France

Title: **Structural Peculiarities of the Polymer- DNA Assembles**
Ana-Maria ALBU, POLITEHNICA University, Romania

Title: **High pressure synthesis of new superhard nanostructured boron compounds**
Yann Le Godec, UPMC Sorbonne Universite, France

Title: **Physicochemical properties of Ti based MXenes obtained from SHS synthesized MAX phases and their application for energy storage**
Sergii A Sergiienko, National University of Science and Technology MISiS, Russia

Title: **Fabrication of electronically active hybrid photosynthetic reaction center proteins and metals**
Chanoch Carmeli, Tel Aviv University, Israel

Title: **Combined Effect of 830 nm Laser Irradiation and Silver Nanoparticles in WS1 Wounded Cells**
Sathish Sundar Dhilip Kumar, University of Johannesburg, South Africa

Title: **Investigation of Friction and Wear Properties of Silicon Nitride reinforced polycarbonate nanocomposites**
Anil Kumar Bhargava, Malaviya National Institute of Technology, India

Title: **Synthesis and Characterization of TiO2 Nanoparticles by Sol- gel Method**
Rajendra Duchaniya, Malaviya National Institute of Technology, India

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Raffaella Signorini et al., Nano Res Appl, Volume:4
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SEMICONDUCTOR QUANTUM DOTS FOR LIGHT EMITTING APPLICATIONS

Raffaella Signorini[1], Francesco Todescato[1], Ilaria Fortunati[1], Alessandro Minotto[1], Jacek J Jasieniak[2] and **Renato Bozio[1]**

[1]INSTM - University of Padova, Italy
[2]Monash University, Australia

One of the emerging applications exploring the potentialities of fluorescent nanomaterials is related to light emitting technologies. In particular for the realization of practical light- emitting diodes and large-area displays, semiconductor nanomaterials may overcome many issues of such challenging technologies. A critical aspect of semiconductor nanoscaled materials is related to the large Coulomb interaction between electrons and holes, and their strong spatial confinement, with respect to their bulk analogues. When the size is reduced to levels smaller than the exciton Bohr radius, size-dependent absorption and emission properties develop. Upon formation of excitons within quantum dots (QDs) through optical or electrical processes, Coulomb interactions play a key role in subsequently determining their radiative and nonradiative decay rates, fluorescence quantum yields, multi-exciton generation and its decay. Appropriate engineering of QDs, through the colloidal synthesis of core/shell heterostructures, has emerged as the most facile manner to gain control of these Coulomb processes. The strong electronic coupling between the core and shell in core/shell QDs, ensures that the electronic structure, composition and thickness of the shell must be considered in parallel with the properties of the core in order to predictably manipulate the electron and hole probability densities to obtain the desired optoelectronic characteristics. This spatial control of carriers affects the direct Coulomb interaction between electrons and holes, but also influences the rate and carrier selectivity of trapping at surface and, possibly interfaces defects. The latter is highly dependent on the core/shell structure, for which lattice mismatch between materials must be carefully managed to avoid defect formation stemming from excessive interfacial stress. The above structural and electronic factors define the dynamics of single and multi excitons in QDs, which directly influences aspects such as recombination lifetimes, luminescence efficiency and optical gain properties. Considering the importance of each of these properties for light emitting applications, in this presentation we compare different approaches for the enhancement of light emission quality in terms of high fluorescence efficiency, high color quality, enhanced photostability under prolonged irradiation and easy implementation of solution processable methodologies. All these excellent features make the use of QDs materials a promising way for the realization of optically and electrically pumped light emitting devices.

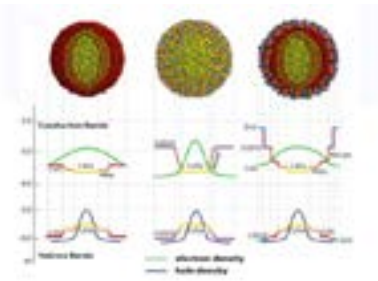

Figure 1: Cross- sectional core- shell structure depiction and a schematic representation of the electronic (hole) density distribution of CdSe- CdS, CdSe- Cd0.5Zn0.5S and CdSe- CdS- Cd0.5Zn0.5S- ZnS QDs.

Recent Publications

1. Minotto A, Todescato F, Fortunati I, Signorini R, Jasieniak J J and Bozio R (2014) Role of Core-Shell Interfaces on Exciton Recombination in CdSe-CdxZn1-xS Quantum Dots. The Journal of Physical Chemistry C 118(41):24117-24126.
2. Fede C, Fortunati I,Weber W, Rossetto N, Bertasi F, Petrelli L, Guidolin D, Signorini R, De Caro R, Albertin G and Ferrante C (2015) Evaluation of gold nanoparticles toxicity towards human endothelial cells under static and flow conditions. Microvascular Research 97:147-155.
3. Vittadello L, Zaltron A, Argiolas N, Bazzan M, Rossetto N and Signorini R (2016) Photorefractive direct laser writing. Journal of Physics D: Applied Physics 49:125103-125111.

4. **Todescato F, Fortunati I, Minotto A, Signorini R, Jasieniak J J and Bozio R (2016) Engineering of semiconductor nanocrystals for light emitting applications. Materials 9(8):672.**
5. **Scian C, Todescato F, Signorini R, Agnoli S, Cesca T, Bozio R and Mattei G (2017) Oxidation effects on the SERS response of silver nanoprism arrays. RSC Advances 7(1):369--378.**

Biography

Raffaella Signorini has been working as an Associate Professor in Physical Chemistry at the Department of Chemical Sciences of the University of Padova since October 2015. Her research activity: (i) Characterization of the optical properties of chromophores characterized by reverse saturable absorption (RSA) and two photon absorption (TPA), and development of an optical limiting device capable to protect from pulsed and CW laser radiation in a wide frequency band; (ii) Investigation of the up-converted stimulated emission of chromophores in suitable laser cavities and development of an integrated laser device; (iii) Characterization of the two photon induced fluorescence of organic multipolar chromophores; (iv) Investigation of hybrid sol-gel materials properties, displaying photocatalitic activity; (v) Micro and sub-micro fabrication via two photon induced polymerization of polymeric and sol-gel materials; (vi) Realization and characterization of plasmonic nanostructures for sensing applications. She is an author of almost fifty papers on international journals and books, and two patents.

