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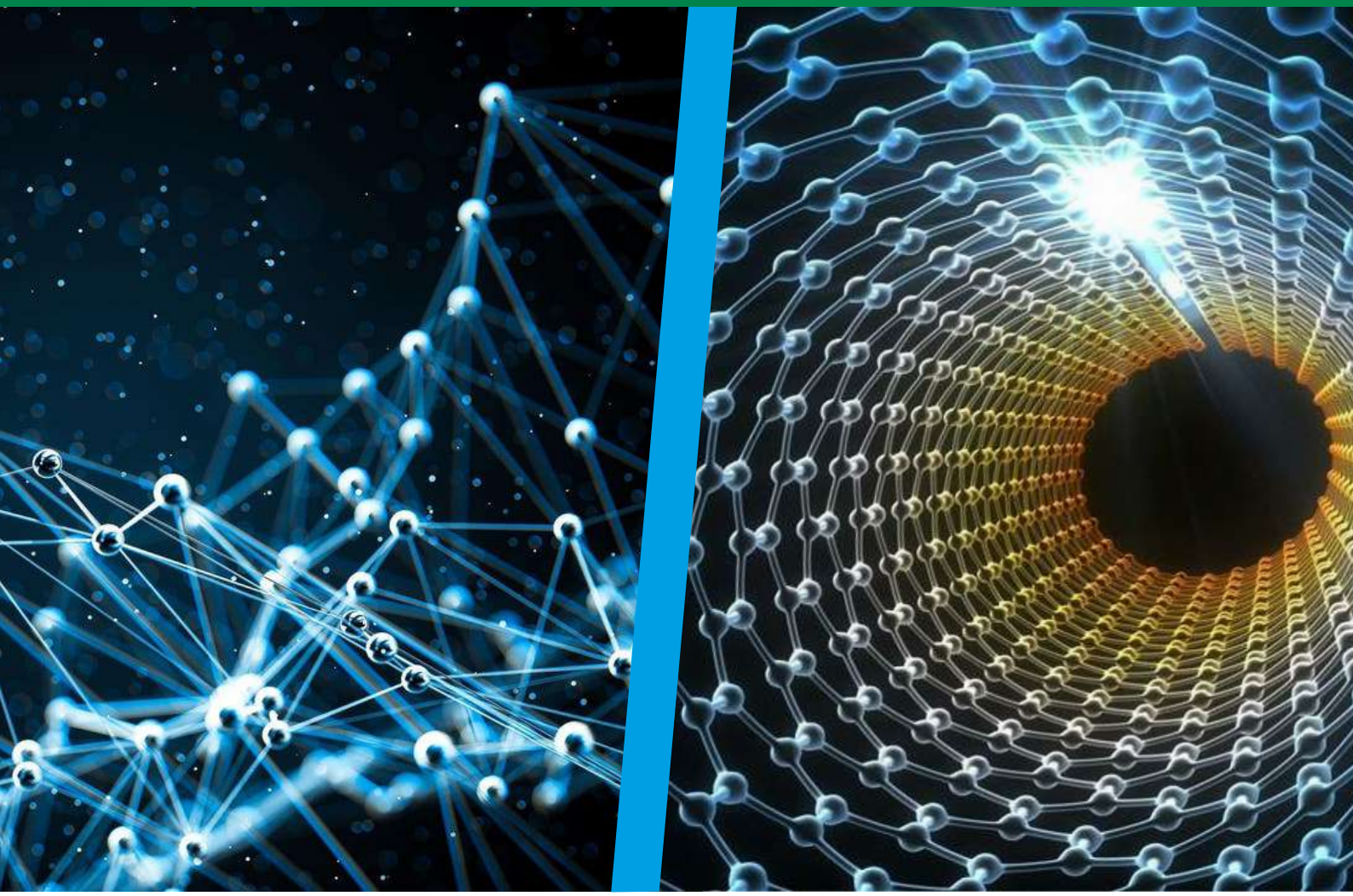
CONMAT2022

2nd Global Summit on Condensed Matter Physics

GSEMSN2022

2nd Global Summit and Expo on Materials Science and Nanoscience

October 17-19, 2022 **Dubai, UAE**



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FOREWORD

Conference Chair Welcome Message:

On behalf of the Organizing Committee it is our pleasure to welcome all the participants of the 2nd Global Summit on Condensed Matter Physics (CONMAT2022) to be held in Dubai, UAE during October 17-19, 2022.

As is well-known - Condensed Matter Physics has a specific goal of understanding the structure and properties of all kinds of solids and liquids (including liquid crystals). It is a very broad and lively area of research in modern physics, where one observes frequent occurrence of novel phenomena, relating to exotic properties of matter in metals, semiconductors, superconductors, magnets, insulators, and mesoscale systems among many others.

Due to intense research all over the world in the whole CMP area, new ideas and novel materials are created every now and then. Needless to say, today CMP is one of the main pillars of high technology. In this highly active area CONMAT2022 intends to cover a few selected topics to be presented by well-known experts of this field. We also encourage young researchers to participate, present their recent research work and interact with other co-participants.

Prof. Dr. Mukunda P. Das
Chair, CONMAT2022
The Australian National University
Canberra, Australia

FOREWORD

Dear Colleagues,

It is a great pleasure to announce that The Scientistt will host the 2nd Global Summit and Expo on Materials Science and Nanoscience (GSEMSN2022) will be held in Dubai, UAE during October 17-19, 2022.

GSEMSN2022 aims to bring together the renowned researchers, scientists and scholars to exchange ideas, to present sophisticated research works and to discuss hot topics in the field and share their experiences on all aspects of Materials Science and Nanoscience.

The GSEMSN2022 will be a 3 days event that means to gather the key players of the materials science and nanoscience community and related sectors. This event is launched with the aims to become an established event, attracting global participants, intent on sharing, exchanging and exploring new avenues of Materials Science and Nanoscience-related scientific and commercial developments.

A wide-ranging scientific program consisting of plenary lectures, keynote lectures, Invited lectures, parallel sessions, as well as poster sessions for young scientists covering all topics in Materials Science and Nanoscience will be scheduled. This conference provides a wonderful opportunity for you to enhance your knowledge about the newest interdisciplinary approaches in Materials Science and Nanoscience.

Moreover, the conference offers a valuable platform to create new contacts in the field of Materials Science and Nanoscience, by providing valuable networking time for you to meet great personnel in the field.

We look forward to seeing you at GSEMSN2022 in Dubai, UAE.

COMMITTEES

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N.R. Cameron
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Porous Polymers as Scaffolds for Tissue Engineering and 3D Cell Culture

Abstract
The presentation will discuss some of our work on the development of highly porous polymeric materials as scaffolds for 3D cell culture, tissue engineering and regenerative medicine. The materials are produced by a technique known as emulsion templating, which generates porous polymers (polyHIPEs) with a very well-defined and fully interconnected network of pores in the size range 10-100 microns. Features such as the pore diameter, degree of interconnection, porosity, mechanical properties and surface chemistry can be varied to produce materials tailored for different applications. The main focus of the presentation will concern recent work on the development of degradable materials intended for tissue engineering and regenerative medicine applications. These are produced by light-activated thiol-ene network formation, which, due to the speed of cure, can be adapted to 3D printing (stereolithography) platforms. Recent results from current projects focussing on a range of tissue engineering/regenerative medicine applications, including human neural precursor cells, human pluripotent stem cells, hematopoietic stem cells, osteoblastic cells and endometrial cells, will be presented.

Keywords
Polymers, tissue engineering, scaffolds, biomaterials

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Biography
Prof. Neil Cameronis Head of the Department of Materials Science & Engineering at Monash

University (Australia) and is also the Monash Warwick Alliance Professor of Polymer Materials. His research is focused on the preparation of novel polymeric materials, with particular emphasis on scaffolds for 3D in vitro cell culture and tissue engineering, self-assembling polypeptides, peptide-synthetic polymer hybrids and sugar-containing polymers (glycopolymers). His research has led to the publication of >170 papers and he has given >160 invited lectures at conferences and colloquia.

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Magnesium Alloys as the Third Generation of Human Implants

Abstract
The Magnesium alloys are considered as the third generation of novel promising materials to design biodegradable and resorbablehuman medical implants, which combine bioactivity and biodegradability of their surfaces during their exposure to physiologial environments. The recent advancement in reducing the rapid degradation of Mg-implants is linked with the introduce of Ca as an alloying elements. The increasing fight against bacterial infections during the surgery requires the development of medical devices and materials with antimicrobial properties. Several studies have revealed the antimicrobial efficiency of Ag-nanoparticles (NPs), although the mechanism of their effect is not yet fully understood. Thus, the deposition of Ag-NPs on Mg-alloys surface could be one approach to provide antimicrobial protection for the implantable medical device surface, to combat associated infections.This work resumes the application of several non-destructive electrochemical techniques, used to characterize the dynamic of the initial stages of the corrosion process of Mg, Mg-Ca and AZ Mg-alloys, when exposed to Ringer, Hank and SBF media. The results are correlated with those of surface analysis. The antibacterial effect against the Staphylococcus aureus and Escherichiacoli bacteria on Mg-Ca0.3 in the presence of Ag-NPs deposits in different size is reported also.

Keywords
Magnesium alloys; biodegradation; physiological media; silver nano-particles; antibacterial tests; corrosion tests.

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Biography
Lucien Veleva has completed his PhD at the age of 30 years from Institute of Physical Chemistry in Sofia, Bulgaria. Actually she is Professor at Applied Physic Department (CINVESTAV-IPN, Mexico), since 1994, responsible for Laboratory of Physical Chemistry. She has published more than 80 papers in reputed journals (Impact Factor), Book on Corrosion and Materials Degradation, 4 Patents and chapters in International Books and in 2011 has honored with Doctor Honoris Causa, Francis

LaQue Award of ASTM (2012), International Distinguished Career NACE Award (2013), Service Recognition Award of ASTM for Nondestructive Testing (2017). She has been supervising PhD and MSci thesis.

