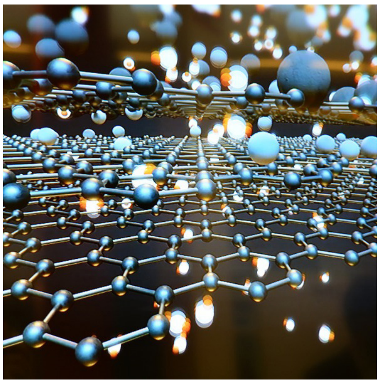
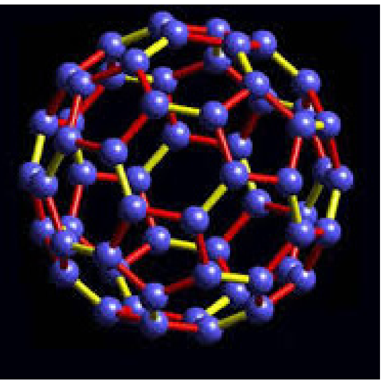
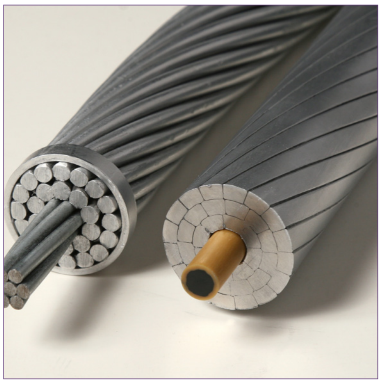
Video Presentations
March 20, 2019

Materials Chemistry 2019







2nd International Conference on

Materials Science and Materials Chemistry

March 20-21, 2019 | London, UK

Room temperature p-orbital magnetism in monoatomic carbon chains

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The study of magnetism without the involvement of transition metals or rare earth ions is considered the key for the next generation spintronic devices. Various recent reports claim that optimizing the occupation number of the mixed p-orbitals is the optimistic way to strengthen the p-orbital magnetism in bulk crystals. We prove experimentally that the kinked monoatomic carbon chains, the so-called linear-chained carbon, allows intrinsic ferromagnetism even above room temperature. According to our ab initio calculations, unconventional magnetism is credited from the p-shells. In contrast, the linear monoatomic carbon chains are non-magnetic. Although the optimized differential spin density of states at the Fermi level (SDOS) of the kinked carbon chains is larger than that of bulk Fe, the magnetic moment is as weak as 0.3µB. In order to reinforce the magnetic response, we tune the p-orbital magnetism by introducing dopants from groups IV to VII of the periodic table. Our best system, the arsenic-doped carbon chain, generates a strong local magnetic moment of 1.5µB, which is comparable to that of the bulk Fe of 2.2µB, with the mean exchange–correlation energy reaching a 63% ratio in comparison to bulk Fe.

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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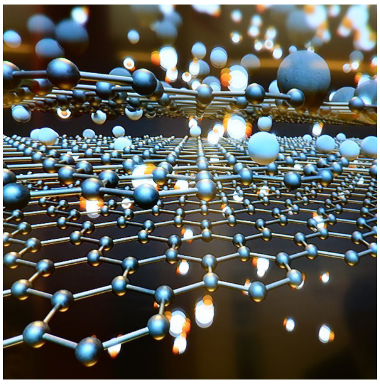
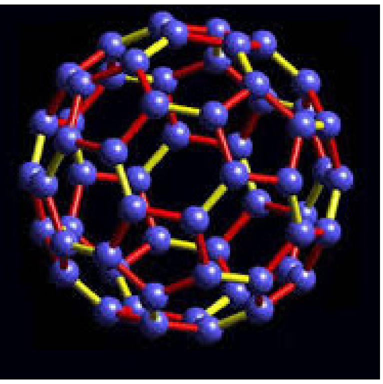
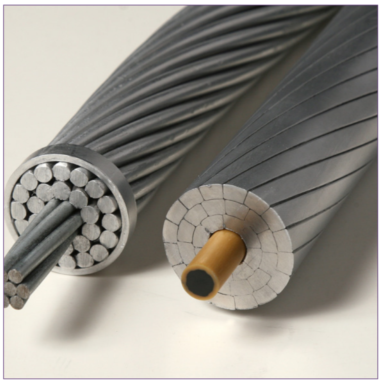
Poster Presentation

Materials Chemistry 2019







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Comparative quantum chemical and dynamic Monte Carlo investigations of the cytisine derivatives as green inhibitors for corrosion protection of carbon steel in HCl medium.