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Rome, Italy

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Garbine Aguirre et al., Nano Res Appl, Volume:4
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DESIGN AND POTENTIAL COSMETIC APPLICATIONS OF MULTI-RESPONSIVE MICROGELS AND SELF-ASSEMBLED MICROGEL FILMS

Garbine Aguirre[1,2], Abdelouahed Khoukh[1], Kamel Chougrani[2], Valérie Alard[2] and **Laurent Billon[1]**

[1]University of Pau and Pays de l'Adour, France
[2]LVMH Recherche, France

In recent years, among the broad research field in materials science, microgel particles have received considerable attention as controlled delivery systems. Microgel particles are environmentally responsive particles with incomparable chemical and physical versatility. These stem from the unique combination of their simple synthesis, large surface area, variation of their volume in response to different stimuli, and their ability to contain different types of small molecules and even macromolecules due to their porous structure. These properties make them an outstanding potential choice to be used as effective smart delivery systems. Although the design of microgels will be dependent on the requirements established by the specificity of the application, current developments tend to prepare multi-responsive microgels that respond simultaneously to a combination of several stimuli in order to obtain more effective delivery systems. In this sense, thermo- and pH-sensitive microgels have received significant attention as smart delivery systems. Concerning delivery applications, the design of innovative delivery systems is resulting in the new product development in cosmetic. The key parameter for achieving the most effective cosmetic and personal care products is the controlled release of active cosmetic molecules to the target site of action on/in the skin. Therefore, the design of the sophisticated and effective targeted delivery systems is considered to be the panacea of modern cosmetic. Herein, the potential application of different multi-responsive oligo (ethylene glycol)-based microgels as smart delivery systems of different cosmetic active molecules (hydrophobic, hydrophilic and macromolecules) has been studied. In addition, those microgels have been taken to the next level producing multi-responsive self-assembled microgel films from a fast bottom-up approach. The results obtained indicate that multi-responsive oligo (ethylene glycol)-based microgels and films are new potential vehicles to design sophisticated and controllable cosmetic active delivery systems.

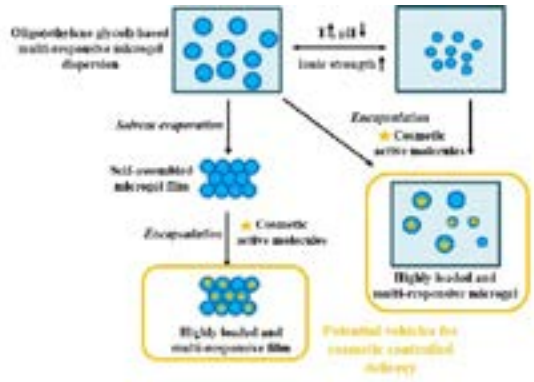

Figure 1: Scheme of cosmetic active molecules encapsulation process into multi-responsive microgel and films.

Recent Publications

1. Aguirre G, Ramos J and Forcada J (2016) Advanced design of T and pH dual-responsive PDEAEMA-PVCL core-shell nanogels for siRNA delivery. Journal of Polymer Science Part A: Polymer Chemistry 54:3203-3217.
2. Aguirre G, Villar-Alvarez E, Gonzalez A, Ramos J, Taboada P and Forcada J (2016) Biocompatible stimuli-responsive nanogels for controlled antitumor drug delivery. Journal of Polymer Science Part A: Polymer Chemistry 54:1694-1705.
3. Pikabea A, Aguirre G, Miranda J I, Ramos J and Forcada J (2015) Understanding on nanogels swelling behavior through a deep insight into their morphology. Journal of Polymer Science Part A: Polymer Chemistry 53:2017-2025.
4. Aguirre G, Ramos J, Heuts J P A and Forcada J (2014)

Biocompatible and thermos-responsive nanocapsule systhesis through vesicle templating. Polymer Chemistry 5:4569-4579.

5. **Aguirre G, Ramos J and Forcada J (2013) Synthesis of new enzymatically degradable nanogels. Soft Matter 9:261-270.**

Biography

Garbine Aguirre has received her BSc in Chemistry from the University of the Basque Country (UPV/EHU) in 2009. She remained at UPV/EHU and undertook her PhD under the supervision of Dr. Jose Ramos and Prof. Jacqueline Forcada, obtaining her Doctorate in 2015 with special mention as International Doctor. During the PhD, she has spent four months in the group of Prof. J.P.A. Heuts, at Eindhoven University of Technology. Her thesis concerned the synthesis and characterization of new stimuli-sensitive biocompatible and biodegradable nanogels that could be potentially useful as nanocarriers in controlled drug/gene delivery. Then, in 2016, she held a Postdoctoral Researcher position at EPCP group, IPREM, Université de Pau & Pays Adour (UPPA) in collaboration with LVMH Parfums Christian Dior to work with Prof. Laurent Billon. Her research focuses on the synthesis, characterization, and biotechnological and cosmetic applications of biocompatible and/or biodegradable stimuli-responsive microgels.