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Integrating Sustainable Practices into Organic Electronics Research

Abstract
Sustainability is becoming a crucial element for companies, because of ever more stringent regulatory requirements worldwide. The efforts in integrating sustainable practices into organic electronics R&D started to become evident in the past decade. However, despite significant results have been already achieved [1,2], there is the need for green organic electronics technologies that can be pursued through diverse but complementary approaches.
Here we present how we arecontributing towards the paradigm shift from traditional organic thin-film transistors (OTFT) production technologies and practices to one that assigns value to waste minimization, avoiding the use of substances that pose serious risk to human health and the environment, and preferring the use of renewable resources and industrial waste streams.[3-6]
Besides the very promising results obtained, this contribution intends to withdraw the attention of researchers from multiple disciplines that green conditions and materialscan be properly selected and adequately play a role in influencing the efficiency of an electronic device, while driving up a more sustainable technology.

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A Network Breakdown Model for a Tumor Microenvironment

Abstract
Tumor hypoxia was discovered a century ago, and the interference of hypoxia with all radiotherapies is well known. Here, we demonstrate the potentially extreme effects of hypoxia heterogeneity on radiotherapy and combination radiochemotherapy. We observe that there is a decrease in hypoxia from tumor periphery to tumor center, due to oxygen diffusion, resulting in a gradient of radiative cell-kill probability, mathematically expressed as a probability gradient of occupied space removal. The radiotherapy-induced break-up of the tumor/TME (Tumor Micro Environment) network is modeled by the physics model of inverse percolation in a shell-like medium, using Monte Carlo simulations. The different shells now have different probabilities of space removal, spanning from higher probability in the periphery to lower probability in the center of the tumor. Mathematical results regarding the variability of the critical percolation concentration show an increase in the critical threshold with the applied increase in the probability of space removal. Additionally, calculations on networks using this key idea of different removal probabilities, also show the hampering of the network breakdown as described in terms of the largest remaining clusters and their size distributions. Such observations will have an important medical implication: a much larger than expected radiation dose is needed for a tumor breakup enabling successful follow-up chemotherapy. Information on the TME's hypoxia heterogeneity, as shown here with the numerical percolation model, may enable personalized precision radiation oncology therapy.

Tayfun Babadagli
University of Alberta, Canada

Use of Nano-Materials and New Generation Chemicals in Heavy-oil and Bitumen Recovery to Improve Efficiency and Reduce GHG Emission

Abstract
Future depletion of heavy-oil reserves requires more efficient (low cost but high recovery) and low GHG (greenhouse gas) emission methods. Steam injection is predominantly used in heavy-oil recovery followed by cold production methods. The former has limitations due to high cost and environmental problems while the latter is more environmentally friendly but less efficient caused by low production. One of the ways to improve the efficiency and reduce the amount of steam injected (and GHG emissioncaused by steam generation) is toapply additives to steam (or hot water) such as nano-materials (nano-metal particles, nano-solutions, and nano-based smart materials) and chemicals (solvents, ionic liquids, polymers, surfactants, alkalis, amines, enzymes, alcohols, and ethers). Some of these materials have also been tested as additives (to water or solvent) during electro-magnetic heating, which is more applicable in unfavorable environmentssuch as deep reservoirs, tight formations, and oil shales. The optimal use of these materials as additives to improve the heavy-oil recovery efficiency is discussed with evidences from laboratory experiments (tube tests, micro model and core flooding tests).Also covered in this talk isthe additives used in non-thermaloperations such as cold production and solvent applications for the depletion of heavy-oil reserves.Specifically, nano-materials used to generate Pickering emulsionsare compared with conventional surfactants. After discussing the performance of the above-mentioned additive materials for different conditions, suggestions are made as to cost efficient field applications and future research work.

Keywords
Heavy-oil, recovery efficiency, nano-materials, new generation chemicals, GHG emission reduction.

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Point Defects in AlN and GaN for Quantum Information Processing: An ab initio Insight

Abstract
Point defects in wide band gap semiconducting materials and insulators have been found as robust and promising candidates for quantum information processing applications. In particular, the negatively charged nitrogen-vacancy centre in diamond (NV^{1-}) is a prototype solid state quantum bit for which a complete theory on spin polarization cycle has been developed and a number of experimental reports demonstrated a coherent optical spin control and readout procedures of individual electron spin in NV^{1-}. Numerous defects exhibiting qubit-like properties were proposed in other semiconductors such as silicon carbide (SiC), hexagonal boron nitride (h-BN) or silicon. Wurtzite aluminium nitride (AlN) and gallium nitride (GaN) are direct wide band gap materials capable of accommodating highly localized defect states; therefore, they can be promising hosts for qubits or single photon emitters. To the best of our knowledge, there are only three defects in AlN that were reported as quantum bits like NV^{1-} in diamond, i.e., V_N^{1-}, $Ti_{Al}V_N^{1-}$ and $V_{Al}O_N$. Although the level structure and spin state of these complexes is indeed similar to NV^{1-}, a significantly lower photoionization threshold than internal optical excitation energy of $V_N^{1-}$and $Ti_{Al}V_N^{1-}$, poor charge stability of the defects with respect to Fermi energy and the necessity of p type AlN to stabilize the desired charge and spin state of $V_{Al}O_N$ rule them out from the family of qubits. Here, we investigate a serious of point defects in AlN and GaN by using the-state-of-the-art hybrid spin-polarized density functional theory (DFT) calculations. We determine the level structure, stability, optical and magnetic properties of these defects. We report a singlet spin state positively charged nitrogen-vacancy defect (V_N^{1+}) in AlN that exhibits remarkable stability across wide range of Fermi energies and possesses proper electronic structure to act as quantum memory like qubit similar to ST1 center in diamond and recently reported carbon defect in two-dimensional WS_2. We further develop defect engineering procedure by complexing V_N^{1+} with isoelectronic scandium cation substitution (Sc_{Al}) to further localize the defect wavefunctions and enhance the intersystem crossing rates by spin orbit coupling (SOC). We find the exceptional charge and optical stability of $Sc_{Al}V_N^{1+}$ and relatively low formation energy that can facilitate the introduction of this complex in desired concentration. When it comes to single photon emitters, native point defects are highly unlikely to be responsible due to significant electron-phonon coupling and as a result, large Huang-Rhys factors. On the other hand, the first raw transition metals at cation site of AlN or GaN have a proper electronic structure and exhibit a very narrow emission originating from spin flip transition within 3d manifold. We demonstrate a positively charged Cr_{Al} in AlN and Cr_{Ga} in GaN as a source of strong single photon emission around 1.2 eV reported experimentally.

Keywords
Point defects; AlN; GaN; ab initio; quantum information processing

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Development of VO2 -based Composite Thin films, Related Apps

Abstract
VO2, a famous Phase Change Materials (PCMs), exhibits an insulator-metal transition (MIT) characterized by the reversible switching between two crystalline phases (monoclinic to rutile), which generates huge variations of the physical properties in a relatively narrow range of temperatures, near 68°C. Due to this strong non-linear behavior and it associated hysteresis, vanadium dioxide is of great interest for many applications where the successful integration of this “smart” material leads to achieve “smart” micro-devices in microelectronics, photonics or thermal applications.Pulsed Laser Deposition (PLD) is well recognized for the synthesis of thin films and composites presenting very good quality, particularly for oxide materials and consequently for VO2. We developed conventional classical PLD set-up and a more specific Pulsed LaserNanoparticle Source (PLNS).In this communication, we will emphasize the efficiency of the laser-based processesto buildVO2-based specific architectures. In the temperature range of 20°C-90°C,VO2composites with large magnitude of change in physical properties will be investigated(up to 5 orders for resistivity, more than 75% at 3µm for near-IR optical transmission[1] and variation of 43% for the emissivity). Related to these composites, thermal[2], electrical or optical activations will be discussed. Different VO2-based smart micro-devices will be presented, from the first realized Radio Frequency-Switchesto more complex recent Phase Shifters, Reflect-Array Antennae or Thermal Diodes.

Keywords
VO2 thin films & composites, Pulsed laser-based processes, VO2 micro-devices

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Study of High Power Impulse Magnetron Sputtering (HiPIMS): Application to Cr deposition thin film.

Abstract
An alternative Physical Vapor Deposition (PVD) process based on a pulsed discharge has emerged in recent years [1-2] for thin film deposition. This PVD process called High Power Impulse Magnetron Sputtering (HiPIMS) has the advantage of producing a very dense plasma with a very high degree of ionization over a pulse duration of few tens microns at a frequency of the order of KHz. In this study, we use a HiPIMS-PVD process to deposit chromium metal thin film Cr and chromium nitride thin film CrN. For Both cases, Cr target on the cathode is used. To deposit only Cr thin film, argon plasma discharge is used while the argon-nitrogen plasma discharge is used to deposit CrN. On the other hand, a global model of plasma discharge applied to the ionization region is developed to quantify the density of each activated species created in the plasma as well as the electron density and temperature [3]. A satisfactory agreement between the simulation results and the experiments is obtained.

Keywords
Plasma – Thin Films - PVD – HiPIMS – Chromium – Chromium Nitride.

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Biography
Ahmed Rhallabi is Professor in Nantes University France. He received the Ph D degree in Material Science in 1992. He is a supervisor in the development of multiscale simulation approaches for plasma etching and deposition processes in Institut des Matériaux de Nantes, France.

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Photophysical Study of New Small Molecules Presenting Thermal Activated Delayed Fluorescence (TADF) and Room Temperature Phosphorescence (RTP) for OLEDs Devices Applications

Abstract
Control of photophysical properties is crucial for the continued development of optoelectronic devices and luminescent materials. Thermally activated delayed fluorescence (TADF) is a realistic mechanism to efficiently harvest the (dark) triplet excitons, created upon electroluminescence, in last generation OLED devices[1-2]. This allows obtaining internal quantum efficiency (IQE) close to 100% without using any highly expensive, rare, and toxic heavy-atom complexes. Such a triplet to singlets process conversion is possible when the energy difference between them (ΔE_{ST}) is very small[3] (<0.2 eV). Besides the TADF phenomena, another strategy to harvest triplet-excited states using pure organic small molecules is to take advantage of the room temperature phosphorescence[4] (RTP). RTP has been observed when small molecules are dispersed in solvents or materials in which molecular motion is hindered. In particular, the most relevant methods to obtain efficient RTP are aggregation-induced or crystallization-induced emission[5] (AIE or CIE).
This talk presents the photophysical study of several new original molecules based on the popular donor-acceptor design[6-7] used for achieving TADF and RTP. The new acceptor introduced in this work can induce very different and complex photophysical properties in solution and solid-state by only subtle changes in their structure, which greatly affect the competition between different photophysical decay mechanisms. Interestingly, these materials also show the possibility to tune their emission by modulating the supramolecular organization through the sample preparation. In particular, they present AIE, excimer emission, mechanochromic luminescence (change of the emission colour when the external stress is applied), and polymorphism. It will be demonstrated how it is possible to trigger the TADF inducing a change of the molecular conformation through crystallization or excimer formation. It is also demonstrated how the molecular design and rigidity of the medium, are crucial to determine whether the molecule emits through TADF or RTP.
In conclusion, our study uncovers design rules and strategies to control of photophysical properties while concomitantly fully understanding the photophysical effects driven by TADF and RTP phenomena. This will likely enable the development of new efficient emissive materials in future.