Aziz Aboulmouhajir, K Sadik and **N El Hamdani**
Hassan II University, Morocco

The corrosion of metals and their alloys, which is harmful to the environment, limits industrial processes by efficiency as well as by cost. Green corrosion inhibitors are currently the most sought after, because of their availability, their lower cost, their biodegradability, the respect of health and environmental standards and, above all, their extremely high efficiency. This work focused on the theoretical study of the reactivity of the three major constitutive of alkaloids namely Cytisine, Dehydro cytisine and N-methyl cytisine - extracted from seeds of *Retama Monosperma (L.) Bois*s, a very abundant medicinal plant in the Abda-Doukkala region of Morocco - as green metal corrosion inhibitors [1-2], with the aim of rationalizing the relationship between their molecular structure and their inhibitory efficiency. In addition to the investigation of regioselectivity and competitiveness between neutral and protonated entities in aqueous media, global reactivity was quantified by a variety of molecular quantum descriptors, while local reactivity was followed by Fukui indices and molecular electrostatic potential. Both global and local reactivity show a notable competition between the three inhibitors, with a priority of Cytisine in both gas and aqueous phases. Moreover, in order to approach the interaction mechanics between molecule and metal surface and quantify the nature and the adsorption strength of the complex formed, we have used quantum mechanics as well as dynamics Monte Carlo simulation. All quantum calculations were done in B3LYP with the aug-cc-pvdz basis set and the C-PCM solvation model.

Speaker Biography

Aziz Aboulmouhajir has completed his PhD in Molecular Modeling and spectroscopy, at the age of 25 years from Instelling Antwerpen University in Belgium with High Distinction. He is holder of the STAS Prize of the Royal Academy of Sciences, Letters and Arts of Brussels, in Belgium. For the last ten years, he was head of the Molecular Modeling and Spectroscopy E2MS Team at Chouaib Doukkali University. He is currently professor and director of several thesis projects in Molecular Recognition and spectroscopy in Hassan II University (Morocco).

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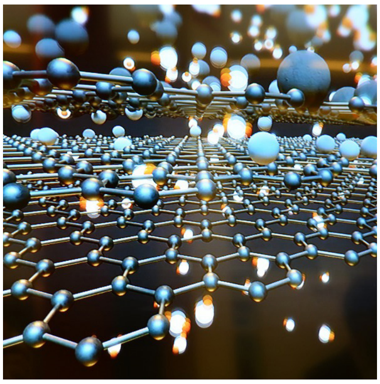
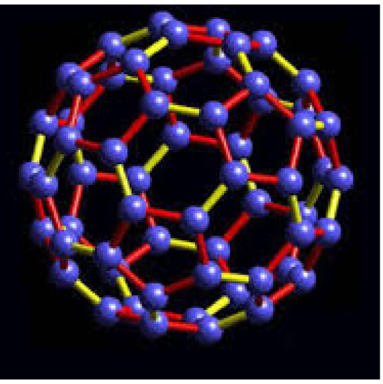
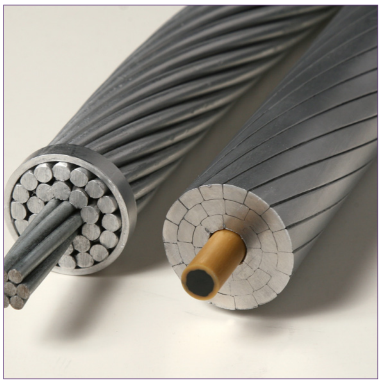
Video Presentation
March 21, 2019

Materials Chemistry 2019







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Global crisis/sustainability technologies - in actuator/piezoelectric devices

Kenji Uchino
The Penn State University, USA

There are four factors that have influences on engineering: Social/culture/religion, Technology/science, Economics, and Politics/law. The strength of the impact of these factors becomes different according to history. Alchemy of the 16th century is an example of “Socio-Engineering”. From the Christian doctrine, “Heliocentric model” was denied, but “alchemy” was approved. Religion was controlling science. In the 17th-18th centuries, people were solved from the spell of religion and engineering based on science and technology, so-called “Techno-Engineering” is respected instead. In the 18th-19th centuries, technologies for mass production at low manufacturing cost were required and “Econo-Engineering” became mainstream to enhance national strength. The intention of increasing national wealth and military strength increased friction and that led to the First and Second World War in the 20th century. Engineering of this period is mainly government-led production of war weapons, and it was a beginning of “Politico-Engineering”. After the wars, mass production technologies for the reconstruction/recovery revived, but when the 21st century began, as a consequent result, environmental degradation, resource depletion, and food famine have become major problems. Global regulations are strongly called, and the government-initiated technology (“politico-engineering”) has become important again in order to overcome the regulations. Politico-Engineering covers (1) legally-regulated normal technologies such as sustainability, and (2) crisis technologies.