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STRUCTURAL PECULIARITIES OF THE POLYMER-DNA ASSEMBLES

Ana Maria Albu
Politehnica University of Bucharest, Romania

The last decade of past century was marked by a revolution in the field of materials synthesis for optical and photonic applications. It is noteworthy that major dispute regarding the origin of these materials: inorganic or organic, natural or synthetic, hybrid or pure? The goal of our work is that attempting to obtain a controlled structure and then improving the properties by adding small amounts of DNA or chromophores. The idea for using these partners is to get desired applications which regard the biophotonic / nonlinear optical (NLO) field. The used chromophores were synthesized starting from NLO sequences and contains both azo-benzenes and carbazole groups in order to induce a response to an external and/or internal stimulus. DNA is also used in NLO application but has another important property and that is targeting specific molecules/cells/tissues. This study was made to understand the perfect combination between the monomers (amides) and DNA/chromophores. The importance of this work is to highlight the best conditions and the mechanism to obtain new polymers with induced properties in order to be applied in specific fields. Moreover, we have a shot to prove the structure and properties control by reaction parameters. The molecular interaction and the surrounding media play an important role in changing of the fundamental properties of materials. So the electronically behaviors at molecular level are principally determined by the concentration of the NLO constitutive sequences. Demonstrating how such materials respond to a sensitive stimulus which affects the polar ordering is given by the solvatochromic, VCD, FT-IR and Raman studies. The physical - chemical characterization of novel compounds, proposed by us, foreshadows the potential applications of polymer materials, with such sequences, in the biophotonic and NLO field.

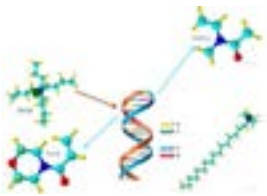

Figure 1: The chemical structures of the main materials used to make polymer-DNA Assembles.

Recent Publications

1. J B Lee, A S Shai, M J Campolongo, N Park and D Luo (2010) Three-dimensional structure and thermal stability studies of DNA nanostructures by energy transfer spectroscopy. ChemPhysChem 11: 2081-2084.
2. A Rodriguez-Pulido, A I Kondrachuk, D K Prusty, J Gao, M A Loi and A Herrmann (2013) Light-Triggered Sequence-Specific Cargo Release from DNA Block Copolymer–Lipid Vesicles. Angewandte Chemie International Edition 52:1008-1012.
3. R M Zadegan and M L Norton (2012) Structural DNA nanotechnology: from design to applications. International Journal of Molecular Sciences 13:7149-7162
4. A Czogalla, H G Franquelim and P Schwille (2016) DNA nanostructures on membranes as tools for synthetic biology. Biophysical Journal 110:1698-1704.
5. Aldea, A M Albu and I Rau (2016) New polymeric materials for photonic applications: Preliminary investigations. Optical Materials 56:90-93.

Biography

Ana Maria Albu has her expertise in the field of Polymer Science and related fields such as: organic synthesis, smart materials, design and manufacture of the new architecture materials with peculiar applications like optic, opto-electronic, micro-electronics, photonic; biomaterials. Two main directions are distinguished: particular aspects in macromolecular synthesis and synthesis of polymeric materials with non-conventional applications. For her, the research activity is closely related to didactic activity, her being devoted teacher to training and orientation of students to specialized technical domains. It is a recognized presence in the field's conferences through the interdisciplinary approach of its research. In recent years, she has focused her activity to the synthesis and characterization of polymer materials with applicability in the biophotonic field. At the same time, by interdisciplinary approaches, it is looking for solution for novel, eco-friendly polymer materials with applications in the field of fuel cells, selective recovery of metallic ions, specialized coating.

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Yann Le Godec, Nano Res Appl, Volume:4
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HIGH PRESSURE SYNTHESIS OF NEW SUPERHARD NANOSTRUCTURED BORON COMPOUNDS

Yann Le Godec
IMPMC, CNRS - Sorbonne Université, France

Superhard materials are widely employed in industry for production of cutting and polishing tools, as well as anti-abrasive coatings. The synthesis of man-made superhard phases started from the early 1950s, as soon as the development of high-pressure techniques allowed reaching the pressures necessary for diamond synthesis. However, the experimental and theoretical design of novel superhard materials still remains a great challenge to materials scientists. To this aim, experimental observations and simulations suggest that for many polycrystalline materials there is an optimal grain size (usually in the range of dozens of nanometers) which results in a significant, up to 50-70%, increase of hardness of the material in comparison with that of its coarse grain counterpart. This increase in hardness is known as the Hall–Petch effect. That's why the synthesis of bulk nanostructured materials remains the least-explored but challenging domain that allows combination of desired physical, chemical, and mechanical properties and gives rise to nanoelectronics, nanomechanics, band gap engineering, etc. Boron-based materials comprise many covalent diamond-like and boron-rich compounds whose structures are three-dimensional nets of short and strong covalent bonds responsible for their extreme hardness. In this talk, I will show that the use of very high pressures and temperatures combined with the *in situ* probe by x-ray diffraction with synchrotron radiation is the methodological key to control the composition and microstructure of new bulk nanostructured and superhard boron compounds and I will give many examples from our recent studies, leading to patent some new strategic compounds.

Recent Publications

1. **J P Itié, E Girard, N Guignot, Y Le Godec and M Mezouar (2015) Crystallography under high pressure using synchrotron radiation, Journal of Physics D: Applied Physics 48, 504007.**

Biography

Yann Le Godec is a CNRS Researcher and experienced user of large-scale instruments (ESRF, SOLEIL, DESY, DIAMOND, ILL, ISIS, etc.) for high pressure research. During last years, he has used high pressure to create new solids with advanced mechanical and physical properties. His activities led him to patent numerous new dense materials with light elements that have aroused considerable interest in search for novel superhard phases all over the world. He has been also leading in the development of *in situ* high pressure - high temperature diffraction techniques, both for x-rays and neutron studies. For his work, he has received the CNRS "Medaille de Bronze" Award.