Keywords
Thermally activated delayed fluorescence (TADF); room temperature phosphorescence (RTP); Charge Transfer (CT); aggregation-induced emission (AIE).

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Biography
I graduated with a master's in Physical Chemistry from the Faculty of Industrial Chemistry "TosoMontanari", Bologna. I hold my first PhD in Physics and NanoSciences at the University of Salento (Italy), at my second European Marie Curie PhD in Chemical Sciences: Molecules, Materials, Tools and Biosystems at EcoleNormale Paris Saclay (France). Actually, I work as a senior researcher at the Nanotechnology centre of CNR Nanotec in Lecce (Southern Italy). I do research in photophysics and photochemistry and optoelectronic devices. My current project is based on the photophysical study of new small molecules presenting Thermal activated delayed fluorescence (TADF) and Room temperature phosphorescence (RTP) for optoelectronic and biological applications.

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Laser-Assisted Generation of Ultra-small Iron Nanoparticles

Abstract

The current contribution explores the implications of using laser fragmentation in liquids (LFL) to synthesize ligand-free ultra-small iron nanoparticles (NPs) in solvents with different dipolar moments. As extensively discussed by the community interested in generating nanomaterials at the ultra-small scale (1-3 nm), the employment of large amounts of hazardous chemicals, often needed for their production, shall be suppressed [1]. In addition to the environmentally detrimental effects of hazardous chemicals management and disposal, their by-products tend to pollute these ultra-small NPs. Since these elements are primarily employed as building blocks to create increasingly complex structures, any polluting agent at their surface or as a part of their structure heavily changes the materials' behavior, thus, making their production noncontrollable and irreproducible. In response to such a challenge, we explore the implications of using a methodology that replaces hazardous reducing agents' usage with light. In LFL, nanosecond pulsed laser radiation is employed to irradiate micrometric particles, and depending on the irradiation dosage, it is possible to heat, melt, and eventually evaporate the particles' surface.

Moreover, as recently suggested in various works, the selection of polar solvents while employing LFL should enable the production and stabilization of these appealing nanomaterials while suppressing chemical waste production [2]. Besides, unlike most traditional synthesis approaches, it also brings a ligand-free surface, a fundamental matter in application sectors requiring a large number of chemically active sites [3]. Given the importance of iron ultra-small NPs as contrast agents for magnetic resonance imaging, we proved this hypothesis by reducing the size of micrometric carbonyl iron to the regime of 1-3 nm. Besides, we also found that the solvent's selection can enable precise control over the synthesized nanomaterial's chemical structure (Fe, Fe2O3, and Fe3O4) and production rate. These findings culminated in the evidence that solvents with a large dipolar moment like ethylene glycol or polyethylene glycol 400 are the most optimal liquid environments for producing highly stable colloids composed of ligand-free ultra-small iron NPs.

Keywords

Iron nanoparticles; ultra-small nanoparticles; nZVI; stabilization effect; laser fragmentation in liquid

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Biography

Dr. Rafael Omar Torres Mendieta obtained his Ph.D. degree in 2016 at the University Jaume I, Spain, in Applied Physics. Afterward, he worked as a postdoctoral researcher at the same university in the GROC group co-leaded by Prof. Gladys Mínguez-Vega and Prof. Enrique Ataulfo Tajahuerce Romera. Later in 2017, he joined the Institute for Nanomaterials, Advanced Technologies and Innovation in the Czech Republic to work as an Assistant Professor in the field of nanomaterials development by sustainable technologies. He is currently the leader of the FEMTONANO research team, which focuses on unveiling the most complex details behind the synthesis and study of nanomaterials using ultrafast laser radiation. In addition, his interests extend to possible applications where laser-synthesized nanomaterials can be used, such as catalysis, bacteria eradication, water treatment, energy storage and conversion, smart fluids, and drug delivery, among others.

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Inhibition Impact of Cement Composite Admixtures on Fungi Activity

Abstract

Biodegradation of construction materials is still current issue [1]. Microorganisms such as bacteria, algae or microscopic fungi are present on the surfaces of cement composites and can disrupted compact structure of material [2]. This action can influence sustainability parameters such as durability and service-life of the material [3]. To investigate the potential inhibition impact against fungi, various admixture in cement composites as secondary raw materials were used. Cement composites made of cement as a reference sample, blast furnace slag, microsilica, fly ash, bypass dust, eggshells, and recycled glass were investigated. Hence, the effort to combine inhibition impact and utilization of industrial waste were established.

To investigate proposed goals the petri dishes with Sabouraud Dextrose Agar were prepared. Nutrient agar was inoculated by microscopic fungi Cladosporium previously cultivated in laboratory of Department of Environmental Engineering at Technical University of Ostrava, Faculty of Mining and Geology. Six secondary raw materials as admixtures and cement were sterilised with UV light and mixed up with agar and with constant stirring poured to same sized Petri dishes. After the agar has cooled down the inoculum was stirred at Vortecx mixer, VorTech and poured on prepared agar. The inoculum consisted of 10 ml of distilled water and spores taken from growth Cladosporium. There were 23 Petri dished prepared. For each raw material there were two sets of culture media (second one served as a parallel medium) with inoculum and on set of culture media without inoculum, just with raw materials. One Petri dish just with agar to prove clear preparation and one Petri dish with agar and inoculum to compare growth of fungi with growth with raw materials.

Results had shown growth of fungi on each inoculated medium except of eggshell parallel medium. It is known [4] that eggshell added to cement has inhibition impact. To prove that theory it is necessary to provide more research. Some Petri dishes had not spread inoculum all over the surface that is the reason why some of the dishes had empty spaces. Three of the control media set (microsilica, eggshells, glass) had shown slightly contaminated culture media. According to visual assessment, it was possible to compare each inoculated culture media with raw material with culture media with inoculum but without raw material (CMI). All the results had just lightly differences, despite of that there were observed dissimilarities. Following scale was created: (1) growth with smaller number of colonies and slighter mycelium than CMI, (2) Growth with smaller number of colonies and larger mycelium than CMI (3) Growth with higher number of colonies and slighter mycelium than CMI (4) Growth with higher number of colonies and larger mycelium than CMI. Cement, slag, bypass dust and eggshells corresponded to scale 3, microsilica and glass corresponded to scale 4 and fly ash to 1.

With further research it is achievable to consider proper admixtures in fight against biodegradation of materials caused by microscopical fungi.

Keywords
Fungi, Cladosporium, Admixtures, Cement, Biodegradation

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Biography
Ing. Miriama Hološová is a doctoral student at Technical University of Košice in second grade of four. At Faculty of Civil Engineering, she is providing research at the Department of Material Engineering focusing on cement composites. The name of the thesis is “Durability of waste-based cement composites and their resistance against biocorrosion.” Miriama graduated from the Technical University of Košice in 2017 in bachelor’s degree with final work focused on parameters of indoor quality environment and in 2019 in engineer’s degree focused on diagnosis of historical constructions solving salinity and humidity issues. In 2022 Miriama absolved two-month mobility traineeship at Czech Technical University in Prague at Department of Materials Engineering and Chemistry with focus on another secondary raw materials from industrial production used in cement composites and their utilization.

Satoshi Ejima
University of Greifswald, Institute of Physics, D-17489 Greifswald, Germany

Photoinduced Insulator-to-Metal Transition of Excitonic Insulators

Insulator-to-metal transition is one of the most exciting phenomena in condensed matter physics. A new route to realize such a phase transition is to apply optical pulses on insulators, which can be observed by the time-resolved photoemission spectroscopy.
In this talk, we numerically demonstrate such a photoinduced metallization of excitonic insulatorsin the extended Falicov-Kimball model (EFKM) at half filling both with and without the internal SU (2) structure.By simulating the time-dependent photoemission spectrain the SU(2)-symmetric EFKM utilizing the time-dependent density-matrix renormalization technique,we demonstrate the emergence of an extra band above Fermi energy after pulse irradiation, reflecting the enhanced pair correlations. Even in the absence of the SU (2) structure, the pair correlations are enhanced during the pump, while they decrease over time. This implies the possible metallization of Ta2NiSe5, a strong candidate material for an excitonic insulator, whose minimal theoretical model isconsidered to be the EFKM without internal SU (2) structure. Optimizing the pulse parameters, we demonstrate the photoinduced metallization, reflecting recent findings in time- and angle-resolved photoemission spectroscopy experiments on Ta2NiSe5.

Biography

Dr. Satoshi Ejima obtained his PhD degree in 2006 at the University of Marburg, Germany. After working as Postdoc, he moved to University of Greifswald (UG), Germany in 2008. He received his habilitation in 2017 and is working now as a senior researcher at the UG and a visiting researcher at RIKEN (Japan). His research interests are focused on the theoretical investigations of strongly-correlated quantum many-body systems, such as electron-phonon coupled systems and models with Hubbard-type interactions, with an emphasis on new emergent phenomena not only in thermal equilibrium but also in nonequilibrium and driven situations.

Abhishek Sharan
Khalifa University, UAE

Hetero structural Interface Atomic Structure Prediction from First Principles Methods and Application to CdTe Solar Cells

Abstract
Designing and control of interfaces between dissimilar materials is central to advancing optoelectronic and emerging technologies. Using first-principles insight into designing incommensurate interfaces is particularly challenging, as these interfaces are notoriously defective and explicit interface atomic structure models rarely exist. In this work using modified bulk crystal structure prediction algorithm based on first-principles density functional theory, we predict the interface atomic structure between SnO2 and CdTe without and with the addition of CdCl2 that have different bulk atomic structures. Optimization of SnO2/CdTe and SnO2/CdCl2/CdTe interfaces are crucial at enhancing the performance of CdTe based thin-film solar cells. We find that SnO2/CdTe interface is highly defective, while we discover a unique two-dimensional structure of CdCl2 interpahse between SnO2 and CdTe. Addition of CdCl2 facilitates transition from rutile SnO2 structure to zinc blende CdTe structure, thereby removing defect states from the CdTe absorber band gap. Implementing the interface atomic structures into device simulations, we show the theoretical feasibility of high efficiency buffer less oxide-CdTe heterojunction solar cells. Our results demonstrate a broader potential of designing defect free incommensurate interfaces with the addition of atomically designed interlayer, and potential of using first principles methods for designing and optimizing heterostructural interfaces.

