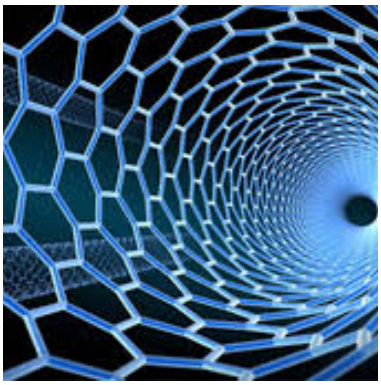
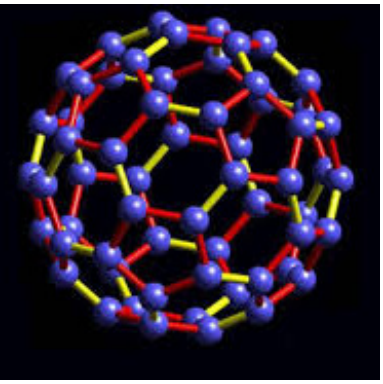
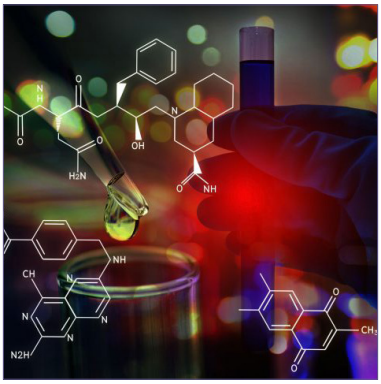
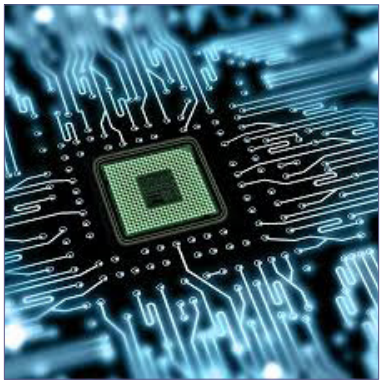
Video Presentations

Materials Chemistry 2018



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Antiferromagnetically assisted electron-phonon coupling as a mechanism of Fe-based superconductivity

Wong Chi Ho and **Rolf Lortz**
Hong Kong University of Science and Technology, Hong Kong

While there is still no self-consistent theory on the mechanism in iron-based superconductors, we develop a novel theoretical ab-initio approach that allows us to explicitly calculate the superconducting transition temperatures (Tc) of $LaFeAsO_{1-x}F_x$, $SmFeAsO_{1-x}F_x$ and $NdFeAsO_{1-x}Fx$ that perfectly agree with experiments. We consider recent evidence that electron-phonon coupling may have been previously underestimated where the hidden force owing to anti-ferromagnetism can greatly enhance the electron-phonon coupling through the localized orbitals of iron d-like xz or yz orbitals. We then include the contribution of these localized orbitals in a McMillan formalism with modified pairing potential that additionally considered the dipole-dipole attraction between the spin-polarized electrons on the Fermi surface and the iron orbitals in combination with the exchange Hamiltonian. With this approach we can not only calculate a theoretical Tc of $LaFeAsO_{0.9}F_{0.1}$ as a series of pressure corresponding to the experimental values, but also get the correct doping dependence.

Speaker Biography

Wong Chi Ho studied bachelor program in Department of Applied Physics in the Hong Kong Polytechnic University from 2009 to 2011. In 2010, he went to United Kingdom as a research trainee (particle physics) in Lancaster University. In 2011, he obtained full PhD scholarship from Hong Kong. In 2015, he has completed his PhD degree in the field of experimental and computational superconductivity at the age of 28 years from Hong Kong University of Science and Technology. In 2016, he was a postdoctoral researcher in Ural Federal University in Russia. Now he returns to Hong Kong to serves as postdoctoral researcher in Hong Kong University of Science and Technology. He registered two patents in China Patent Office and published many high-impacted journals such as ACS Nano.

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Notes:

GxP/GMP and its consequences for documentation and information technology systems

Eleonora Babayants
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Documentation is a critical tool for ensuring GxP/GMP compliance. This is what GMP states about document control: each manufacturer shall establish and maintain procedures to control all documents that are required. In the regulated environment which must be GxP/GMP compliant, document control is the cornerstone of the quality system. It is so important that if an external audit identifies deficiencies in the document control system, the entire organization can be shut down.There are also GMP requirements for information technology. For a drug to be produced in a GxP/GMP compliant manner, some specific information technology practices must be followed. Computer systems involved in the development, manufacture, and sale of regulated product must meet certain requirements. Change control within quality management systems (QMS) and information technology (IT) systems is a formal process used to ensure that changes to a product or system are introduced in a controlled and coordinated manner. In the regulated industries, manufactures are required to use a change control procedure. In this workshop, we will discuss the connection between GxP/GMP and document control. We will describe details of document control procedures, and the role of Quality Assurance in the documentation systems. We will review GMP requirements for information technology and how computer systems including documentation management systems must meet GxP/GMP requirements. We will also review change control procedure and how it should be used in GxP/GMP environment.

Speaker Biography

Galaxy Consulting Founder and President Eleonora Babayants is a documentation management professional and hands-on consultant with over 25 years of experience in documentation and records management, document control, regulatory compliance, internal and external auditing, electronic document management systems, information governance, and change management. Eleonora's past work includes development and implementation regulatory compliance processes and procedures, leading implementation and administration of document control systems in full compliance with regulatory requirements, enabling enterprise search, improving systems information architecture, creating and implementing users training programs. She led electronic document management systems selection and deployment, administered and supported these systems, web information portals, knowledgebase applications, recommended and implemented re-structuring of the content and the information architecture of these systems. She worked very closely with IT to do feasibility assessment and to capture users' requirements. She wrote technical documents and created documents templates. Eleonora's experience spans multiple industries including biomedical, pharmaceutical and medical devices companies.