Speaker Biography

Kenji Uchino a pioneer in piezoelectric actuators, is Director of International Center for Actuators and Transducers. He is also the founder and Senior VP & CTO of Micro-mechatronics, Inc. Prior to joining Penn State in 1991, he was a Research Associate in the physical electronics department at Tokyo Institute of Technology. He joined Sophia University, Japan, as an Associate Professor in physics in 1985. He was also involved with Space Shuttle Utilizing Committee in NASDA, Japan, and Vice President of NF Electronic Instruments, USA. He is the Chair of Smart Actuator/Sensor Study Committee sponsored by Japanese MITI. He was the associate editor for Journal of Advanced Performance Materials, J. Intelligent Materials Systems and Structures, and Japanese Journal of Applied Physics. He has authored 550 papers, 54 books and 26 patents in the ceramic actuator area.

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Notes:

Plasmonic nanostars: A golden platform for medical diagnostics and photo immunotherapy

Tuan Vo-Dinh
Duke University, USA

An overview of recent developments in our laboratory for plasmonics-active gold nanostars (GNS) have been developed and applied for multifunctional cancer diagnostics and therapy (theranostics) will be provided. Plasmonics refers to the research area of enhanced electromagnetic properties of metallic nanostructures that produce ultrasensitive and selective detection technologies. The technology involves interactions of laser radiation with metallic nanoparticles, inducing very strong enhancement of the electromagnetic field on the surface of the nanoparticles. These processes, often called 'plasmonic enhancements', produce the surface-enhanced Raman scattering (SERS) effect that could enhance the Raman signal of molecules on these nanoparticles more than a million-fold. The SERS technology can be used to directly detect chemical species and biological species with exquisite sensitivity for biomedical diagnostics.

A SERS-based nanoprobe technology, referred to as 'Molecular Sentinel' nanoprobes, has been developed to detect DNA targets of pathogenic agents (e.g., HIV) and biomarkers of diseases (e.g., BRCA1, ERB2 breast cancer genes). Other plasmonic platforms, such as gold nanostars, offer plasmon properties that efficiently transduce photon energy into heat for photothermal therapy. Nanostars, with their small core size and multiple long thin branches, exhibit intense two-photon luminescence, and high absorption cross sections that are tunable in the near infrared region with relatively low scattering effect, rendering them efficient efficient photothermal agents in cancer therapy. A theranostic nanoplatform construct was created, allowing SERS imaging and photodynamic therapy. SERS-based plasmonic nanoprobes and nanochip systems have also been developed for use as diagnostic systems for point-of-care personalized nanomedicine and global health applications.

Gold nanostars can be used for photothermal therapy and immunotherapy. GNS- mediated photothermal therapy combined with checkpoint immunotherapy —a treatment we referred to as Synergistic Immuno Photothermal Nanotherapy (SYMPHONY)— has been found to reverse tumor-mediated immunosuppression, leading to the treatment of not only primary tumors but also cancer metastasis as well as inducing long-lasting immunity, i.e. an anti-tumor 'vaccine' effect in murine model.

Speaker Biography

Tuan Vo-Dinh is a distinguished Professor of Biomedical Engineering, Professor of Chemistry, and Director of the Fitzpatrick Institute for Photonics. His research activities and interests involve biophotonics, nanophotonics, plasmonics, laser-excited luminescence spectroscopy, room temperature phosphorimetry, synchronous luminescence spectroscopy, surface-enhanced Raman spectroscopy, field environmental instrumentation, fiber optics sensors, nanosensors, biosensors and biochips for the protection of the environment and the improvement of human health.