Biography
Abhishek Sharan is a Post-Doctoral fellow at Khalifa University, Abu Dhabi UAE. Prior to this role, he worked at National Renewable Energy Laboratory (NREL), Colorado USA as a Post-Doctoral fellow from where he continues to work in collaboration. He received PhD in Physics from University of Delaware, USA in 2019 and Bachelor of Technology in Engineering Physics at Indian Insititute of Technology (IIT) Delhi, India in 2011. He has experience in industrial R&D in the area of photovoltaics at Bharat Heavy Electricals Limited (BHEL) Gurugram, India. His research is focused on using first principles computational methods at understanding and engineering properties of materials. Dr. Sharan has expertise in the area of photovoltaics, materials discovery, defect physics, emergent phenomena in materials, two-dimensional materials etc. He has keen interest in energy related materials for green energy production and storage. Dr Sharan holds 2 patents and 20 research articles published in international peer-reviewed journals.

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Exotic Magnetic Flux Patterns In Superconductors between Type I and II

Abstract

The Ginzburg-Landau theory distinguishes two superconductivity types: ideally diamagnetic type-I materials and type-II superconductors that allow magnetic flux forming the mixed state with Abrikosov vortices. However, this dual classification does not exhaust all possibilities even for the standard BCS theory, which reveals a special regime of inter-type (IT) superconductivity. It has very distinct characteristics and should be regarded as a separate superconductivity type. Its intermediate mixed state (IMS) carries a manifold of exotic vortex patterns ranging from clusters of vortex lattices, to vortex stripes, labyrinths, and liquid droplets.

It is shown that the IT superconductivity regime is a generic phenomenon generated by proximity to the super-critical Bogomolnyi point, at which the superconductive state is self-dual and infinitely degenerate. The IMS phase diagram is determined by the degeneracy-breaking mechanism, and is not sensitive to the microscopic details of the system. The generic nature of the phenomenon explains qualitatively similar vortex patterns appearing in a wide class of superconductors including single- and many-band compounds, magnetic materials, thin films and hybrid devices. These link superconductivity phenomenons with the world of spontaneously emerging complexity.

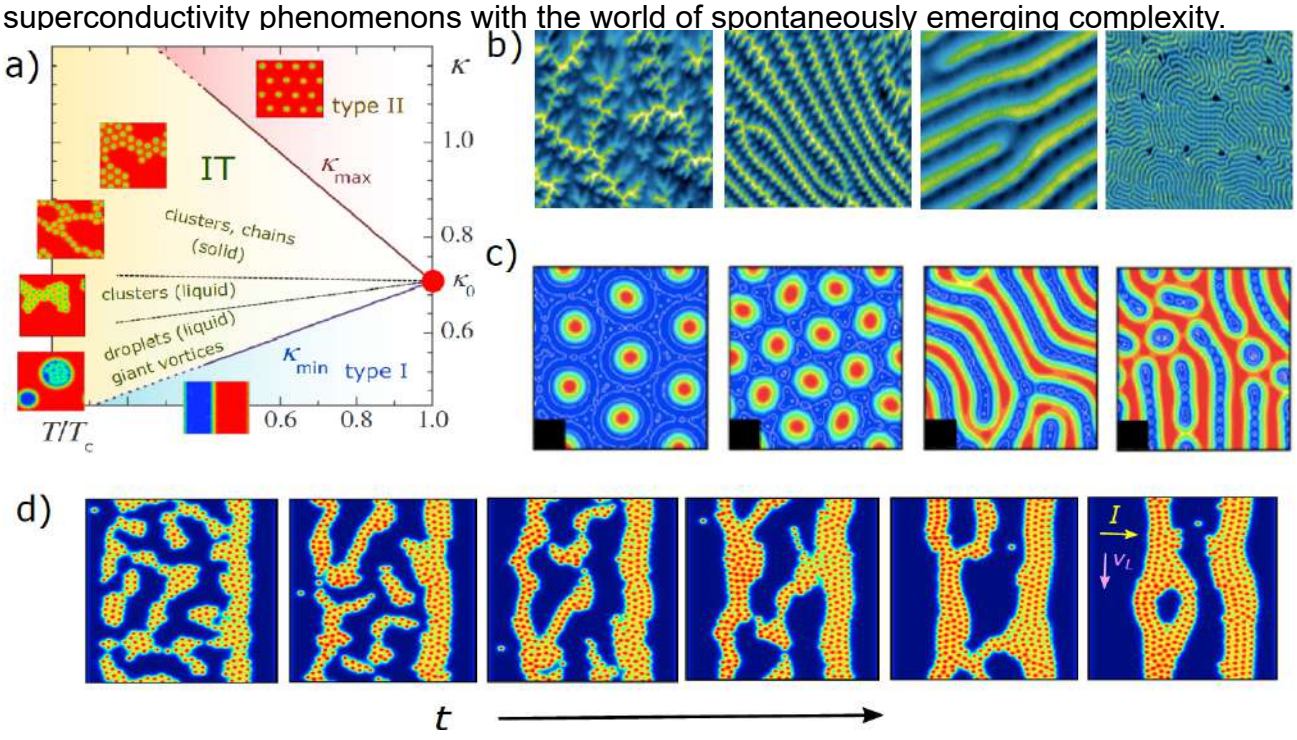

Figure: a) Phase diagram of IMS's with examples of flux configurations [1], b) magnetization profile in EuFe2(As0.79P0.21)2 [2], c) flux profile in a thin superconducting film [3], d) the current driven time evolution forming IMS vortex stripes in Nb [4].

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Novel Ag0(NP)/TiO2 Supported Bentonite Thin Film in the Efficient Degradation of Bisphenol a using Visible Light

Abstract

The persistent endocrine-disrupting chemical bisphenol A is posing serious health concerns; hence, it is known to be an emerging and potential water contaminant [1]. Bisphenol A is having widespread use as raw material and intermediary in the manufacture of epoxy resins, polycarbonate plastics, and food packages [2]. The harmful effects on various targets in the human body via estrogen response pathways are documented elsewhere [3]. It is a typical chemical of endocrine-disrupting chemicals (EDC) that can lead to damage the reproductive organs of aquatic organisms [4]. The present investigation aims to synthesize novel cubical Ag(NP) decorated titanium dioxide supported bentonite (Ag/TiO2@Clay) nanocomposite using a novel synthetic process. The nanocomposite materials were characterized by several analytical methods viz., transmission electron microscopy (TEM), X-ray diffraction (XRD) analyses, Energy-dispersive X-ray spectroscopy (EDX), atomic force microscopy (AFM), scanning electron microscopy (SEM), Brunauer-Emmett-Teller (BET) and diffuse reflectance spectroscopy (DRS). Further, the photocatalytic removal of bisphenol A was conducted utilizing the thin film catalyst under the LED (Light Emitting Diode; Visible Light) and UV-A (Ultra Violet-A) light sources. The parametric studies solution pH (6.0-8.0), pollutant concentrations (1.0-20.0 mg/L), and the interaction of several scavengers and co-existing ions are studied extensively to demonstrate the insights of the removal mechanism. The mineralization of bisphenol A and repeated use of the thin catalyst showed the potential usage of photocatalyst in the devised large-scale operations. Similarly, the natural matrix treatment was performed to evaluate the suitability of the process for real implications.Therefore, the thin film catalyst exhibited high potential in order to devised large-scale operations to decontaminate water contaminated with bisphenol A.

Keywords

Novel nanocomposite thin film; photocatalytic degradation of bisphenol A; mineralization rate; stability of nanocomposite thin film; natural matrix treatment

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Biography

Seung-Mok Lee is a Full Professor of the Department of Environmental Engineering at Catholic Kwandong University in Korea since 1990. He has a B.S. degree in Chemical Engineering fromHanyang University, M.S. degree in Chemical Engineering from the Yonsei University, Korea and a Ph.D. degree in Environmental Engineering from Kansas State University, USA. His research and teaching activities focus on adsorption of heavy metal ions in aqueous environment by using various advanced materials. He has published 300 research articles in several professional journals, including 200 international professional journals. He is chapter author for the Stochastic Modeling of Adsorption Kinetics, Marcel Dekker (2002) and Ferrate(VI) in the Treatment of Wastewaters, InTech (2011). He has received various awards, including a Prime Minister's Award from Korean Government (2009), and awards for the outstanding research paper from the Korean Society of Environmental Engineers (2007, 2012, 2014).

Masataka Matsumoto

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Phase Transitions and Critical Phenomena in Non-Equilibrium Steady States From Holography

Abstract

One of the natural extensions from an equilibrium system is a non-equilibrium steady state (NESS) with a constant flow of current, such as a heat current or an electric current. However, the construction of thermodynamics for NESS is not at all straightforward.A new parameter in the NESS, the current, should be one of the essential parameters that may characterize the NESS's universal features. Natural phenomena to look for the universal features of NESSs are critical phenomena. A natural question is how the current affects the critical phenomena.Motivated by this, we investigate critical phenomena of NESSs whose microscopic theory is explicitly defined by quantum gauge theory. To do this, we employ the gauge/gravity duality (holography), which conjectures the equivalence between a strongly coupled gauge theory and a classical gravity theory.In this talk, I will present our recent works on the phase transition and critical phenomena in the NESS with holography.We find a phase transition associated with a spontaneous chiral symmetry breaking in a current-driven system.The phase diagram contains both the tricritical point and critical points, which appear in the presence of the current [1]. We find that the system exhibits an inverse symmetry breaking at low temperatures.Furthermore, we also report asymmetric critical phenomena at the tricritical point [2], characteristic of the NESS.

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Biography

Masataka Matsumoto has completed his Ph.D from Chuo University in 2020. He is the postdoctoral researcher at Shanghai University.He is working on the application of the gauge/gravity duality to condensed matter physics, especially non-equilibrium systems and phase transitions.