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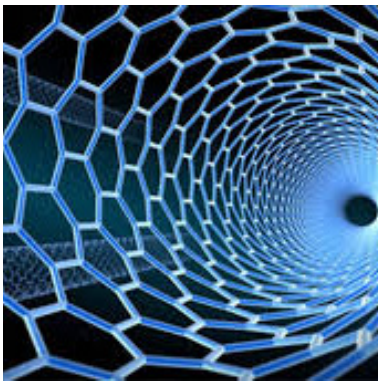

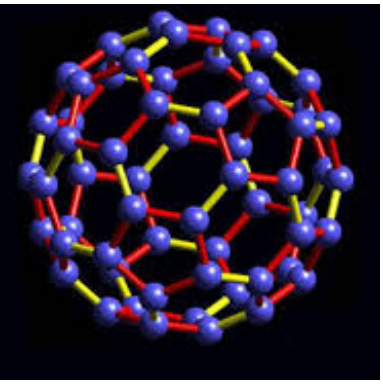
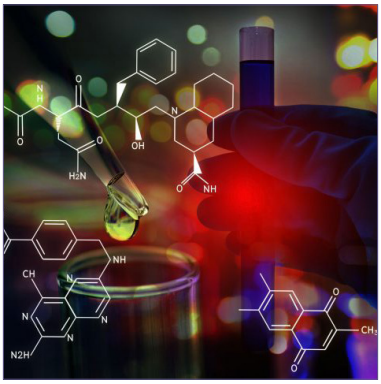
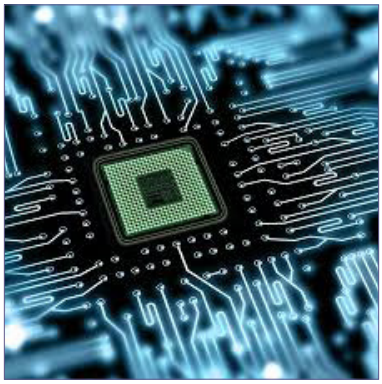

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Forsterite porous nanoceramics as a novelty in medical applications

Alexandra Avram, Adriana Marieta Naghiu, Maria Gorea and **Maria Tomoaia-Cotisel**
Babes-Bolyai University of Cluj-Napoca, Romania

The main purpose of this study is to develop novel nanoceramics based on forsterite (F) with high bioactivity and enhanced mechanical properties for medical applications. Forsterite nanoceramics were obtained by two methods using solid state (FS) and sol-gel (SG) synthesis. Their powders were pressed into pellets and thermally treated at different temperatures, 1200°C, 1300°C, and 1400°C. The compactness characteristics of the obtained forsterite ceramics were determined. The median apparent porosity of FS ceramics falls in the range of 17-46%, while that for SG ceramics is of 27-39%. With the increase in temperature, the apparent porosity of FS ceramics decreases comparatively to that of SG ceramics. In vitro bioactivity testing was performed by immersing the FS and SG ceramic pellets into simulated body fluid (SBF) for 1 week to several months. The formation of hydroxyapatite on the surface and within the pores of FS and SG-derived forsterite ceramics is confirmed even after 1 week, by X-ray diffractions (XRD). After 3 months of immersion in SBF, the surface of forsterite ceramic is covered by an organized fibrous network of hydroxyapatite elongated crystals. This fibrous hydroxyapatite was evidenced by atomic force microscopy (AFM). Mechanical characteristics were also determined, both by compression, flexural strength and Young modulus by nanoindentation. FS ceramics showed a median flexural strength of about 24 MPa, about 4 times higher than that of SG ceramics (6 MPa). The value of the Young modulus determined through nanoindentation falls in the range of 40 to 50 MPa for SG ceramics, and between 87 to 101 MPa, for FS ceramics. The novelty element of this investigation is also represented by the use of forsterite at nanometric scale, as porous nanomaterials with improved mechanical properties for bone grafts, as coatings for innovative metallic implants, and as drug delivery systems for orthopaedic medical applications.

Speaker Biography

Alexandra Avram is an Ph.D. candidate and a research assistant at the Physical Chemistry Center, Faculty of Chemistry and Chemical Engineering, Babe-Bolyai University. Her research interests include nanomaterials, biomaterials for bone tissue engineering (glass, ceramics, and composites) and drug delivery.

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Functionalized silver nano-sensor for colorimetric detection of Hg2+ ions: Facile synthesis and their docking studies

Shiva Prasad Kollur, Govindaraju Shruthi and **Chandan Shivamallu**
Manipal Centre for Natural Sciences, India

In the present study, we describe the facile synthesis of silver nanoparticles (AgNPs) and their functionalized nanostructures with 2-aminopyrimidine-4,6-diol (APD-AgNPs) for Hg^{2+} ion detection. The promising colourimetric response of APD-AgNPs to detect Hg^{2+} ions were noticed with naked eyes and spectroscopic changes were examined by using UV-Visible spectrophotometer. The aggregation of APD-AgNPs up on addition of Hg^{2+} ions was due to chelation effect of functionalized nanostructures and exhibit colour change from pale brown to deep yellow colour. The probing sensitivity was observed within five minutes with a detection limit of about 0.35 µM/L. The TEM images of APD-AgNPs showed poly-dispersed morphologies having hexagonal, heptagonal and spherical nanostructures with average size between 10 to 40 nm. Furthermore, the sensing behaviour of APD-AgNPs towards Hg^{2+} ions detection was investigated using docking and interaction studies.