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PHYSICOCHEMICAL PROPERTIES OF TI-BASED MXENES OBTAINED FROM SHS SYNTHESIZED MAX PHASES AND THEIR APPLICATION FOR ENERGY STORAGE

Sergii A Sergiienko[1], Vladislav A Kolotygin[2] and **Nataliya D Shcherban[3]**
[1]National University of Science and Technology MISiS, Russia
[2]Institute of Solid State Physics RAS, Russia
[3]L V Pisarzhevskii Institute of Physical Chemistry, Ukraine

MXenes attract attention as electrodes for energy storage applications e.g. for supercapacitors due to combination of large theoretical electrochemically active surface; high theoretical conductivity; and hydrophilic nature of their surfaces. The problem is that the methods of MXenes preparation described in the literature are often multi stage and complicated. So the purpose of our work is the development of more simple and technologically acceptable method of MXenes preparation. In the literature the synthesis of MAX phases (precursors for MXenes synthesis) has been realized by different methods. So we used one stage self-propagating high-temperature synthesis (SHS) that seems most suitable because of this method has several advantages like simplicity; short reaction time; cost-effective; and little demand on external energy. For SHS commercially available Ti, Al and carbon black powders were used. Several phases (mainly Ti_3AlC_2, Ti_2AlC, TiC, Al_2O_3) were among the products after SHS. Obtained products are crushed in a roll crusher and then automatic agate mortar. For Al etching from the MAX phase a dilute solution of HF was used. Then delamination of MXenes in N,N-dimethylformamide and isopropanol mixture with sonication were lasted during three days. The content of unreacted MAX phase particles in MXene powder can be reduced by using hydrocyclone assembly and alcohol medium instead of water. Suspension stability of MAX phase particles decreases rapidly while suspension of MXene particles is fairly stable. Also alcohol medium can protect $Ti_3C_2T_x$ MXene from oxidation. Then MXene powder was washed with water several times and to remove residual water vacuum filter was used. Since both layered $Ti_3C_2T_x$ and Ti_2CTx obtained can be used as electrodes for super capacitors, SHS method is suitable for Tix+1AlCx phase preparation. In neutral aqueous electrolyte (1 M solution of Na_2SO_4) obtained electrodes demonstrated gravimetric capacitance up to 220 Fg^{-1} at charge-discharge rates 2 mVs^{-1}.

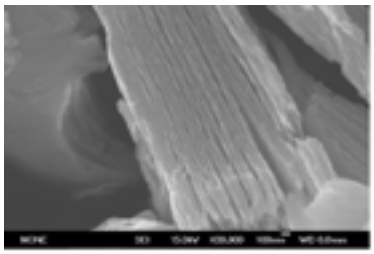

Figure 1: SEM images of Ti3C2 MXene

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5. S Sergiienko, K Moor, K Gudun, Z Elemessova and

R Bukasov (2017) Nanoparticle-nanoparticle vs. nanoparticle-substrate hot spot contributions to SERS signal: studying Raman labeled monomers, dimers and trimmers. Physical Chemistry Chemical Physics 19:4478–4487.

Biography

Sergii A Sergiienko has ten years of working research experience at L V Pisarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine. His research projects mainly devoted to synthesis and investigation of functional properties of ordered porous materials. He has published 14 international research papers. His current research project deals with synthesis and characterization of novel nano-hetero-structured MXene-based materials for electrochemical energy storage at National University of Science and Technology MISiS, Russia.

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FABRICATION OF ELECTRONICALLY ACTIVE HYBRID PHOTOSYNTHETIC REACTION CENTER PROTEINS AND METALS

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[1]Tel Aviv University, Israel
[2]Bar-Ilan University, Israel

Efficient electronic junctions were fabricated by covalent binding of photosynthetic reaction center proteins to metals, semiconductors polymer poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and solid semiconductor ITO. The primary stages of photosynthesis take place in nanometric-size protein-chlorophyll complexes photosystem I (PSI). PSI generates a photo voltage of 1 V with an absorbed light-energy conversion efficiency of 47% (~23% solar energy) and a quantum efficiency of ~100%. The robust cyanobacterial PSI was used in the fabrication of optoelectronic devices by forming oriented multilayers from genetically engineered cysteine mutants. Oriented multilayers were fabricated by covalent binding of successive layers of PSI using cross-linking molecules. Photosystem I layers were bound to metal and transparent conducting semiconductor electrodes under dry environment. The devices generated sizable photocurrent and photo voltage. The rate of photocurrent indicated the formation of a good electronic coupling between PSI and the electrodes. These devices can serve in the fabrication of hybrid bio-solid-state optoelectronic devices.

Recent Publications

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Biography

Chanoch Carmeli is a Prof. Emeritus at Tel Aviv University, Israel. He has served as Chair & Head at the Department of Structural Biology. His research interests include nano-technology of biological molecules, photosynthetic reaction center, structural biology (EXAFS) of biological metal canters and proton turbine ATP synthase. He was a Visiting Professor at UCLA, London University, UCSB, Curie Institute, Roche Institute, Cornell University and University of California, Berkeley. He has 106 scientific publication and six patents.