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Nagative Capacitance MOSFET with a Multiferroic Gate Dielectric

Abstract
Negative capacitance field effect transistor (NCFET) has gained intensified attention for its prospects to make subthreshold swing (SS) below 60 mv/dec and application in low power consumption devices. Moreover, devices based on GaAs substrates are widely used for their high-electron-mobility and relatively wide energy gap. In this work,a detailed simulation was first made on GaAs NCFET to clarify key structure factors, including channel length, polysilicon gate length, doping concentration, ferroelectric film thickness, and voltage bias, on the performanceof NCFET. The performance of the NCFET is not only on the structure factors but also onthe other factors (e.g., applied voltage bias, etc.)Mobility, band energy diagram, electric potential along channel surface, and substrate capacitance are then investigated to make detailed analyses of simulation results. Finally, we have built an NCFET with 0.85BiTi0.1Fe0.8Mg0.1O3-0.15CaTiO3 (BTFM-CTO) multiferroic film as a dielectric gate layer which shows large polarization in our previous work. Optimization of the NCFET has achieved a valueSS of 44.9 mV/dec, and a high ION/ IOFF value of 1.2×109 with a low supply voltage of 0.6 V, which demonstrates the BTFM-CTO film is a competitive candidate for a ferroelectric layer of GaAs NCFET. The current work may generate new insights into advanced NCFET based on GaAs with low power consumption, which would benefit the device design and application.

Keywords
Multiferroicgatedielectric,Negative capacitance FET (NCFET), GaAs, low power dissipation, subthreshold swing (SS), negative differential resistance (NDR)

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Biography

Dr. Jia got her PhD. Degree in Shanghai Institute of Optics and Fine Mechanics, CAS in 2011. Then she joined Shanghai Institute of Microsystem and Information, CAS and National Institute for Materials Science from 2011 to 2016. Now, she is the Associate Professor of Shenzhen Institute of Advanced Technology, CAS. Dr. Jia's research concentrates on multifunctional materials and devices for Information technology, especially on the multiferroics, ferroelectrics, semiconductors, etc. She has published 70 papers, applied 20 patents, and 2 academic books.

Abdullah Yar
Abdullah Yar and Jasra

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Hexagonal Warping Induced Non-linear Hall Effect in Topological Insulator Bi2Te3

Abstract
Non-linear Hall effect is investigated theoretically in topological insulator Bi2Te3. Particular emphasis is given to the role played by the hexagonal warping in the energy band structure of topological insulators. Remarkably, the Hall response exhibits central minimum with a width set by the band gap, followed by two resonance peaks. We also investigate the role of proximity-induced Berry curvature. We find strong dependence of the non-linear Hall effect in topological insulator on the strength of hexagonal warping, Fermi energy level, band gap in the energy spectrum, and temperature of the system.
This work may be potentially utilized in realizing electronic devices.

Keywords
Topological Insulators, Nonlinear Hall Effect, Hexagonal Warping, Berry Curvature

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Biography
Dr Abdullah Yar is currently working as an Associate Professor, Department of Physics, Kohat University of Science and Technology (KUST), Kohat-26000, Khyber Pakhtunkhwa, Pakistan. He has also worked in this university as a lecturer and assistant professor as well. He also worked as a visiting lecturer, Department of Physics, Islamia College University Peshawar, Khyber Pakhtunkhwa, Pakistan. He also worked as a lecturer, Department of Physics, University of Malakand, Chakdara, Dir (Lower), Khyber Pakhtunkhwa, Pakistan, and visiting lecturer, University Girls College, University of Malakand. He has also served as a Chairman, Department of Physics, Kohat University of Science and Technology, Kohat. He received Best University Teacher Award 2019-20 from Kohat University of Science and Technology, Kohat. He has supervised many graduate research students and two research funded projects.
He is working on electronic transport in interacting quantum dot systems, magneto transport in 2DEG systems, graphene, Weyl semimetals, topological insulators, electron-vibron effects in interacting quantum dot systems and has published many papers in this field. His field of research is Condensed Matter Theory.

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Environmental Impacts of Wooden Panels with Various Thermal Insulations

Abstract

The construction industry participates to a significant degree in air pollution [1], but by applying the approaches of environmental assessment of projects and the design of more environmentally suitable constructions, it is possible to reduce these environmental burdens [2]. The optimal design of materials can reduce the environmental impact of the structure or even the entire building by up to 60% [3]. The LCA approach is most often used to compare the environmental impacts of materials, structures and buildings [4].

In the paper, five variants of the wooden wall structures made of panels with a cross of glued wood were evaluated, where the main goal was to vary different thermal insulation while keeping the same thermos-physical performance of the wall in terms of achieving a heat transfer coefficient U with a value of 0.1 ± 0.01 W/(m2.K). The U parameter was set to meet a requirement for a passive house. Material composition and individual layers of the wooden wall was: thin-layer plaster, reinforced mesh, thermal insulation, cement adhesive, wooden cross laminated timber (CLT) panel, supporting metal (wooden) grid, and plasterboard. The thermal insulation materials varied in particular alternatives from conventional (white polystyrene-OS1, mineral wood-OS2) to rarely used materials as polyurethane boards (PIR)-OS3, wooden boards- OS4 or hemp insulation-OS5. The environmental impacts of the proposed wall variants were compared in the SimaPro software using the Recipe and CML methods. The following mid-point environmental categories were selected for the assessment of the impacts of the walls: climate change, primary energy consumption, fossil resource consumption and water consumption. For the overall impacts, three end-point damage categories were chosen for comparison, namely: human health, ecosystem and depletion of resources. All values of environmental indicators were expressed for 1 m2 of perimeter structure. The wall with hemp thermal insulation had the lowest impact on climate change, on the contrary, the highest impacts were found for the wall with polyurethane insulation (Fig. 1). The difference between the lowest and the highest environmental impact of structures was 24.57%.

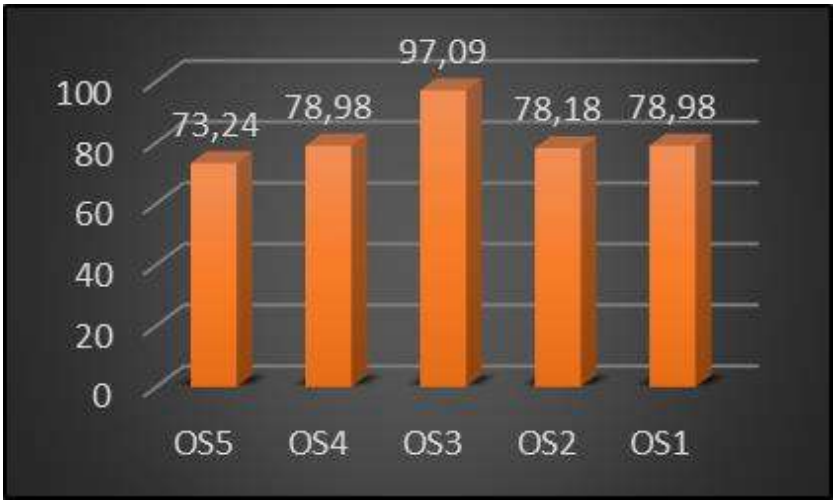

Fig. 1 The influence of structures on climate change

The hemp-based wall structure was found to be the best alternative also in all other environmental categories.

Keywords
Carbon footprint, CLT panel, climate change, resource depletion

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Biography
Prof. Adriana Eštoková is a full professor at Technical University of Kosice, Faculty of Civil Engineering and her research is in the field of environmental and material engineering. She focuses more closely on the study of the environmental properties of cement composites based on various wastes and their potential risks, such as the leachability of dangerous metals and natural radioactivity, as well as on the study of the durability of materials and their chemical and biological corrosion processes. Another area of research is the assessment of the impact of building materials on the environment during the life cycle of the building and the impact on the quality of the internal environment of buildings.

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Possibilities of Critical Raw Materials Recovery by Extracellular Precipitation

Abstract

Critical raw materials (CRMs) can be defined as materials of which the risks of supply shortage and their impacts on the economy are higher compared to most of other raw materials. The European Commission (EU) has created the three lists of CRMs for the EU (in 2011, 2014 and 2017) [1]. To tackle the supply risk challenge, innovation is required with respect to sustainable primary mining, substitution of critical metals, and urban mining. In these three categories, bio-hydrometallurgy can play a crucial role [2].

The natural biogeochemical cycles of elements under the microorganisms (MO) influence are the base of the bio-hydrometallurgical methods. Bio-hydrometallurgy is the advanced technology of the mineral raw recovery and processing as well as the environmental protection. Basic processes of bio-hydrometallurgy are biomining, extracellular precipitation of metals with biogenic compounds, intracellular biosynthesis of solid metals, bio-electrochemical recovery of metals, microbial sorption and methylation [3].

Some MO in the effort to avoid metal entrance to the cell release different compounds into the environment which participate in the formation of insoluble compounds (organometallic complexes, metal sulphides or oxides). This process is called extracellular precipitation of metals, which belongs to the most significant process for recovery metals/metalloids from primary and secondary sources [4]. Extracellular precipitation involves several mechanisms such as:Physical-chemical interactions with cell surface – precipitation of metals does not depend on the metabolism and are probably results of the chemical interactions between metal and cell surface [5]; Direct metal reduction – metals are removed from the environment by bioreduction to lower oxidation stage,bacteria use organic compounds as a source of electrons for the reduction. Organic pollutants as well as metals are simultaneously remove [6];Release of precipitating agents into solution – by sulphate-reducing bacteria (SRB), which are to able realize the conversion of sulphates to hydrogen sulphide under anaerobic conditions. H2S produced by SRB consequently reacts easily in aqueous solution with the cations of heavy metals, forming metal sulphides that have low solubility. Selective precipitation by bacterially produced H2S has been demonstrated on a limited number of critical (Co) and economically important metals (Fe, Zn, Ni and Mn). Notably, selective precipitation and metal recovery can be well combined with bioremediation needs, for instance in the treatment of acid mine drainage [7];Release of oxidation agents – metal precipitation is also possible by the mechanism

when cell synthesizes oxidation agents such as molecules O2 or H2O2, which diffuse to its outer environment [8].