Speaker Biography

Shiva Prasad Kollur received his Ph.D. degree from the University of Mysore, Mysuru in 2012. He persued his post-doctoral studies at Indian Institute of Science, Bengaluru. He joined as an Assistant Professor in Chemistry at Manipal Academy of Higher Education, Manipal in 2015. His research interests include Coordination Chemistry, Bioinorganic Chemistry, Materials Chemistry, Sustainable Chemistry and development of novel green synthetic approach for the production of nanomaterials.

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Antimicrobial activity of Vancomycin loaded in biomimetic hydroxyapatite and poly (Lactic acid) microcapsules

Gertrud-Alexandra Paltinean, Aurora Mocanu, Gheorghe Tomoaia, Sorin Rapuntean, Ioan Petean, Ossi Horovitz and **Maria Tomoaia-Cotisel**

Babes-Bolyai University of Cluj-Napoca, Romania

Any orthopaedic surgical procedure carries possible bone infection risks, which might be prevented by using bone cement based on combining pure hydroxyapatite, HAP or biomimetic hydroxyapatite, bHAP, poly (lactic acid), PLA, and antibiotic drugs, like vancomycin, VCM, for local drug delivery, and thus overcoming the disadvantages of systemic antibiotic therapy. The goal of the current study was to determine the vancomycin antimicrobial ability by using hydroxyapatites, HAPs, and PLA microcapsules that are biocompatible and nontoxic. Our results show that the initial burst release and total release of active VCM agent can be controlled by using VCM/HAP/PLA or VCM/bHAP/PLA composites in aqueous dispersions. Among bone cement, the biomimetic hydroxyapatite, like multi-substituted hydroxyapatite with Mg, Zn, Sr and Si, HAP-Mg-Zn-Sr-Si, has attracted increased interest due to its osteoconductivity in vivo, thus opening the new opportunities for orthopaedic surgical procedures. In the current investigation, both pure HAP and HAP-Mg-Zn-Sr-Si were prepared by wet chemical methods, without surfactants or template molecules and characterized by XRD, FTIR, TEM, SEM-EDX and AFM. The PLA microcapsules were synthesized and morphologically characterized, by TEM, SEM and AFM. Then, HAPs mixed with vancomycin loaded in PLA microcapsules were synthesized and structurally characterized by XRD, FTIR, TEM, SEM-EDX and AFM. Further, the vancomycin release into the water dissolution medium was quantitatively measured by UV-Vis spectrum, which is characteristic for vancomycin. The vancomycin was released into the dissolution medium from composite microcapsules, within of 4 weeks, compared to vancomycin loaded in pure HAP, where drug release was observed for only about 2 weeks. The release of vancomycin is dependent of the microcapsules (i.e. solid) and dissolution liquid ratio and can be controlled with precision. The antibacterial activities of aqueous dispersions of VCM/HAP/PLA or VCM/bHAP/PLA composites were determined using the inhibition zone assay. High level of inhibition zone was obtained for the aqueous dispersions of both VCM/HAP/PLA and VCM/bHAP/PLA composites, used individually, against four pathogenic species: Staphylococcus aureus, Salmonella typhimurium, Bacillus cereus and Micrococcus luteus. Additionally, a distinct inhibition zone was clearly formed in methicillin-resistant Staphylococcus aureus media for up to 3 weeks incubation, for these composites. This approach can be used for further development of controlled delivery systems of therapeutic vancomycin molecules, for biomedical applications as the coating of metallic implants and as bone grafts in orthopaedic surgery.

Speaker Biography

Gertrud-Alexandra Paltinean graduated from the Faculty of Chemistry and Chemical Engineering of Babes-Bolyai University (bachelor degree, master degree and doctorate). Her activities are focused on the preparation and characterization of nanomaterials based on multisubstituted hydroxyapatite and air pollution, using advanced technologies (UV-Vis, lyophilizer, AFM, STM) from the Physical Chemistry Center where she is a member.

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Low cost membrane for efficient microbial fuel cell

Shrok Allami, Mohammed Abed Hamid and **Bayan Saad**
Ministry of Science and Technology, Iraq

Electric energy generation from the association of organic materials in the wastewater by microbes using microbial fuel cell (MFC) is one of the developing techniques used to gain high efficiency for some applications. The goal of this project is to construct low-cost, double-chambered MFCs that harvest electricity and produce reclaimed water from wastewater. MFCs were constructed from cheap alternatives to traditionally used expensive Nafion membranes and platinum cathodes. Low-Density Polyethylene, aluminium and graphite for membrane, cathode, and anode respectively were used to construct double chamber MFC. The double-chambered consist of wastewater and salt solution at the anode and cathode sides respectively. The MFC produced about 0.087 mA/cm2 of anode area at a potential of more than 0.642 V. MFC efficiency produced 0.49%. A 3 MFCs series connected produce 2.232 V and 67% fuel cell efficiency.

Speaker Biography

Shrok Allami is a scientific researcher in the ministry of science and technology-renewable energy directory of the department of hydrogen and biofuel. She has completed her PhD in 2007 from University Technology, Iraq. She has published more than 25 papers in reputed journals, participated in more than 16 national and international conferences as a researcher and has been serving as an editorial board member in Iraqi scientific journals.