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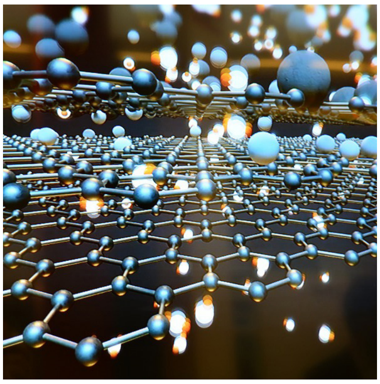
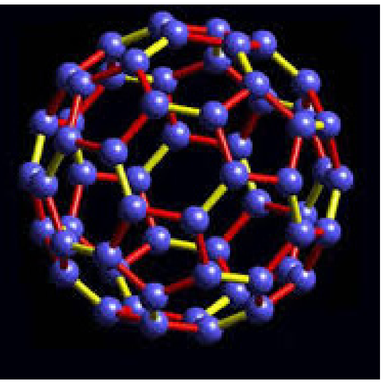
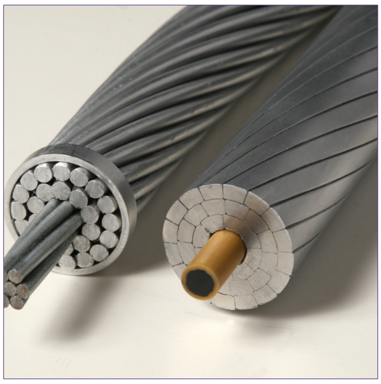
Accepted Abstracts

Materials Chemistry 2019







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Comparative study of cytotoxic and genotoxic effects of uncoated and poly-ethylene glycol-coated gold nanoparticles on human kidney cells

Tchounwou PB, Rogers C and **Patlolla A**
Jackson State University, USA

Gold nanoparticles (AuNPs) have generated a substantial amount of scientific and technological interest due to their ease of synthesis, chemical stability, and unique optical properties. Numerous empirical studies demonstrate their biomedical applications in chemical sensing, biological imaging, drug delivery, and cancer treatment. In considering these applications, biocompatibility and the absence of cytotoxicity of AuNPs are essential. Comparative studies were conducted to investigate whether 25-35 nm poly (ethylene glycol) (PEG) coated and uncoated AuNPs are more or less cytotoxic and genotoxic to human kidney(HK-2) cells. Cytotoxicity, oxidative stress, and genotoxicity were evaluated by the MTT assay, dichlorofluorescein (H_2DCF) assay, and single cell gel electrophoresis, respectively. Results showed that uncoated Au particles significantly reduced cell viability and were cytotoxic with an IC50 concentration of 100µM whereas, the PEG coated AuNPs displayed low toxicity even at a high dose of 200µM after 24-hour exposure. Uncoated AuNPs increased reactive oxygen species concentration (ROS), decrease GSH production, and depolarize the mitochondrial membrane potential in a concentration-dependent manner. PEG AuNPs produced no notable increase in ROS or deceased in GSH along with negligible polarization of the mitochondrial membrane potential. PEG AuNPs showed insignificant genotoxic effect of DNA damage represented by 1.07% in comparison to 37.4% exerted by uncoated AuNPs. Overall these findings show that uncoated AuNP appear to be more cytotoxic and more genotoixis than PEG coated AuNPs. of cytotoxicity and genotoxicity of PEG coated AuNP compared to uncoated AuNP will have beneficial clinical implications for application in nanobiotechnology and nanomedicine.

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Thread-like CMOS logic circuits using SWCNT transistors for e-textile systems

Insoo Kim
University of Connecticut, USA

Recently, wearable electronic textile (e-textile) devices have been spotlighted for next generation smart devices and systems because of their unique advantages such as light, deformability in movement, and wide range application with various fields. Fibre-based electronics, formed directly on textile substrates, is the one of most desirable features required for wearable e-textile since we can integrate sensing and processing circuitry onto the garments.

Typical fibre-based electronics can be formed on a premade two-dimensional (2-D) fabrics. The most advantage of this approach is that device fabrication process is similar and compatible with conventional silicon-based process technology. However, due to the rough surface morphology and weakly interfacial adhesion between the deposited film and fabric, 2-D fabric electronics are limited in terms of device performance and integration with a large scale electronics. Another approach is forming transistors on a thread-like cylindrical single fibre. Since the transistors are formed on the thread, there is no performance degradation due to the rough surface. Furthermore, the fabrication process of the thread-like fibre electronics is compatible with the existing textile fabrication process - a simple reel-to-reel process and weaving technology. Thus, we can easily integrate e-textile with conventional garments.