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Keywords

Bio-hydrometallurgy, heavy metals, extracellular precipitation

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Biography

Dr. Alena Luptakova- holds an MSc in the field of chemical engineering. Since 1986 she has worked in the Department of Mineral Biotechnologies, Institute of Geotechnics of Slovak Academy of Sciences. She has over 35 years of experience in the field of biohydrometallurgy, especially bioremediation and bioleaching, becoming an expert in bioremediation of acid mine drainage (AMD) using sulphate-reducing bacteria (SRB). She is experienced in the preparation and application of bionanosorbents produced by SRB, bioleaching of sulphide minerals and electronic waste by sulphur- and iron-oxidizing bacteria (SFeOB) and the microbiologically influenced corrosion of cement composite materials by SFeOB and SRB. She is the author of 3 monographs, 2 student books, 2 chapters in monographs, 88 scientific publications in Wos/Scopus, over 90 papers in national/international conference proceedings and 16 invited lectures. In database Wos has H-index 10. She is experienced in preparation and management of national (10) and international (11) projects.

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Increasing the Recovery Rate of Reservoir Sediments as a Waste Through their Re-use in Construction Industry

Abstract
Bottom sediments, silting the watercourses and reservoirs, pose a significant water management problem. Sediment extraction is an essential part of maintaining the functionality and flow of water structures, which creates a considerable amount of material that needs to be properly managed in accordance with waste management. The sediment itself is not considered as a waste. However, the problem arises with contaminated excavated material from water structures, which is categorized as waste in the European Waste Catalog, throwing a generally negative picture on sediments[1].
Due to the perpetual availability of sediments extracted from reservoirs, it is common practice to use them in construction industry. In several studies the extracted sediments have been applied as the main or supplementary material. They can be used as a raw material for the production of lightweight aggregates, in the production of bricks, ceramics and can also be used as a partial replacement of binder in the production of concrete[2-5].
In our study, bottom sediments extracted from reservoir were used as 20 and 40 wt% replacement of cement in concrete. The technological properties of prepared composites as compressive and flexural strength after 28, 90, 180, and 365 days of hardening were tested compared to the control concrete mixtures prepared with cement, natural aggregate and water(Fig. 1).

Fig. 1: Research methodology

The results showed that the use of a 20% sediment cement replacement contributed to an increase in the strength of the composites after 28 days of curing by more than 35% compared to the use of a higher (40%) sediment cement replacement. However, after 365 days, the compressive strength of the composites with less weight replacement was only 6% higher and stabilized at about 34

MPa. The development of the tensile strength of the sample with 20% cement sediment was even higher after 28 days of setting than the tensile strength of the comparative sample. With higher weight replacement of cement by sediment, the flexural tensile strength decreased by 20% after 365 days of setting. In conclusion, it can be stated that the use of higher mass replacements of cement with sediment from water reservoirs seems to be more advantageous from an environmental and economic point of view.

Keywords
Binder, cement, sediment, concrete, strength

Acknowledgement
This research has been supported by the Slovak Grant Agency for Science (Grant No. 1/0419/19) and by the Slovak Research and Development Agency under the contract No. APVV-20-0140.

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Biography
Natalia Junakovais an associate professor in the field of Environmental engineering at the Institute of Sustainable and Circular Construction, Faculty of Civil Engineering at the Technical University of Košice with 18 years of professional experiences in civil and environmental research and education. Her research interest is focused on the Sustainable materials and constructions, Sustainable water management, Sustainability assessment and certification of buildings. The results of her research work have been published in more than hundred national and international journals and scientific conference proceedings. She is an author and co-author of scientific monograph, three academic textbooks, four educational textbooks, more than 120 research outputs, 30/44 publications registered in the WoS / SCOPUS databases with the number of citing articles 91/170 WoS / SCOPUS (Scopus H-index 7). She has successfully led an educational project and she has also actively participated in solving of national and international research and educational projects. In practice she cooperates as a sustainability consultant during the design and construction of buildings certified by BREEAM method and as a consultant for sustainable blue-green infrastructure in urban landscape.

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Vanadium Dioxide Thin Films for Thermal Micro-Systems

Abstract
This work proposes to take benefit of the properties of a Phase Change/Transition Material (PC/TM), namely vanadium dioxide (VO2) to tune thermal properties. This oxide material well-known for its first order Semiconductor to Metal transition (SMT) close to room temperature (341K), presents drastic physical variations and consequently huge modifications in its optical[1,2]using an adapted Langmuir–Blodgett (LB, electrical and thermal[3]using an adapted Langmuir–Blodgett (LBproperties. Vanadium dioxide thin films are deposited on c-cut sapphire substratesusing the Pulsed Laser Deposition (PLD) method with the aim to investigate their thermophysical propertiesas an effort to develop new thermal micro-systems[4]using an adapted Langmuir–Blodgett (LB. High quality VO2 thins films with a homogenous thickness on arelatively large surface (2×2cm2) are fabricated and the significant temperature variation of the thermal diffusivity and emissivity of the VO2 films is explored across the SMT. The measuring, analysis, and comparison of the electrical and morphological characteristics of the VO2 films are used to prove the reliability of the PLD as a method that provides ideal materials for applications in micro and nano scale. Electrical abrupt transitionsare obtained with very strong associated amplitude (5 ordersin magnitude) between semi-conductor and metallic states. The thermal diffusivity of the VO2 films during their heating and cooling measured by infrared photothermal radiometry andthe emissivity measured by ellipsometry allowed to determine the heat capacity and thermal conductivity. These thermophysical properties of the VO2 thin films are taken as an input value for the theoretical approachtopredict the thermal amplification factor, which establishes the efficiency of thermal micro-systems like athermal transistor.

Keywords
Phase Change Materials, Thin Films, Pulsed Laser Deposition, Thermal Diffusivity

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Structural Studies of NdBa[Co]_2 O_(5.75)

Abstract
We report here, the temperature dependent structural studies carried out on oxygen-deficient double perovskite NdBa (δ~0.75). The samples were characterized using x-ray diffraction and dc magnetization techniques. All the diffraction patterns were analyzed using Rietveld profile refinement software. At room temperature (RT) the compound stabilizes in tetragonal structure with space group P4/mmm. Careful diffraction studies reveal the signature of superlattice peaks having the lattice parameters 2apx2apx2cp where ap and cp are lattice parameters of its perovskite structure. The magnetic measurements show transitions at 110 K and 45 K, which correspond to paramagnetic to ferromagnetic and ferromagnetic to antiferromagnetic transitions, respectively.The compound shows signatures of Griffith's phasein the temperature range 250 K - 125 K. Our detailed structural studies reveal signature of these transitions thereby suggesting significant connectivity between magnetism and crystal structure.

Keywords
Double perovskite, x-ray diffraction, Griffith's phase

Biography
Mr. Himanshu Pant is currently a senior research fellow at Indian Institute of Technology, Mandi work in gunder the supervision of Dr. Bindu Radhamany. He earned his master's degree (M Sc) from Kumaun University, S. S. J. Campus, Almora (Uttarakhand) in 2018 and bachelor's degree from the Kumaun University, S. S. J. Campus, Almora (Uttarakhand) in 2016. He is currently pursuing his research in cobalt based double perovskites compounds at School of Basic Sciences in Indian Institute of Technology, Mandi.

Day-02 Virtual Presentations

Raman Singh

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Graphene Coatings for Remarkable Corrosion Resistance

Abstract

Corrosion and its mitigation costs dearly (any developed economy loses 3-4% of GDP due to corrosion, which translates to ~$250b to annual loss USA). In spite of traditional approaches of corrosion mitigation (e.g., use of corrosion resistance alloys such as stainless steels and coatings), loss of infrastructure due to corrosion continues to be a vexing problem. So, it is technologically as well as commercially attractive to explore disruptive approaches for durable corrosion resistance. Graphene has triggered unprecedented research excitement for its exceptional characteristics. The most relevant properties of graphene as corrosion resistance barrier are its remarkable chemical inertness, impermeability and toughness, i.e., the requirements of an ideal surface barrier coating for corrosion resistance. However, the extent of corrosion resistance has been found to vary considerably in different studies. The author's group has demonstrated an ultra-thin graphene coating to improve corrosion resistance of copper by two orders of magnitude in an aggressive chloride solution (i.e., similar to sea-water). In contrast, other reports suggest the graphene coating to actually enhance corrosion rate of copper, particularly during extended exposures. Authors group has investigated the reasons for such contrast in corrosion resistance due to graphene coating as reported by different researchers. On the basis of the findings, author's group has succeeded in demonstration of durable corrosion resistance as result of development of suitable graphene coating. The presentation will also assess the challenges in developing corrosion resistant graphene coating on most common engineering alloys, such as mild steel, and presents results demonstrating circumvention of these challenges.

Biography

Professor Raman Singh's expertise includes: Alloy Nano/Microstructure-Corrosion Relationship, Stress Corrosion Cracking (SCC), Corrosion/SCC of Biomaterials, Corrosion Mitigation by Novel Material (e.g., Graphene), Advanced and Environmentally Friendly Coatings, High Temperature Corrosion. He has supervised 50 PhD students. He has published over 245 peer-reviewed international journal publications, 15 books/book chapters and over 100 reviewed conference publications. His professional responsibilities include editor-in-chief of two journals, Fellow ASM International and Engineers Australia, over 40 keynote/plenary talks at international conferences (besides numerous invited talks), leadership (as chairperson) of a few international conferences.

Mukunda P Das

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High Temperature Superconductivity under High Pressure in Hydrides

Abstract

Superconductivity is an unanticipated phenomenon and its hundred ten years of history is a fascinating subject in physical sciences. The fact that certain materials below a critical temperature lose their electrical resistance, exhibit a persistent current without decay for a long period and repel a magnet, remained a miracle until a microscopic explanation was found in 1957. In this talk I shall present a brief overview of the important landmarks and discuss major recent advances in this fundamental, stimulating and at the same time a difficult area of research.

Particularly I shall discuss our current understanding of high temperature superconductivity under high pressure in various Hydride materials. A key idea is due to Neil Ashcroft who proposed that the critical temperature of metallic hydrogen should be high because its phonon frequencies are high. In 2004 he further proposed hydrogen-rich materials can be considered chemically “precompressed” and with less external pressure they have the potential to superconduct at higher Tc for the same reasons that hydrogen does at extreme pressures. Since then a lot of developments has happened both in experiments and theories, particularly issue like near-room temperature superconductivity.

In this talk I shall try to cover most of the crucial and relevant aspects at a pedagogic level.