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Sathish Sundar Dhilip Kumar et al., Nano Res Appl, Volume:4
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COMBINED EFFECT OF 830 NM LASER IRRADIATION AND SILVER NANOPARTICLES IN WS1 WOUNDED CELLS

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University of Johannesburg, South Africa

In recent years, silver nanoparticles (AgNPs) have attracted significant attention in medicinal, biomedical and pharmaceutical research owing to their valuable physicochemical and antibacterial properties. The objective of this study was to prepare, characterize and evaluate the potential of green synthesized silver nanoparticles (G-AgNPs) against human pathogenic bacteria and evaluate their cellular responses in WS1 wounded cells in combination with laser irradiation (830 nm, fluence of 5 J/cm^2). When the mixture of silver nitrate solution and leaf sap extract (LSE) was exposed to direct sunlight, it yielded a rapid color change from colorless to reddish-brown, indicating the formation of G-AgNPs. Physicochemical characterization such as single particle inductively coupled plasma mass spectrometry, high resolution transmission electron microscopy and surface chemistry studies (Fourier transform infrared spectroscopy and x-ray diffraction) revealed a small size of 38±2 nm, smooth surface and existence of LSE on the G-AgNPs. G-AgNPs possessed good antibacterial activity against both *Pseudomonas aeruginosa* and *Staphylococcus aureus*. *In vitro* wound healing studies such as cell morphology, cell migration, cell proliferation, cell apoptosis and nuclear morphology studies were investigated in WS1 cells. Overall, these results suggest that the use of G-AgNPs and in combination with laser shows great potential to heal wounds in in vitro, and this combined therapy did not show any toxicity to the cells. Thus, the present study reveals that the novel G-AgNPs demonstrated effective antibacterial properties against both gram-negative and gram-positive bacterial strains, and G-AgNPs in combination with photobiomodulation showed excellent wound healing properties in WS1 cells.

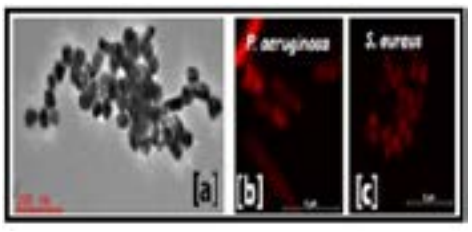

Figure 1: [a] HRTEM image of G-AgNPs, [b] and [c] confocal image of G-Ag-NPs treated Pseudomonas aeruginosa and Staphylococcus aureus.

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Biography

Sathish Sundar Dhilip Kumar has completed his BSc degree in Botany from Bharathidasan University, India; MSc degree in Biotechnology from Bharathidasan University, India; and PhD in Nanobiotechnology from Anna University, India. He is currently working as a Claude Leon sponsored Postdoctoral Researcher in the Laser Research Centre, Faculty of Health Sciences, University of Johannesburg, South Africa. His field of research is mainly focused on preparation and characterization of nanoparticles and their applications in biological sciences. He has published 10 research articles including one review paper in accredited international journal with a Google scholar H-index of seven, i10-index three with the overall citations of 127 and Research Gate score of 16.90 and one book chapter. He also acted as a Reviewer for *Drug Delivery, Informa Healthcare, Process Biochemistry, Elsevier,* and *Pharmaceutical Biology, Taylor and Francis Online*.

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INVESTIGATION OF FRICTION AND WEAR PROPERTIES OF SILICON NITRIDE REINFORCED POLYCARBONATE NANOCOMPOSITES

A K Bhargava[3], Santosh[1], P K Sain[2], Aman Kabra[3], Nimu Chand Reger[3] and **Dhanraj Solanki[3]**

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[2]Government Polytechnic College, Bharatpur, India
[3]Malaviya National Institute of Technology, India

Polycarbonate (PC) matrix nanocomposites containing 0-20 Vol% nanosized silicon nitride (Si3N4) particles have been prepared by solution mixing method followed by hot pressing at 228°C under a pressure of 45 MPa. To characterize phase purity, particle size and morphology of Si3N4 nanoparticles, a combination of x-ray diffractometry and transmission electron microscopy have been used. The prepared nanocomposites have been investigated for density, microhardness, microstructure and wear resistance. Density and microhardness have been found to increase with increasing volume percent of nanoparticulate. The experimental values of density of composites fall close to those of theoretical values predicted from rule of mixtures thereby suggesting that prepared nanocomposites nearly pore free. The maximum improvement of microhardness of 189% has been observed for nanocomposite with 20 Vol% Si3N4 particles as compared to neat PC. It correlates well a modified rule of mixtures with strengthening efficiency factor of 0.09. Scanning electron micrographs indicated good dispersion of nanoparticles in PC matrix. Friction and wear properties have been evaluated using pin-on-disc method. It has been found that PC-20% Si3N4 nanocomposite exhibits lowest friction coefficient (about 0.2) and highest wear resistance as against pure PC for normal load of 20 N. The improvement of wear resistance has been found to be as high as 68% with PC containing 20 Vol% Si3N4 as against neat PC.

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Biography

A K Bhargava has thirty eight years of teaching and research experience at Malaviya National Institute of Technology Jaipur (India). Currently, he is working as a Professor and Head, Department of Metallurgical and Materials Engineering, MNIT Jaipur, India. His areas of specialization include composite materials, rapid solidification of steels, and tribology. He published several research papers and two books namely, "Polymers, Ceramics and Composites" and "Mechanical Behaviour and Testing of Materials". He contributed two book chapters in Elsevier publication.