However, integration of logic-gates and large-scale circuits using the thread-like electronics is still challenging. This limitation greatly prohibits the use of the thread-like electronics in practical applications. We previously demonstrated thread-like single-walled carbon nanotube (SWCNT) fibre-type thin-film transistors (TFTs) as well as CMOS logic circuits using the SWCNT TFTs using partial reel coating and selective doping process. In this talk, we will introduce the fabrication process of SWCNT TFTs and dynamic operation of the CMOS logic circuits based on SWCNT TFTs. We will also discuss SPICE simulations techniques about how to optimize threshold voltage, contact resistance, off-/gate leakage current of the TFTs.

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Notes:

Device for testing the performance of a hydrogen sensor modified from the morris prototype

Jair Gibran Arenas Salcedo
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A hydrogen permeation sensor based on the Morris prototype was designed, constructed and tested in this work. The cylinder was changed from a disc shape to a parallelepiped shape to facilitate the adhesion of the Nafion membrane and to decrease the potential H leakage on the edges of the cylinder. To test the ability of the sensor to detect hydrogen permeation, a device was designed that comprised two interconnected cells operating simultaneously. This device detects the permeation of H by the sensor and the potential reduction of a passive film. The sensor was calibrated, and the calibration curve was shown to be consistent with the Nernst equation.

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Magnetic field influence on the silica particles size utilizing modified sol-gel method

Amer Karnoub
University of Aleppo, Hungary

In this study, well-dispersed silica nanoparticles with a diameter reach less than 1 nm were prepared via a modified sol-gel method. The modulation of particles size was utilized through directing strong magnetic fields (0.5- 3T), on the silica sol, during the polycondensation process. Through controlling the preparation conditions; pH, magnetic field strength and exposure time, the silica nanoparticles size, which suspend in the sol, were decreased or increased accordingly.

Effects of magnetic field on the particle size and particle size distribution of silica sols were examined by means of dynamic light scattering. XRD spectra showed crystalline features for some silica sol coated films that were dried at room temperature.

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Computer analysis of the microporous structure of activated carbons prepared from plant materials by chemical activation

Mirosław Kwiatkowski
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The work presents results of the analysis of the microporous structure of activated carbons obtained from plant materials by chemical activation with potassium hydroxide. The aim of the research was to evaluate the impact of the hydroxide to biomass mass ratio on the microporous structure of the obtained activated carbons. The calculations were carried out using the BET and DR methods, as well as the new LBET method with the unique fast multivariant identification adsorption systems procedure. The obtained results of the research highlighted the significant potential of the production of activated carbons with very high adsorption capacity and large specific surface area from plant materials, by chemical activation with potassium hydroxide. Moreover the presented research yielded a broad spectrum of information and shed a new light on the issues pertaining to the assessment of the effect of carbonaceous adsorbent production technology on the obtained parameters of the porous structure.

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Mechanical behaviors of gas hydrate system: Ongoing development of phase-transition mechanics

Fulong Ning
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Natural gas hydrates are ice-like crystalline substances in which gas molecules are physically trapped inside the polyhedral cavities of water molecules1–3. They occur abundantly in both petrochemical production lines4 and hostile environments such as seafloor sediments, arctic or permafrost regions and even the surfaces of other planets. Natural gas hydrates distribute widely in the offshore marine sediments and onshore permafrost area under specific low temperature and high-pressure conditions. Over the last few decades, much attention has been directed toward them as energy resources and for their environmental impact. Understanding the mechanical behaviors of gas hydrate-bearing sediments (GHBS) is important for their associated applications in wellbore stability, stratum deformation during exploitation, geological disaster prevention, and the risk assessment of replacing CH_4 with CO_2 in hydrate reservoirs and CO_2 sequestration in oceans. In our work, we reveal the mechanical mechanism of gas hydrate system at microscale level using molecular dynamic simulations, AFM and CT scan, investigate the static and dynamic mechanical responses at the lab scale using direct shear tests and sonic measurements. Then we used our mechanical correlation into the wellbore and reservoir stability evaluation at the filed scale. Here we firstly propose the conception of phase transition mechanics which mainly investigate phase transition behaviors caused by force, and mechanical response and flow behavior during phase transition procedure by taking gas hydrate for instance.