Biography

Mukunda P Das is Honorary Professor in Theoretical Physics of the Australian National University. He is Fellow of American Physical Society, Institute of Physics (UK) and Australian Institute of Physics. His research interest spans the fundamental aspects of condensed matter, which include Superconductivity, Vortex Matter, Bose-Einstein Condensation, Strongly Correlated Electrons, Meso- and Nanoscopic Systems, Density Functional Theory and Theory of Disordered States. He is also interested in the professional ethics, an important subject of philosophy. He has been member of Editorial Boards of several international journals, J. Physics: Condensed Matter (IOP)(2002-2012), ANS: Nanoscience and Nanotechnology, GSTF Journal of Physics and Applications, Condensed Matter- Open Acess Journal, Inter. J Condensed Matter, Advanced Materials and Superconductivity Research, Nova Sc., New York and others.

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Spectroscopic Manifestations of Electron Fractionalization in The Pseudo Gap State of Cuprates

Abstract
The origin of the pseudogap in cuprates has been debated for decades, but still remains enigmatic. In this talk, we demonstrate that the concept of electron fractionalization based on Mott physics explains recent spectroscopic data related to the pseudogap. Angle-resolved photoemission spectroscopy (ARPES) studies have shown that, upon electron doping, the upper Hubbard band (UHB) is fractionalized into a coherent UHB and an in-gap band (IGB) with a pseudogap in between [1]. Upon hole doping, the lower Hubbard band (LHB) is fractionalized into a coherent LHB and an IGB with a pseudogap in between.Excitonic excitation from the LHB to the IGB across the pseudogap is observed using resonant x-ray inelastic scattering (RIXS), and exhibits a temperature dependence characteristic of the pseudogap originating from the electron fractionalization [2].

Collaboration with H.-Y. Huang, J. Okamoto, M. Hashimoto, Z.-X. Shen, T. Watanabe, T. Adachi, and Y. Koike is gratefully acknowledged.

Keywords
High-Tc superconductivity, Pseudogap, ARPES, RIXS, Electron fractionalization

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Biography
Atsushi Fujimori is a Professor Emeritus at the University of Tokyo, a Visiting Professor at National Tsing Hua University, and a Distinguished Visiting Scholar at National Synchrotron Radiation Research Center, Taiwan. He received his B.S., M.S., and D.Sc. degrees from the University of Tokyo in 1976, 1978, and 1981, respectively. He was a research scientist at National Institute for

Research in Inorganic Materials, Tsukuba, Japan, between 1978-1988, and a visiting assistant professor at the University of Minnesota, USA, between 1984-1985. He has been studying the electronic structure of correlated electron systems, including high-temperature superconductors, transition-metal oxides, and magnetic semiconductors by photoemission, absorption, and scattering methods using soft x rays.

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Hydrodynamic Effects in Electron Fluids on Spintronics

Abstract

In metals with disorder, the electron transport isdescribed as diffusive. On the other hand, in those with electron-electron interaction being the dominant source of scattering, the motion of the electrons resembles the flow of classical liquids with shear viscosity, namely, the hydrodynamic fluids. The recent progress of nano-technology has made it possible to extend the study on such hydrodynamic electron fluids in nano-devices and low dimensional materials. In such fluids, the angular momentum of the fluid vorticity and electron spins couple each other due to the angular momentum conservation, i.e., the spin-vorticity coupling[1]. Combining the Novier-Stokes and the spin diffusion equations in the presence of the spin-vorticity coupling, we examine a variety of spintronic phenomena[2-4].
We present that metals with nano-structure provide unique spintronic devices due to the local hydrodynamic nature.
The hydrodynamic phenomena of electron fluids open a door to “Hydrodynamic spintronics”.

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Biography

Professor, Dr. Sadamichi Maekawa is a Senior Advisor of RIKEN Center for Emergent Matter Science, Japan and Visiting Chair Professor of Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences. His achieved many awards, those are in November 2018: Clarivate Analytics Highly Cited Researchers, December 2013: Honoris Causa Doctorate of University of Zaragoza, Spain, October 2012: Honorary Member of the Magnetic Society of Japan, July 2012: IUPAP Magnetism Award and Néel Medal April 2008: the title of Distinguished Professor, Tohoku University, November 2007: Fellow of the American Physical Society, April 2005: the title of Honda Professor, September 2003: Magnetics Society of Japan Award, March 2001: Humboldt Award (Germany), April 1999: Fellow of Institute of Physics (UK). His Main Research Topics: Solid State Theory: Theory of electronic properties in strongly correlated electron systems, Theory of transport in magnetic nanostructures and spintronics

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Development of Magnetic Tunnel Junctions for Magnetic Sensor Applications

Abstract
Magnetic tunnel junction (MTJ) based on a CoFeB/MgO/CoFeB trilayer structure exhibit a giant tunnel magnetoresistance (TMR) effect. In addition, theCoFeB/MgO/CoFeB-based MTJ can be grown on a Si wafer and can be combinedinto a multilayered structure with various materials. These advantages drive us to apply the CoFeB/MgO/CoFeB-MTJ to a variety of magnetic sensor (hereafter called TMR sensor). The TMR sensor can be used at room temperature, can be microfabricated into a nanometer-scale, and can be driven with a small power consumption. Very recently, its magnetic field detectivity has reached a sub-pT level which enables us to detect a human bio-magnetic fields [1]–[3].We believe that the TMR sensor that shows these outstanding characteristics will be an essential device to construct a next-generation smart society. In the presentation, we will introduce our recent works on the development of MTJswith a multilayered structure designed especially for the TMR sensor applications.

Keywords
Spintronics, magnetic tunnel junction, tunnel magnetoresistance, magnetic anisotropy, magnetic sensor, sputtering technique

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Biography
TakafumiNakano received his Ph.D. degree at the Department of Applied Physics, Tohoku University in 2017. Since 2020, he has been an assistant professorat the Department of Applied Physics, Tohoku University. His research interestincludes the development of multilayered structures for

spintronic devices by a sputtering technique.MikihikoOogane received his Ph.D. degree at the Department of Applied Physics, Tohoku University in 2003. Since 2022, he has been aprofessor at the Department of Applied Physics, Tohoku University. His research interestlies in the development of novel spintronic materials and devices.

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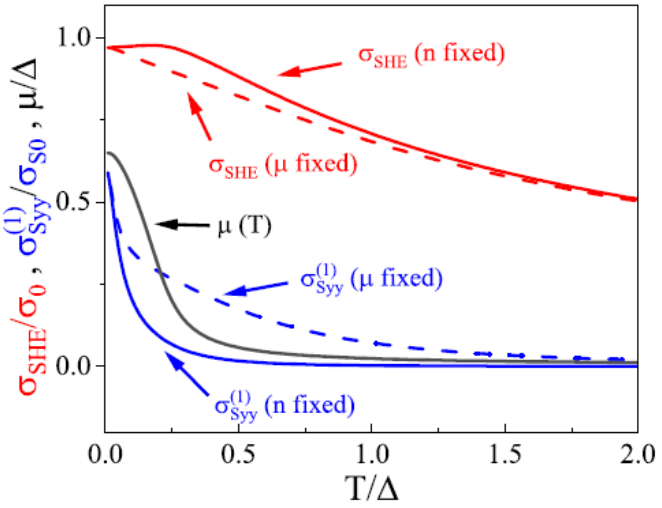
Topological Nature and Anomalous Spin Transport Properties of Dirac Electrons in Organic Conductors

Abstract
The anomalous spin transport coefficients of gapped Dirac electrons are studied considering a quasi-two dimensionalorganic conductor α-(BETS)2I3 [1]. In the presence of a gap induced by spin–orbit interaction, weshow that the effective Hamiltonian is similar to the model considered by Kane and Mele [2] with additional tilting. This Hamiltonian contains the spin-orbit interaction proportional to the z-component of spin. Conductivity tensors up to the linear order of the applied magnetic field are obtainedanalytically using the microscopic linear response theory or Kubo formula. It is shown that spin Hall conductivity σSHE andanomalous diagonal spin conductivity proportional to the magnetic field σSyy(1) become nonzero, which arewritten in terms of the Berry curvature and orbital magnetic moment (see Fig. 1 below) representing the topological nature of the system. The estimated values of spin conductivities usingtypical parameters turn out to be comparable to the spin Hall conductivity in Pt.



Keywords
Spin Hall effect, gapped Dirac electrons, organic conductor, Kane-Mele model, Berry curvature

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Electronic Correlations of CeSb under The Devil's Staircase Transition

Abstract
Solids with competing interactions often undergo complex phase transitions with a variety of longperiodic modulations. Among such transition, devil's staircase is the most complex phenomenon, and for it, CeSb is the most famous material, where a number of the distinct phases with long-periodic antiferromagnetostructures sequentially appear below the Néel temperature [1]. An evolution of the lowenergy electronic structures and underlying electronic correlations going through the devil's staircase is of special interest to understand its mechanism, which has, however, been elusive despite 40 years of intense research.
In my presentation, I will talk about our recent investigations of the electronic properties undergoing the devil's staircase by using laser-based angle-resolved photoemission spectroscopy. We reveal the paramagnetic electronic structure with the semimetallic feature [2]. The high-energy resolution and bulk-sensitivity achieved by utilizinglow-energy laser source reveals the significant reconstruction of these itinerant bands and the many-body interactions, which have so far evaded from the experimental detection. The reconstruction of itinerant bands to the 4f order is dramatically changed at each distinct transition of the devil's staircase, and it exposes the strong electronic anisotropy across T_N [3]. Moreover, we discovered a new type of electron-boson coupling between the mobile electrons and crystal-electric-field excitations of the 4f-orbitals, which renormalizes the Sb 5p band prominently, yielding a remarkable kink at very lowenergy. This coupling strength of the many body state is exceedingly strong and anomalously enhanced during the devil's staircase transition [4].

Keywords
Magnetism, phase transition, photoemission, band structures

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Biography
I have received a doctoral degree in physics in 2014 from Hiroshima University, Japan. After spending a year as a visiting scientist at Prof. Ulrich Höfer's group of Phillips-Universität Marburg, Germany, I have joined Prof. Takeshi Kondo's group at the University of Tokyo, Japan. In 2021, he became an associate professor for experimental physics at Hiroshima University. My main research interests are laser photoemission spectroscopy of solid states and their ultrafast phenomena.