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SYNTHESIS AND CHARACTERIZATION OF TIO2 NANOPARTICLES BY SOL-GEL METHOD

R K Duchaniya[1] and **Niresh Kumari Choudhary**[2]
[1]Malaviya National Institute of Technology, India
[2]University of Rajasthan, India

Titanium dioxide nanoparticles are used for variant applications which can be well chosen by size, thermal and electrical properties. The TiO_2 nanoparticles are not new for photo catalytic activity, in degrading organic contaminants and germs, making of cosmetic products and paper industries. Titanium dioxide nanoparticles are prepared by different techniques in which sol gel is most used. The sol-gel synthesis method of nano TiO_2 can be through different molar ratio of TTIP: ethanol: distilled water. Characterization of TiO_2 nanoparticles are done by x-ray diffraction analysis, UV–Vis spectroscopy, FTIR and FESEM (with EDS). The average crystalline size of TiO_2 nanoparticle is obtained value of 4.5 nm by XRD. Surface morphological studies have been concluded from SEM images. FT-IR peaks of Ti-O bond were observed around 630-770 cm-1 for both samples. Electronic energy band gap of TiO_2 nanoparticles was observed 3.149 eV and 3.293 eV in respect to one and the other sample. A mixture of both brookite and the small amount of anatase form of TiO_2 nanoparticle has been found in the couple of samples nano TiO_2.

Recent Publications

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3. **Komal Yadav and Vibha Uttam (2016) Study of corrosion behavior of Ni-P-TiO_2 nanocomposite coating on mild steel deposited by electroless deposition process. Journal of Materials Science and Surface Engineering 4:410-414.**
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5. **Ravi Agarwal, Kamlesh Verma, Narendra Kumar Agarwal, Rajendra Kumar Duchaniya and Ramvir Singh (2016) Synthesis, characterization, thermal conductivity and sensitivity of CuO nanofluid. Applied Thermal Engineering 102:1024-1036.**

Biography

R K Duchaniya has his expertise in Nanomaterials, Engineering Materials, Corrosion and Surface Coatings. He has published 32 papers in national and international journals and conferences. He has expertise in the field of nano composite which can be used for solar cell. His work in the field of Electroless Plating Method is considerable for improving surface and corrosion resistance properties of materials by developing nano-composite coating on materials. He has developed a different field related to melt coolability of materials which can be used in nuclear reactor. He built collaboration of MNIT Jaipur with different institutes and research organizations.

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Ilya Zharov et al., Nano Res Appl, Volume:4
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BORON AND GADOLINIUM RICH NANOPARTICLES FOR NEUTRON CAPTURE THERAPY OF CANCER

Ilya Zharov and Yulia Yegeris
University of Utah, USA

Neutron capture therapy (NCT) is a suggested treatment for cancer. Species with large amounts of boron-10 or gadolinium-157 are required for an effective NCT. Gadolinium-containing nanoparticles might also be useful in MRI imaging, thus leading to theranostic agents. Dopamine-modified boron nanoparticles (BNPs) were prepared by ligand exchange on the surface of hydrophobic BNPs formed by ball milling. The boron core-silica shell nanoparticles were prepared by first performing a hydrosilylation reaction to convert the double bonds of the hydrophobic BNP ligands into trialcoxysilane moieties, followed by a sol-gel reaction to form the silica shell. The latter imparts hydrophilicity to the boron nanoparticle and provides a surface that can be further modified with various functionalities for targeted delivery. Furthermore, silica encapsulation results in particles that are uniform in shape and size, and are easy to manipulate. Silica nanoparticles (SNPs) grafted with carborane containing polymer brushes were prepared by modifying the silica surface with initiator moieties, followed by surface-initiated atom transfer radical polymerization of reactive monomers. After the formation of the polymer brushes, they are treated with carboranyl alcohols or acids, resulting in an almost complete modification of the polymer side-chains with the carboranyl moieties. Finally, silica nanoparticles were prepared with internal functional groups and microporosity, suitable for the incorporation of modalities for both MRI imaging and cancer treatment by neutron capture therapy using boron-10 and gadolinium-157 nuclei. These modalities were incorporated by preparing ORMOSIL particles with reactive functional groups throughout the nanoparticle body, followed by their conversion into the metal chelating and boron-containing moieties inside the nanoparticles.

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4. Gao Z and Zharov I (2014) Tannic acid-templated mesoporous silica nanoparticles with large pores. Chemistry of Materials 26:2030-2037.
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Biography

Ilya Zharov is an Associate Professor at the Chemistry Department, University of Utah. He obtained his BS degree in 1990 from Chelyabinsk State University; MS in 1994 from the Technion; and PhD in 2000 from the University of Colorado, Boulder. In 2000-2003, he was a Beckman Postdoctoral Fellow at the Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign. His research focuses on novel nanoporous materials, ion conductive membranes, and on theranostic agents. Among his awards are Camille and Henry Dreyfus Foundation New Faculty Award and the National Science Foundation CAREER Award. He was named an Emerging Investigator by the *Chemical Communications* in 2011 and serves on the Editorial Board of *Current Smart Materials*.

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S Moradi et al., Nano Res Appl, Volume:4
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EVALUATION OF HEMOSTATIC BEHAVIOR OF GELATIN-SILICA NANOHYBRID BY CHANGING THE PH OF INJURY IN SEVERE BLEEDING

S Moradi[1], M Chenani[1] and **S A Ahmaditabatabaei[2]**
[1]Islamic Azad University, Tehran, Iran
[2]Imperial College London, UK

After trauma, fast hemostasis is an essential strategy in extensive bleeding, in this decade, much effort has been made to develop the hemostatic agents, but the existent options have ample restrictions, including failure to maintain the structure of the styptic in the face severe bleeding and rapid changes in pH. Since the changes in pH of injury site is an important factor in the failure of styptic and their structural damage, in this study gelatin-silica nanohybrid behavior in severe bleeding was evaluated under different pH. Experiments including blood absorption, zeta potential measurements, and poly disparity index by GPC tests were studied. By changing the pH of environment, structural integrity and there upon nanohybrid hemostatic behavior changed dramatically. So that nanohybrid showed the most blood absorption (440%) and acceded to a coherent structure with tendentious to alpha helix and beta-sheets (the secondary structure of a protein), that also provide ability to maintain integrity of structure in severe bleeding. These results obtained, in alkaline or acidic environment nanohybrid hemostatic behavior was limited, so that in the acidic pH, the blood absorption was reduced to 110% and 1.6 times the normal clotting time delayed. Based on the results of this study, it was found that changes in nanohybrid behavior in acidic pH were much more than in alkaline pH and nanohybrid can also maintain the structural integrity with rapid hemostasis. According to the desire of injury site to change the pH to alkaline side, the resulting nanohybrid has an ideal ability to control excessive bleeding and can be proposed for further studies *in vivo* as a novel styptic.