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Novel composites based on nanoceramics and silver nanoparticles with antimicrobial activity for biomedical applications

Reka Balint, Gheorghe Tomoaia, Sorin Rapuntean, Aurora Mocanu, Ossi Horovitz and **Maria Tomoaia-Cotisel**
Babes-Bolyai University of Cluj-Napoca, Romania

Recently, the increasing resistance of microorganisms to antibiotics has triggered intense research for finding alternatives. Moreover, the apparition of microbial strains with multiple resistance has determined numerous studies on the efficiency of metal ions, especially Ag+and silver nanoparticles, AgNPs, on various microorganisms, mainly bacteria and fungi. In this work, we describe first the synthesis of spherical AgNPs in aqueous media via reduction of silver nitrate using glucose in alkaline media in the absence and the presence of TEOS. Also, an aqueous dispersion of AgNPs was prepared by using a solution of silver nitrate and a mixture of two chemical agents: sodium citrate and tannic acid in alkaline media. The size, shape and size distribution of AgNPs were determined by UV–Vis spectroscopy, dynamic light scattering (DLS), atomic force microscopy (AFM) and scanning transmission electron microscopy (STEM). The compounds present on the surface of the AgNPs were identified using FT-IR spectroscopy. Obtained data indicated that the use of TEOS and the combined use of sodium citrate and tannic acid produced spherical AgNPs dispersions, as they allow the control of nucleation, growth and stabilization of the synthesis process. Therefore, synthesis of new nanostructured composite materials made from the mixture of HAP ceramics and AgNPs at different ratios (from 0.1 to 5 wt% Ag) is realized. The HAP ceramics was previously obtained by a wet precipitation method, while AgNPs were prepared by reduction of silver nitrate as described above in alkaline media. HAP and HAP & AgNPs composites were characterized by X-ray diffraction, different imagistic methods (TEM, SEM and STEM, AFM), UV-Vis spectroscopy and zeta potential measurements. The antimicrobial effect of the AgNPs alone in aqueous dispersions and in their composites with HAP ceramics was tested on five pathogenic species: Escherichia coli, Staphylococcus aureus, Salmonella typhimurium, Bacillus cereus and Micrococcus luteus and important results were obtained for biomedicalapplications.

Speaker Biography

Balint Reka graduated from the Faculty of Chemistry and Chemical Engineering at Babes-Bolyai University in Cluj-Napoca, where she got chemistry diploma. Now, she is a PhD student and assistant researcher at the Chemistry Physics Center at the Babes-Bolyai University.

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Accepted Abstracts

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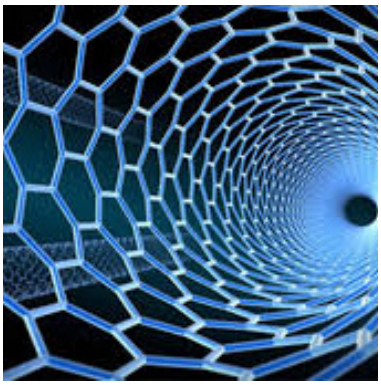

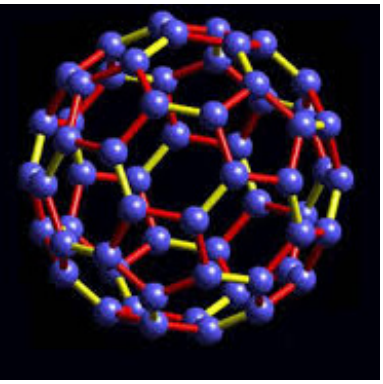
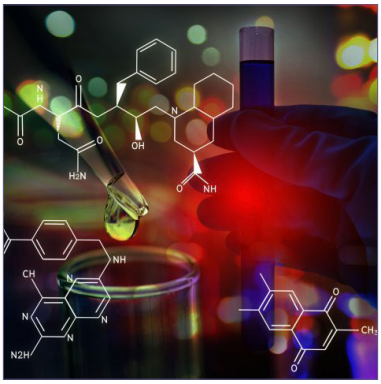
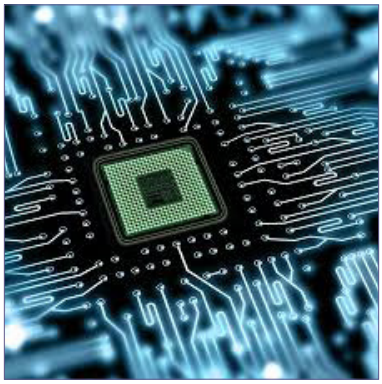

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Identifying, developing and moving sustainable communities through application of bioenergy for energy or materials: Future perspective through energy efficiency

Abdeen Mustafa Omer
Energy Research Institute, UK

The demand for energy continued to outstrip supply and necessitated the development of biomass option. Residues were the most popular forms of renewable energy and currently biofuel production became much promising. Agricultural wastes contained high moisture content and could be decomposed easily by microbes. Agricultural wastes were abundantly available globally and could be converted to energy and useful chemicals by a number of microorganisms. Compost or bio-fertiliser could be produced with the inoculation of appropriated thermophilic microbes which increased the decomposition rate, shortened the maturity period and improved the compost (or bio-fertiliser) quality. The objective of the present research was to promote the biomass technology and involved adaptive research, demonstration and dissemination of results. With a view to fulfill the objective, a massive field survey was conducted to assess the availability of raw materials as well as the present situation of biomass technologies. In the present communication, an attempt had also been made to present an overview of present and future use of biomass as an industrial feedstock for production of fuels, chemicals and other materials. We may conclude from the review paper that biomass technology must be encouraged, promoted, invested, implemented, and demonstrated, not only in urban areas but also in remote rural areas.