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Morphology of silver particulate films on polymer composite

Pratima Parashar Pandey
IILM, India

The morphology of silver particulate films, can be characterized by their size, size distribution, shape and inter-particle separation. These can be modified by blending of polymers along with the amount of silver deposited. on them. Polymer blends (PS/PVP/P2VP/P4VP) were prepared through solution blending by mixing in a common solvent, Dimethylformamide (DMF). and distilled water. at room temperature. Blends of polymer composite with different compositions ranging from 0 to 100 % were prepared. Silver films of various thicknesses were deposited on these polymer composites held at 457 K in a vacuum better than 8×10^{-6} Torr at the deposition rate of 0.4nm/s. Morphological studies were carried out by Optical absorption spectra and Scanning electron micrographs of the silver particulate films.

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Role of trioctylphosphine on quantum size effect in Ni nanolattice

Gunadhor S Okram
UGC-DAE Consortium for Scientific Research, India

Nickel nanoparticles are of special interest for their attractive potential applications in magnetic resonance imaging, magnetic fluids, catalysts, magnetic recording media, rechargeable batteries, optoelectronics, conducting paints, magnetic hyperthermia, and other biomedical applications. When these nanoparticles are dispersed in a liquid medium for example, they tend to agglomerate/ disperse due to van der Waals or other attractive forces. Similarly, what kind of forces they may need to form their own periodic lattice in solid state and how this will influence their overall properties may be intriguing. We have investigated some of these aspects. They revealed that trioctylphosphine is responsible for their nanolattice formation, how the Ni atoms are arranged in these nanoparticles, how their electronic density of states changes, nearest-neighbour atoms are changed with particle size and why their quantum size effect is unique in heat capacity, not in electronic or magnetic properties. Some of these shall be discussed briefly.

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Polymer - Lipid hybrid nanovehicles designed for synergistic drug delivery for solid tumor management

Madhu Gupta
Delhi Pharmaceutical Science and Research University, India

Efficient dual targeted chemotherapy is an attractive approach for killing the tumor cells and tumor endothelial cells, while sparing the normal tissue. Herein, we investigated whether encapsulation of paclitaxel (PTX) within polymer–lipid hybrid nanoparticles conjugated with kNGR (PLNs-kNGR) achieved this goal in a subcutaneous tumor induced Balb/c mice bearing HT-1080 tumor model with nanocarrier-modified biodistribution and toxicity. The dual targeted PLNs-kNGR was prepared by modified nano-precipitation technique combined with self-assembly and evaluated for different parameters. Compared with other tested NPs, PLNs-kNGR-NPs revealed more cytotoxicity by inducing more apoptosis, higher intracellular uptake and % tumor volume inhibition rate that was 59.7%. These findings substantiate the importance of rational design of nanoparticles for dual targeting synergistic therapy. As a consequence, the PLNs-kNGR-NPs play a key role in enhancing tumor therapeutic efficiency for treatment of CD13 receptor specific solid tumor.

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The Hajjar regional transpressive shear zone (Guemassa Massif, Morocco): Consequences on the deformation of the base-metal massive sulfide ore

Safouane Admou
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The genesis of the base-metal massive sulfide deposits hosted within the Moroccan Hercynian Jebilet and Guemassa Massifs is still under debate. No consensus currently exists between the two models that have been proposed to explain the deposits, i.e., (1) syngenetic volcanogenic massive sulfide mineralization, and (2) synmetamorphic tectonic fluid-assisted epigenetic mineralization. Conversely, researchers agree that all Hercynian massive sulfide deposits in Morocco are deformed, even though 3D structural mapping at the deposit scale is still lacking. Therefore, while avoiding the use of a model-driven approach, the main aim of this contribution is to establish a first-order structural pattern and the controls of the Hajjar base metal deposit. We used a classical structural geology toolbox in surface and subsurface mining work to image finite strain at different levels. Our data demonstrate that: i) the Hajjar area is affected by a single foliation plane (not two) which developed during a single tectonic event encompassing a HT metamorphism. This syn-metamorphic deformation is not restricted to the Hajjar area, as it is widespread at the western Meseta scale, and it occurred during Late Carboniferous times; ii) the Hajjar ore deposit is hosted within a regional transpressive right-lateral NE-trending shear zone in which syn- to post-metamorphic ductile to brittle shear planes are responsible for significant inflexion (or virgation) of the foliation yielding an anastomosing pattern within the Hajjar shear zone. Again, this feature is not an exception, as various Late Carboniferous-Permian regional scale wrenching shear zones are recognized throughout the Hercynian Meseta orogenic segment. Finally, we present several lines of evidence emphasizing the role of deformation in terms of mechanical and fluid-assisted ore concentrations.