Figure 1: APTT chart, plasma and nanohybrid interaction in different pH

Figure 2: M_n, M_w and PDI changes for nanohybrid samples

Recent Publications

1. Chenani M and Ahmadinejad M (2016) Preparation and characterization of novel gelatin/silica nano-hybrid as a styptic for massive bleeding. Journal of Nanomaterials and Biostructures 4:1277- 1288.

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MULTIPLEX DETECTION OF PROTEIN BIOMARKERS WITH SURFACE ENHANCED RAMAN SPECTROSCOPY

Lei Wu
International Iberian Nanotechnology Laboratory, Portugal

As the expression level of proteins in human body is closely related to the occurrence and progression of cancers, the development of highly sensitive, high-throughput, rapid and low-cost optical technology for multiplex protein detection is of great significance to the fundamental research in oncology and the clinical applications in early cancer diagnosis and therapeutics. We focus on the development of a novel multiplex protein detection platform which combines surface enhanced Raman spectroscopy (SERS) technique with the microfluidic chip. This study aims to improve the detection sensitivity, multiplexing ability, efficiency as well as to reduce the overall costs. Here, the spectral-spatial joint encoding method has been proposed to develop a novel analytical platform for high-throughput protein detection, which is further employed for the detection of tumor markers and the study on the interaction mechanism of anti-cancer drugs. This platform provides a new technological route for the early cancer diagnosis and therapeutics. The main content of this presentation are listed as follows: gold@silver core-shell nanorods were adapted to develop a SERS-based immunoassay with highly increased sensitivity; SERS spectral encoding technique was employed for multiplex detection of cancer biomarkers; SERS spectral-spatial joint encoding method was proposed to develop a SERS-assisted 3D barcode chip for multiplex protein detection; and a versatile microfluidic platform for the detection of tumor secretions was presented, in which the mechanism of anti-cancer drugs and the process of intercellular communication were studied..

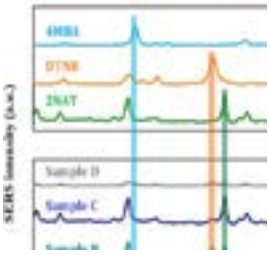

Figure 1: (up) SERS spectra of nanoparticles labeled with different Raman reporters (4MBA, DTNB and 2NAT); (down) Multiplex detection of protein biomarkers with encoded Raman probes.

Recent Publications

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Biography

Lei Wu is currently a Postdoctoral Research Fellow in International Iberian Nanotechnology Laboratory (INL). He obtained his Bachelor's and PhD degree from School of Electronic Science and Engineering, Southeast University, China in 2012 and 2017, respectively. His research interests include Biophotonics, Nanophotonics and Optofluidic Systems. He has published 14 research papers with total citations over 200 times, and has delivered five oral presentations on international conferences.

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MECHANICAL AND THERMAL BEHAVIOR OF NANO-TiO_2 ENHANCED GLASS FIBRE REINFORCED POLYMERIC COMPOSITES AT VARIOUS CROSSHEAD SPEEDS

Kishore Kumar Mahato[1], Krishna Dutta[2] and **Bankim Chandra Ray[3]**

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Fibre reinforced polymeric (FRP) are used in different components of aerospace, space, marine, automobile and civil infrastructure. These materials are becoming prime choice of materials in the field of structural components. During their in-service period different structural components experience a wide range of loadings. The current investigation was focused on the assessment of mechanical and thermal behavior of glass FRP composite on the addition of nano-TiO_2 particles. The control glass/epoxy(GE) composites and nano-TiO_2 modified GE composites were tested at different crosshead speeds viz. 1, 10, 100, 500 and 1000 mm/min. nano-TiO_2 was used as filler material and the epoxy matrix was processed with different nano-TiO_2 contents (0.1, 0.3 and 0.5 wt. %). Addition of 0.1 wt. % nano-TiO_2 particles exhibited an improvement in strength of nano-TiO_2 /GE composites at all crosshead speeds. Different failure patterns of nano-TiO_2 enhanced GE composite tested at 1, 10, 100, 500 and 1000 mm/min crosshead speeds were identified. Scanning electron microscopy (SEM) was carried out to know the main cause of failure that induced different morphologies. Furthermore, the viscoelastic behavior of the material was carried out using dynamic mechanical thermal analyzer which correlated the mechanical and thermo-mechanical behavior of the FRP composites.

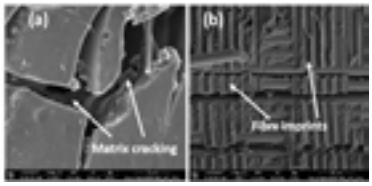

Figure 1: Scanning electron micrographs showing (a) matrix cracking (b) fibre imprints.