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Temperature dependent interplay between emitting species in highly ordered poly(thiophenes) as revealed by optical spectroscopy

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In this study, the temperature dependent PL spectra measurement has provided us a feasible means to elucidate the nature of the emissive species and the melt transitions in different polythiophenes. The effects of thermal fluctuation on different phases of a bulky substituted poly (3-(2, 5-dioctylphenyl) thiophene) (PDOPT) and Poly(3 hexylthiopne-2 5diyl) (P3HT) have been systematically investigated using photoluminescence spectroscopy. This has been achieved by performing in-situ temperature dependent photoluminescence measurements followed by detailed spectral analysis. For PDOPT, the intensities of the emitted species varied as a function of temperature that determine degrees of order. Well-ordered crystals emitted strongly in lower energies as opposed to less ordered films and spherulitic crystals. From the deconvoluted PL spectra, it was revealed that, the emitting energy bands remained constant with shift of intensity with ordered crystals emitting strongly in higher wavelengths as compared to their disordered counterparts that emit strongly in lower wavelengths. On the other hand, for P3HT, the spectrally resolved PL lineshapes through multipeak Gaussian functions simulating 0-0, 0-1, 0-n peaks have revealed multiple vibrational replicas yielding different emitting species (states). We suggest that the temperature dependent vibronic progressions arise from different electronic origins i.e. different species (fluorophores) due to multiple crystalline polymorphs within the crystal with varied coupling of the excited states. From our observation, we conclude that it is not sufficient to invoke only the intramolecular interactions in explaining the nature of PL spectra of highly ordered polythiophenes which are widely dominated by both interchain and intrachain interactions.

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Dielectric elastomer artificial muscles

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Growth in world population and further industrialization combined with concerns about global climate change is causing a surge in demand for clean and renewable energy. We discuss the potential of Dielectric Elastomers (DEs), a new energy transduction technology that can be used to harvest energy from the environment or human activities as well as save energy by making light and efficient motors and other devices. At the material level, this material has fast speed of response (over 100,000 Hz has been demonstrated for small strains), with a high strain rate (up to 640%), high pressure (up to 8 MPa), and power density of 1 W/g (for comparison, human muscle is 0.2 W/g and an electric motor with gearbox is 0.05 W/g). Currently, research is moving from the development stage into the commercialization stage through establishment of practical applications. Using a DE actuator makes it possible to achieve a highly efficient transduction from electric energy into mechanical energy, which translates into a considerable energy saving compared with other actuator technologies such as electric motors with gearboxes. Furthermore, its low cost, light weight, softness, and quietness make the actuator suitable for robots, sensors, motors, speakers, pumps, smart materials, and a wide range of other uses that are currently under development. DE has a very simple structure comprised of a polymer film (elastomer) sandwiched between two electrodes made of a flexible and elastic material. Applying a voltage difference between the two electrodes causes a compression in the horizontal direction and a stretching along the surface. Until recently, the possibility of using DE for electricity generation (energy harvesting) was not well known compared with actuator mode. The operating principle for the electricity generator is rather simple. The DE generator mode uses the actuator mode process in reverse, transforming mechanical energy originating from the physical deformation of the film into electrical energy

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Solid state chemistry of Ca and Cr in the processing of Cr^{4+}:YAG laser ceramics

Oleh Vovk and **Mykhailo Chaika**
National Academy of Sciences, Ukraine

Lasers based on Nd:YAG are widely used in military, materials processing, medicine etc. These lasers consist on active element Nd:YAG and Q-switcher Cr^{4+}:YAG. A recent trend in manufacturing of such elements is replacing single crystals with ceramics of high optical quality. The innovation approach to manufacture the laser can be developed, when both elements made from ceramics. In this case, a combined block of the active element and Q-switcher (Nd:YAG-Cr^{4+}:YAG) can be obtained in one technological route that allows both decreasing laser size and avoiding several expensive technological stages. To realize this approach a harmonization of the sintering routes of both types of ceramics should be carried out. Up today the huge progress has achieved in the sintering of Nd:YAG ceramics of high optical quality while the production of the Cr^{4+}:YAG still remains more art than technology. To reveal the possibility of adjusting the sintering routes of Nd:YAG and Cr^{4+}:YAG ceramics, the solid state chemistry of the Ca and Cr ions that are used as main additives to produce Cr^{4+}:YAG ceramics has been investigated. The effect of Cr ion on the formation of Cr^{4+}:YAG ceramics has been investigated and was revealed that Cr ions enhanced the optical properties of the final ceramics due to the appearance of the intermediate, which lowering the rates of solid state reactions under sintering. The dual role of Ca as sintering and charge compensator for Cr^{4+} has been studied and optimal Ca concentration was determined. The kinetics of Cr^{3+} oxidation to the Cr^{4+} under air annealing has been investigated to maximize the Cr^{4+} amount in ceramics Cr:YAG. The significant difference between the ceramics and single crystal has been revealed. It was established that the limitation stage of Cr oxidation is oxygen diffusion in ceramics grains. The results obtained allow designing the combined sintering route of Nd:YAG and Cr^{4+}:YAG ceramics.

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Catalytic effect of Ti-based additives on hydrogenation of MgH_2

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Various Ti-based additives (TiF_4, TiO_2 and TiH_2) were added to MgH_2 by ball milling and their catalytic effect on hydrogenation properties was investigated. All these additives significantly improved the dehydrogenation performances of MgH_2 but among them, TiF_4 shows best catalytic effect followed by TiO_2 and TiH_2 sequentially. The activation energy of dehydrogenation was calculated by using Kissinger's equation. The result shows that activation energy decreases from -170.48 kJ/mol for as- milled MgH_2 to -77.58 kJ/mol for MgH_2-TiH_2 and further lowers to -75.50 kJ/mol to -70.82 kJ/mol for the MgH_2–TiO_2 and MgH_2-TiF_4. Thermogravimetric analysis (TGA) shows the onset desorption temperature of MgH_2 was also reduced by the addition of different Ti-based additives. XPS studies show that the catalytic effect of these additives on hydrogenation/ dehydrogenation kinetics was due to by the formation of different active species.