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Experimental and quantum study of anticorrosive activity and biological activities of natural and synthetic substances

Belkheir Hammouti[1], A Salhi [1,2], A Bouyanzer[1], T Ben Hadda[3], H Amhamdi[2], A Zarrouk[4]
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The present work is devoted to the study of the inhibition of corrosion of mild steel, antioxidant activity and antimicrobial effect for plant extracts and synthetic products. Theobjective is, on the one hand, to contribute to the valorization of three plants that growthspontaneously in the region of the Rif, Morocco. On the other hand, to evaluate the potentialitiesof synthetic compounds. The experimental studies carried out were corroborated by thetheoretical study in order to develop a correlation between the results obtained from theexperimental measurements and the effect of the molecular structure using the DFT method. The anticorrosive effect was evaluated in a molarhydrochloric acid environment using gravimetric and electrochemical methods. Theexperimental results showed that the inhibitors tested showed good corrosion inhibition. In vitro evaluation of the antioxidant activity of the various phenolic extracts of threeplants and the synthetic phenolic compounds was carried out by three methods: trapping the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical, the β-carotene bleaching (βCB) and the ferric reducing antioxidant power (FRAP). Thus, the results obtained have shown that the antioxidant activities are interesting and aredependent on the content of phenolic compounds. The various extracts and synthetic compounds were also screened for their possibleantimicrobial activity against different strains. This evaluation was carried out by the methodof diffusion of the disc on Muller-Hinton Agar (MHA). In this work, the Pistacialentiscus showed good activity antimicrobial against most ofthe strains tested. In addition, the synthetic compounds have been found tobe interesting with encouraging potential. Thus, the study of electronic properties by the DFT method suggested that the antifungal effect of the synthetic compounds is correlated with the molecular structural effect.

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Modification to metal matrix composites designation system

Babalola Philip Olufemi
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Metal matrix composite (MMC) are engineered materials made from a metal and another conventional material like ceramic, carbon and hard or soft metal. However, MMCs with Aluminium as the matrix predominates all other metals combined. Hence, Aluminium Association developed a standard system of designating MMCs to clarify the matrix, reinforcement, percentage composition and the form of reinforcement. This paper reviewed the existing standard by adding information on the size of the reinforcement which was found to have a remarkable effect on the produced MMC. Other researchers corroborated the effect of particle size on MMC and should not be neglected when identifying the composites.

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Study on mechanical properties and corrosion resistance of Mg-Zn-Nd alloys as potential biodegradable implants

Orly Hakimi
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Mg alloys are considered as potential structural materials for biodegradable implants mainly due to their excellent biocompatibility, degradation behavior in in vivo conditions and adequate mechanical properties. However, their accelerated corrosion rate in physiological environments may lead to premature loss of mechanical integrity, gas embolism and cytotoxic effects.

Here we characterized the corrosion behavior and mechanical properties of a novel magnesium-zinc alloy, Mg-5%Zn-0.13%Y-0.35%Zr with up to 3% Nd additions following a homogenizing treatment and extrusion process, with regards to serving as a biodegradable implant. The microstructural characteristics were examined by optical microscopy, scanning electron microscopy (SEM), and X-ray diffraction analysis. The corrosion performance examination was carried out under in in vitro conditions, including immersion testing, electrochemical analysis, and stress corrosion cracking (SCC) assessments in terms of slow strain rate testing (SSRT), all in PBS solution. The mechanical evaluations included hardness and tensile examinations. The obtained results clearly demonstrated an optimal combination of strength and ductility for the new alloy at 2% Nd concentration. This was attributed to an optimal concentration of the secondary phase, W-phase ($Mg_3(Nd,Y)_2Zn_3$), generated at grain boundaries. The addition of different concentrations of Nd to the base alloy, resulted in minor effect on the corrosion resistance, nevertheless, the calculated corrosion resistance of all tested alloys was within the range which can be considered as suitable for biodegradable applications. Therefore it is believed that the new alloy at 2% Nd concentration, Mg-5Zn-2Nd-0.13Y-0.35Zr, can be considered as a potential candidate for biodegradable implants.

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