Recent Publications

1. **Mahato K K, Dutta K, Ray B C (2018) Loading rate sensitivity of liquid nitrogen conditioned glass fiber reinforced polymeric composites: An emphasis on tensile and thermal responses, Journal of Applied Polymer Science, 135:9.**
2. **Mahato K K, Dutta K, Ray B C (2017) High-temperature tensile behavior at different crosshead speeds during loading of glass fiber-reinforced polymer composites, Journal of Applied Polymer Science, 134: 16.**
3. **Mahato K K, Rathore D K, Dutta K, Ray B C (2017) Effect of loading rates of severely thermal-shocked glass fiber/epoxy composites, Composites Communications, 3: 7-10.**
4. **Mahato K K, Dutta K, Ray B C (2017) Static and Dynamic Behavior of Fibrous Polymeric Composite Materials at Different Environmental Conditions Journal of Polymers and the Environment, 1-27.**
5. **Nayak R K, Mahato K K, Ray B C, (2016) Water absorption behavior, mechanical and thermal properties of nano TiO_2 enhanced glass fiber reinforced polymer composites, Composites Part A: Applied Science and Manufacturing 90:736-747.**

Biography

Kishore Kumar Mahato is pursuing PhD at National Institute of Technology, Rourkela, India. He has published around 15 research articles in different SCI and Scopus indexed journals. The research work is focused on failure and fracture behavior of fibre reinforced polymeric Composite in different harsh environments. Investigations are focused on the assessment of mechanical behavior of environmentally conditioned FRP composites through experimental and numerical analysis. Primarily, the polymer matrix and the existing fibre/polymer interface are susceptible to harsh and hostile in-service environments which can alter the durability and integrity of fibrous polymeric composites. The mechanical response of polymeric materials is loading rate sensitive and the precise mode of failure depends on the in-service environment. The environmental parameters which may influence the performance of the composites includes but not limited to temperature, moisture, UV and other high energy radiations.

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LONGITUDINAL CREEP BEHAVIOR OF NANOCRYSTALLINE NI-NIZR GLASS NANOCOMPOSITE

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Longitudinal creep behavior of nanocomposite for nanocrystalline (NC) Ni-NiZr glass has been studied at various temperatures (from 1200 to 1400 K) at 1 GPa stress using molecular dynamics (MD) simulations. A simulation box of the specimen 15.85 × 15.85 × 15.85 nm dimension (contains 312,924 atoms) is taken for performing MD simulation. Common neighbor analysis (CNA), Centro-symmetry parameter (CSP) analysis, Wigner–Seitz defect analysis and radial distribution function (RDF) have been carried out to investigate the structural evolution and deformation mechanism of nanocomposite specimen during creep process. Self-diffusion of nanocomposite specimen has been performed using MD simulation for interface region and whole specimen at different temperature. Average atomic displacement and local stress in the regions (2Å, 4Å, and 6Å) adjacent to the NC Ni-NiZr glass interface is evaluated during creep deformation process to investigate the atomic movement near the interface of NC Ni-NiZr glass. It is found from creep curves that primary and secondary creep regime is reduced with increasing creep temperature. Creep rate for nanocomposite specimen is observed to be shifted downward with increasing creep temperature after 180 ps time period. Creep rate for creep process occurring at 1400 K temperatures are observed to be increased more from starting of tertiary creep regime to 180 ps time period and then decreased to 300 ps.

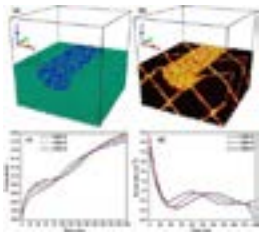

Figure 1: Three dimensional sectional view of nanocomposite for NC Ni-NiZr glass specimen (a) particle type, (b) CSP, (c) creep and (d) creep rate curves of nanocomposite of NC Ni-NiZr glass for different temperatures at 1 GPa stress.

Recent Publications

1. Meraj, M., Yedla, N., & Pal, S. 2016. The effect of porosity and void on creep behavior of ultra-fine grained nano crystalline nickel. Materials Letters, 169, 265-268
2. Pal, S., & Meraj, M. 2016. Structural evaluation and deformation features of interface of joint between nano-crystalline Fe–Ni–Cr alloy and nano-crystalline Ni during creep process. Materials & Design, 108, 168-182.
3. Pal, S., Meraj, M., & Deng, C. 2017. Effect of Zr addition on creep properties of ultra-fine grained nanocrystalline Ni studied by molecular dynamics simulations. Computational Materials Science, 126, 382-392.
4. Meraj, M., & Pal, S. 2017. Nano-scale simulation based study of creep behavior of bimodal nanocrystalline face centered cubic metal. Journal of Molecular Modeling, 23: 309. https://doi.org/10.1007/s00894-017-3481-y
5. Meraj, M., & Pal, S. 2017. Effect of temperature and stress on creep behavior of ultrafine grained nanocrystalline Ni-3 at% Zr alloy. Metals and Materials International, 23(2), 272-282.
6. Meraj, M., & Pal, S. 2017. Healing mechanism of nanocrack in nanocrystalline metals during creep process. Applied Physics A, 123(2), 138.
7. Meraj, M., & Pal, S. 2017. Comparative creep behaviour study between single crystal Nickel and ultra-fine grained nano crystalline Nickel in presence of porosity at 1120 K temperature. Metallurgical Research & Technology, 114(1), 107.

8. Meraj, M., & Pal, S. 2017. Comparative creep behaviour study between single crystal Nickel and ultra-fine grained nano crystalline Nickel in presence of porosity at 1120 K temperature. Metallurgical Research & Technology, 114(1), 107.

Biography

Md. Meraj completed his Master of Technology from National Institute of Technology Durgapur, India in 2014. Presently he is pursuing Ph.D. in Metallurgical and Materials Engineering Department, National Institute of Technology Rourkela, Orissa, India since 2014. He has been working on deformation (such as tensile, compressive, creep, indentation and asymmetrical cyclic deformation) of nanomaterial using molecular dynamics simulations. His scientific interests include high temperature material at nanoscale, nanocomposite of metals and high entropy alloy materials. He has been published 16 SCI research papers and 1 book chapter.

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