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External stimuli-controlled nanosystems towards next generation nanomedicines

Pablo del Pino
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A large fraction of the advances in the nanomedicine and nanochemistry fields aim at developing the safe and efficient delivery of pharmaceutical formulations to targeted cells and/or tissues, thereby improving their bioavailability. However, most of the current nanomedicines have very low specificity in vivo, thus rendering targeted delivery among the most crucial challenges in the fields of nanotechnology and medicine. One of the most straightforward solutions in this context involves the use of external stimuli such as light, magnetic fields or ultrasound to trigger drug release from nanocarriers with spatiotemporal resolution, thereby creating molecular (drug) gradients. In this talk, we present and discuss different nanosystems, which can be controlled by external stimuli such as light, magnetic fields or ultrasounds, to achieve delivery of different macromolecules and/or to control cell behaviour in vitro and/or in vivo.

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Evaluation of fatigue properties of medium carbon low alloy forged steels quenched in polymer

Chandan B R, Ramesha C M and **Prasanna N D**
Ramaiah Institute of Technology, Bengaluru

Medium carbon low alloy forged steels (EN 18, EN19, EN 24 and EN25) have been investigated with respect to their fatigue properties for untreated (Forged) and polymer quenched samples. For heat treatment, the solutionizing temperature of 855^{0}C with a soaking period of 60 min followed by step tempering of 5750 and 2200 was used. Thereafter quenching was carried out in a polymer (polyethylene glycol 10% & 30%) separately. Fatigue tests were carried out for untreated and polymer quenched samples considering the UTS values for various loads; the polymer quenched samples being superior to untreated samples. Simulation of fatigue analysis carried out using ANSYS and corroborated the experimental results for the polymer quenched samples loaded to 30% of UTS, also the specimens quenched in poly ethylene glycol exhibited the best mechanical properties. The heat-treated specimens had a structure of fine tempered martensite with a small amount of ferrite.

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In Vivo Dosimetry in Total Body Irradiation

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Total Body Irradiation (TBI) is a radiotherapy technique that consists of irradiating homogeneously the whole patient's body and it is characterized by an extended source to surface distances and the use of large irradiation fields. The limitations of the available input data and inherent problems with the calculation procedures make it very difficult to accurately determine the dose distributions in TBI. For these reasons, it is highly recommended to use In Vivo Dosimetry (IVD), to guarantee the quality of TBI treatments as a direct measurement of the delivered dose. An IVD QA system was implemented based on semiconductor diodes and radiochromic films. For the commissioning of the system, both detector types were calibrated independently. This guarantees the traceability of the measurements. An assessment was made on the sources of uncertainties. A tolerance level of ±10% was established for the combined contribute on of both computational and experimental uncertainties. An experiment to a phantom was carried out to simulate a clinical TBI procedure. In this way, the calibration of the dosimetry system was corroborated. Finally, the IVD system was applied in TBI of three real patients. The discrepancies obtained between the prescribed and measured doses were below the established tolerance level of ±10 %.

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Novel hererojunction nanostructrures for high efficient solar photo-electrochemical water splitting

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The semiconductor-based generation of hydrogen via water splitting using solar irradiation has attracted great attention since the first report of photoelectrochemical (PEC) water splitting was published by Honda and Fujishima in 1972. To achieve the best efficiency of solar water splitting, the PEC cell must perform multiple functions like light-harvesting, semiconductor/electrolyte interfaces, charge transfer, and chemical redox reactions. The earth-abundant materials that can be used in solar water splitting cells remain an important goal for environmentally challenging methods for energy conversion and storage. Recently many researchers have put potential efforts to develop efficient photoelectrodes, depending on the shape and size of micro and nanoscale features of semiconductors. There are several numbers of traditionally available single semiconducting photoanodes, dichalchogen heterojunction photoanodes, compound semiconductor and heterojunction photoanodes for construction of PEC cell. Among all these photoanodes the nanostructured heterojunction photoanodes exhibits better efficiency. The development of particular nanostructured heterojunction photoanodes material which absorbs visible light efficiently, durability and scalability is a challenging task. The heterojunction nanostructures provide an internal electric field which facilitates the separation of the electron-hole pairs and induces faster migration of charged carriers to enhance the efficiency of the photoelectrochemical cell. In addition to that we have to reduce photo-corrosion, good chemical stability in acidic aqueous solutions (pH < 4) under solar illumination and finally we will get efficient hydrogen generation.

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Impact of renewable technology on lignocellulosic material of physic nut shell: Strategy for climate change and adaptation

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Agricultural residues have the potentials to be used as energy and chemical source and meet its deficit in the country. Physic nut shell is a residue of Jatropha curcas which is a good source of biofuel. This study aims to explore low temperature and pressure to extract the lignocellulosic content of physic nut shell and pyrolyze it for energy (bio-oil) and chemical feedstock productions as alternative technology to improper disposal causing environmental pollution as strategies for climate change and adaptation. The main properties of solid (lignocellulosic) materials were tested and the bio-oil produced was analyzed using GC-MS. Results show proximate analyses (volatile, ash and fixed carbon contents) and ultimate analysis (carbon, oxygen, nitrogen, magnesium, phosphorus and zinc). The pH value of the bio-oil from the residue increased with increase in temperatures. The density, viscosity and calorific value of the physic nut residue oil are 947.5kg/m3, 1.58cPa at room temperature and 14.169kJ/g, respectively. Physic nut shell oil contains aromatic ethers, cyclic ethers, secondary amides and organic halogen compound which are important chemical feedstock. Conversion of these residues to useful products will alleviate the energy supply deficit, improve social and economic development, promote clean and healthy atmosphere of the nation and significantly contribute to global climate change mitigation. Therefore, this study is recommended for policy making on proper disposal and bio utilization of residues in the nation.

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Discrete dipole approximation to determine the optical properties of ZnO polymer nanocomposite

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Optical properties have been simulated by DDA for ZnO NPs and ZnO-PVP composite for different particle size with complex dielectric function as input. The absorption efficiency factor for ZnO NPs of size 26 nm and that for ZnO-PVP of size 28 nm in simulation matches well with the experimentally obtained absorbance data. When ZnO is simulated for the particle size of 26 nm, the electric near-field intensities on the edges show fewer intensities compared with the center. The simulation of ZnO-PVP composites of 28 nm results in a spherical electric near-field with a larger diameter. Since ZnO is a hexagonal structure, the near-field appears to be most intense at the center followed by the edges of the NP. The increase of near electric field due to the presence of local dielectric medium may be the possible reason to behave a particle within the dielectric medium as the particle with higher effective radius. So, in ZnO-PVP composite, ZnO NPs act as a particle with higher effective radius. As a result, in presence of dielectric medium, the absorbance peak of same NPs shifts towards higher wavelength. The dielectric medium perturbs electron-phonon interaction as well as the optoelectronic properties. Moreover, the luminescence properties of the materials are affected due to composite formation. In case of NP-polymer composite, NPs are capped and there is negligible further adsorption and desorption of O_2 molecules occurred on the surface. This increases the photocurrent as well as photosensitivity, which makes the ZnO-PVP composite as a suitable candidate for visible-blind UV detector.

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Rapid and green microwave-assisted synthesis of zinc oxide nanoparticles using aqueous Phoenix dactylifera L. (Date palm) wood extract and evaluation of antibacterial and antifungal activities

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Nanoparticles exhibit completely new or improved properties with larger particles of the bulk materials and these novel properties are derived due to the variation in specific characteristics such as size, distribution and morphology of the particles. Nanoparticles present a higher surface area to volume ratio with decrease in the size, distribution and morphology of the particles Recently, synthesis of NPs via eco-friendly routes have become popular among researchers due to its low cost, synthesis in ambient atmosphere, non-toxicity, environmental compatibility etc. and ease of applications as the resulting particles are highly soluble in water, biocompatible, and devoid of toxic stabilizers. Among the diverse biosynthetic approaches, the use of plant extracts has compensation such as easily available, safe to handle and possess a broad viability of metabolites. The phytochemicals responsible for the synthesis of nanoparticles are Terpenoids, flavonoids, carbohydrates, saponins, alkaloid and protein. In the present study, Zinc Oxide nanoparticles (ZnO NP) were synthesized from palm date wood extract (Phoenix dactiferia L.) in a rapid and eco-friendly microwave-assisted synthesis from zinc nitrate solution. Microwave parameter (irradiation time), wood extract and silver nitrate concentration were optimized. The UV–visible spectroscopy was used to monitor the ZnO NP formation through sampling at time intervals, phyto-synthesized zinc oxide nanoparticles dimensions were characterized using X-ray diffraction analysis. The green synthesized nanoparticles exhibited potent antibacterial activity against the pathogenic bacteria, as evidenced by their zones of inhibition and also a good antifungal activity against the Candida fungus.

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Formulation of Calcium dialuminate ($CaO•2Al_2O_3$) refractory cement from local bauxite

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Three types of bauxites containing aluminium hydroxide of 58.1% gibbsite and 19.3% boehmite for BX3, 95.5% of gibbsite for BX55 and 84.5% of gibbsite for BX8 were used with lime at 95% of CaO through solid state sintering in one stage to prepare a refractory clinker at 1550°C. The powder obtained after grinding the clinker showed in the XRD curves the presence of $CaO•2Al_2O_3$ and $CaO•TiO_2$ phases in the cement samples. The density of cement powder varied between 2.95 and 3.17 g/cm3and the specific area of the powder obtained after grinding was between 0.72 and 0.85 m2/g. The properties of hydrated cement, W/C = 0.33, after stabilization of cement components for 48 h at 105°C were showed by XRD, DTA, DTG and SEM (C_3AH_6, AH_3, CA_2 and $CaO•TiO_2$). The Young's modulus of the cement made varied between 35.5 and 39.4 GPa, and these Young's moduli were compared to conventional CA14M cement.

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Degradation kinetics and stability indicating RP-HPLC method for the estimation of flavoxate hydrochloride in bulk and pharmaceutical dosage forms

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A simple, rapid, economic stability indicating reversed-phase HPLC method was developed, validated and subsequently degradation kinetics in acidic, alkaline, oxidative, thermal, photolytic media are assessed for Flavoxate Hydrochloride (FVH) present in pharmaceutical dosage forms. The proposed RP-HPLC method utilizes a LiChroCART-Lichrosphere100, C18 RP column Hibar (250 x 4 mm, 5µm) in an isocratic separation mode with mobile phase consisting of methanol and water in the proportion of 50:50 % (v/v), at a flow rate of 0.8 ml/min and the effluent was monitored at 315 nm. The retention time of FVH was found to be 2.92 min. Stability of FVH was investigated as per ICH-prescribed stress conditions. Significant degradation of FVH was observed under all studied stress conditions. A kinetic study was conducted to investigate the degradation kinetics of FVH at different temperatures; reaction rate constants, half-life times and activation energy were calculated in all the media. The described method was linear over a range of 1-300µg/ml. The percentage recovery was 99.46. F-test and t-test at 95% confidence level were used to check the intermediate precision data obtained under different experimental setups; the calculated value was found to less than the critical value. The proposed method can thus be used for routine analysis, quality control and for studies of the stability of pharmaceutical tablets containing these drugs.

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One-pot green synthesis of fluorescent carbon quantum dots from vegetable extract for optoelectronic and biomedical applications

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Carbon quantum dots (CQDs) are potential candidates for numerous modern nanotechnologies and biomedical research. Owing to their simple one-pot synthesis, unique excitation-dependent emission, excellent photochemical stability, and high biocompatibility, these water miscible CQDs have shown great potential as an alternative source to conventional organic fluorescent dyes and inorganic semiconductor QDs. Considering these advantages of CQDs, we have synthesized fluorescent CQDs from various natural sources such as pomegranate extract, D-glucose and beetroot aqueous extract in a very simple, green and cost-effective way for white light emitting material, chemical sensing and biomedical applications. The details of the synthesis, photophysical properties and applications of these CQDs are also studied.

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Mechanochemical synthesis of double perovskites materials mediated by ammonium fluoride along with their optical and catalytic role in environmental remediation

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Bond breaking and bond making triggered by stress are usually referred to as mechanochemical reactions. To highlight the power of mechanochemistry to oxidize metal ions leading to the discovery of newer phases, ammonium fluoride mediated synthesis of A_2MF_6 (A =Rb, K; M = Pd, Mn, Ni) has been carried out. Stability of high oxidation state of transition elements using mechanochemical approach has been demonstrated. Grinding reactions of ammonium fluoride with metal (II) acetate and further cation exchange with AF (A = Rb, K) were closely monitored ex-situ characterizations such as high-resolution PXRD, FT-IR and Raman spectroscopy measurements. For the reaction involving AF (A= Rb, K), A_2MF_6 possessing K_2PtCl_6 type structure was confirmed by the Rietveld refinement of PXRD pattern, HR-TEM and SAED measurements. Elemental composition and oxidation state of palladium in Rb_2PdF_6 were examined using XPS analysis. Ligand to metal charge transfer and d-d transitions of Pd (IV) were present in the UV-visible diffuse reflectance spectrum of Rb_2PdF_6 with a band gap of 2.67 eV estimated using the Kubelka–Munk function. Other than LMCT, they also show a broadband in the visible region for d-d transitions. Its role as a photocatalyst to degrade the aqueous dye solutions (MB, RhB, Rh6G and MG) under UV-visible radiation has been evaluated along with their kinetic studies. The reduction of Pd (IV) to Pd (0) by $NaBH_4$ has been favourably used for the efficient and rapid conversion of highly carcinogenic, toxic, mutagenic Cr^{6+} to less toxic Cr^{3+}. Application of Mn^{4+} in K_2MnF_6 as red phosphors has been demonstrated by using PL spectroscopy.

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The potential application of functionalized ZnO nanorod as electrochemical (Glucose and metal ions) biosensors for intracellular environment

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The nanostructure of zinc oxide (ZnO) such as nanorods and nanowires has interesting nanosurfaces in addition to its bulk properties. ZnO has attracted much interest because of its unique piezoelectric, semiconducting, catalytic properties and being biosafe and biocompatible morphology combined with the easiness of growth. This implies that ZnO has a wide range of applications in optoelectronics, sensors, transducers, energy conversion and medical sciences. This abstract relates specifically to electrochemical biosensors based on single and multiple ZnO nanorods especially on a flexible substrate for the extra/intracellular environment. Functionalized zinc oxide nanostructure was used in biological, biochemical and chemical applications. One of the properties is that these nanostructures are very suitable for intracellular measurements of pH, metal ions, glucose and also for cholesterol using potentiometric measurements techniques. To adjust the sensor for intracellular measurements, the ZnO nanorods were grown on the tip of a borosilicate glass capillary (0.7µm in diameter) and functionalized with polymeric membrane or enzymes for intracellular selective metal ion sensors. The sensor in this study was used to detect and monitor real changes of metal ions and glucose across human fat cells and frog cells using changes in the electrochemical potential at the interface in the intracellular microenvironment. The fabrication of such type of device aims to explain the methodology of ions sensing using functionalized ZnO nanorods for the intracellular environment. This nanoelectrode device paves the way to enable analytical measurements in single living cells

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Preparation and evaluation of mechanical properties of fibre reinforced thermoplastic prepregs and optimization of process parameters through mathematical modelling

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Fibre reinforced thermoplastic composites are lightweight materials for making semi-structural parts in automobile, aerospace and home appliances. Nowadays, on account of greater impact resistance, low weight, storage stability, recyclability, infinite shelf life (of prepreg) and shorter processing time, thermoplastics are becoming more popular than thermosetting plastics. Because of high melt viscosity and poor wettability of fibers with thermoplastics, proper impregnation of the thermoplastic matrix into reinforcing fibers is difficult. Development of a suitable process for fabrication and characterization of resultant composites is essential for their usage. FRTP composites are fast gaining importance over fibre reinforced thermosetting composites mainly because of their higher fracture toughness. FRTP prepegs in sheet form produced by film stacking process are ideal for large products like automobile bumper, dashboard etc. The present work involves to preparation, characterization and evaluation of the mechanical properties of graphene-reinforced with Polypropylene thermoplastic by blend mixing method.

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