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Symmetry-Protected Exceptional Rings in The System Described by TheGeneralized Eigenvalue Problem

Abstract
Topological properties of electrons have extensively analyzed in these fifteen years. Remarkably, it turned out that topological band theory can be applied not only quantum systems but also classical systems.The typical example of those classical systems is photonic systems [1].As a notable point, photonic systems are described by the generalized eigenvalue problem (GEVP),in contrast quantum systems described by the standard eigenvalue problem.However, few studies have focused on the above differences from topological physics of quantum systems.

In this talk, we analyze the systems described by the GEVPwith indefinite Hermitian matrices [2].In those systems, symmetry-protected non-Hermitian topological band structure may emerge in spite of the Hermiticity [Fig.1]. We also apply our theory to the photonic system.

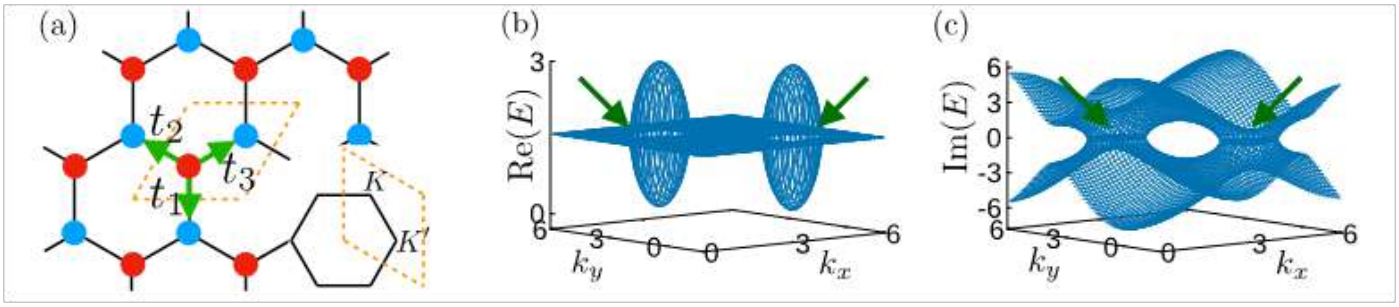

Fig. 1: Panel (a) is the sketch of the honeycomb lattice model.Panel (b) [(c)] is the real part (imaginary part) of the band structure of the GEVP with indefinite Hermitian matrices.

Keywords
Topological Band Theory, Generalized Eigen Value Problem, Photonic Systems

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Biography

Takuma Isobe is a Ph.D. student at the Graduate School of Pure and Applied Sciences,University of Tsukuba. He received his B.E. and M.E. degrees from the University of Tsukuba in 2018 and 2021.

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Universal Critical Behavior in Hubbard Models with Dirac Dispersion: Gross-Neveu-Heisenberg Class

Abstract
We investigate a quantum criticality of an antiferromagnetic phase transition in the Hubbard model on a square lattice with a d-wave pairing field by large-scale auxiliary-field quantum Monte Carlo simulations. Since the d-wave pairing filed induces Dirac cones in the non-interacting single-particle spectrum, the quantum criticality should correspond to the chiral Heisenberg universality class in terms of the Gross-Neveu theory, which is the same as those expected in the Hubbard model on the honeycomb lattice[1], despite the unit cells being different (e.g., they contain one and two sites, respectively). We show that both thesetwo phase transitions, expected to occur on the square and on the honeycomb lattices, indeed have the same quantum criticality. We also argue that details of the models, i.e., the way of counting the total number of fermion components N and the anisotropy of the Dirac cones, do not change the critical exponents. The present estimates of the exponents for the N=8 chiral Heisenberg universality class are =1.05(5), =0.75(4), and =0.23(4)[2], which are compared with the previous numerical estimations[3].

Keywords
Hubbard model, Gross-Neveu model, Dirac fermions, Quantum Monte Carlo, Quantum criticality, Critical exponents

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Biography
Yuichi Otsuka received his Ph.D. from the University of Tokyo in 2002. He is working as a researcher at RIKEN Center for Computational Science. His current research interests include strongly-correlated electrons, quantum Monte Carlo methods, and quantum computing.

Kohei Yoshimatsu
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Electronic Structures of Ti_2O_3 Films Revealed by Soft X-Ray Angle-Resolved Photoemission Spectroscopy

Abstract

Corundum-type Ti_2O_3 exhibited metal-insulator transition (MIT) at approximately 450 K over a wide temperature range of ~150 K. The characteristic MIT originated from the overlap of the Ti 3d a_{1g} and e_g^{π} bands due to lattice deformation [1]. In contrast, the on-site Coulomb repulsion was crucial to reproduce the insulating electronic structures in band-structure calculations. Thus, the importance of electron correlation was also pointed out in Ti_2O_3 [2]. Detailed information on the electronic structures was indispensable to elucidate the mechanism of the MIT in Ti_2O_3. Angle-resolved photoemission spectroscopy (ARPES) is a powerful experimental technique directly investigating electronic structures in momentum (k) space. ARPES experiments required a well-defined surface, which was a large barrier for Ti_2O_3 without any cleavable planes. Recently, we developed a thin-film growth technique to stabilize low-valence titanate films using reductive and non-equilibrium conditions [3]. Soft x-ray ARPES measurements of Ti_2O_3 were carried out using the epitaxial film with a clean and flat surface. We observed clear band dispersions along both k_z and $k_{//}$ directions, indicating that we first revealed k-resolved electronic structures of Ti_2O_3. Band-structure calculations based on GGA + U approximation were conducted to compare the experimental and calculated band dispersions. We found that the electron correlation in the calculation was essential to reproduce the experimental band dispersions.

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Biography

Kohei Yoshimatsu is an Associate Professor at Tohoku University, Japan. He received his B.S., M.S., and D.S. degrees from the University of Tokyo in 2007, 2009, and 2012, respectively. After his Ph. D. student, he became a JSPS post-doc at the University of Tokyo for a year. Then, he was an assistant professor at the Tokyo Institute of Technology between 2013-2018. Since 2018, he has been working in the present position. He has focused on oxide-thin-film growth using pulsed-laser deposition and investigation of electronic structures by using photoemission spectroscopy.

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Thermoelectricity and Topological Phase Transition as a Route to Enhance Thermoelectric Performance

Abstract

Topologically protected materials system generally share commonalities with good thermoelectric materials because of their narrow band gaps and heavy constituent elements. Here we propose that a topological crystalline insulator (TCI) and Dirac semimetal could exhibit a high thermoelectric performance by breaking its crystalline symmetry and tuning chemical potential by elemental doping. As a candidate material, we demonstrate that a weak disordering in the topological crystalline state can enhance thermoelectric performance significantly due to highly dispersive band dispersion and high band degeneracy which guarantee high electrical mobility and a high Seebeck coefficient, respectively. In addition, we demonstrate selective charge Anderson localization as a route to maximize the Seebeck coefficient while simultaneously preserving high electrical conductivity and lowering the lattice thermal conductivity. We confirm the viability of interface potential modification in an n-type Bi-doped PbTe/Ag_2Te nanocomposite, and the resulting enhancement in thermoelectric figure-of-merit ZT. The introduction of random potentials via Ag_2Te nanoparticle distribution using extrinsic phase mixing was determined using scanning tunneling spectroscopy measurements. When the Ag_2Te undergoes a structural phase transition (T > 420 K) from monoclinic β-Ag_2Te to cubic α-Ag_2Te, the band gap in the α-Ag_2Te increases due to the p-d hybridization. This results in a decrease in the potential barrier height, which gives rise to partial delocalization of the electrons, while wave packets of the holes are still in a localized state. Using this strategic approach, we achieved an exceptionally high thermoelectric figure-of-merit in n-type PbTe materials, a ZT greater than 2.0, suitable for waste heat power generation.

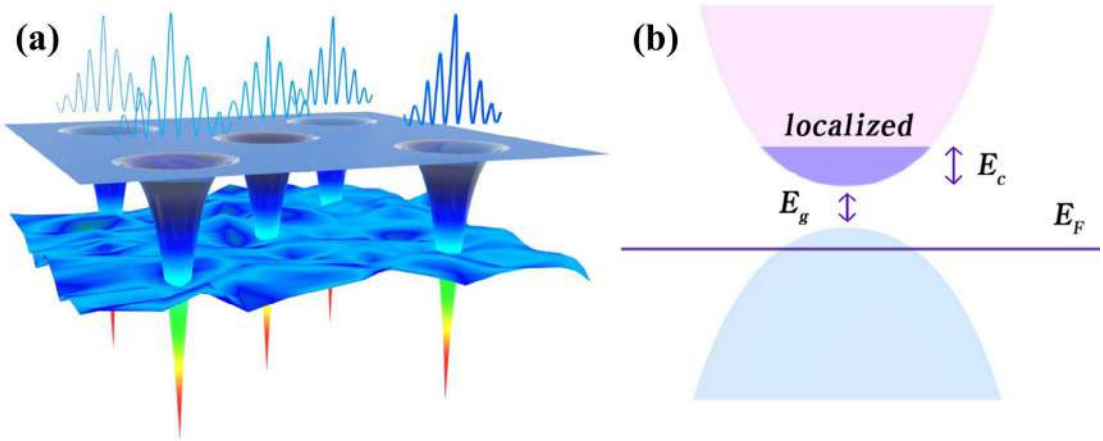

Fig.1.Schematic representation of selective Anderson localization of electron (a) and its band diagram (b)

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Ultrafast Spectroscopy of 3D-Topological Insulators by High-Order Harmonics

Abstract
We observe an anomalous strong-field optical response of the prototypical 3D topological insulator Bi2Se3, re- vealed through the process of high-harmonic generation driven by ultrashort mid-infrared fields. We find that the harmonic yield increases as the polarization of laser field is changed from linear to elliptical and it becomes maximum for a fully circular polarization. With the aid of a microscopic quantum-mechanical theory, we reveal that the observed anomalous enhancement arises from the unique band structure of the gapless topological sur- face states (TSSs). Our results bear implications for the ultrafast probing of topological phase transitions.
In the last decades, high-order harmonic genera- tion (HHG) in gases established itself as a powerful tool for investigating electron structure and dynam- ics [1-2]. Ghimire et al. [3] expanded the HHG process from gases to condensed matter systems [3]. Surprisingly, one of the main features of HHG, the high-energy cut-off exhibits a linear scaling with respect to the laser-field strength in solids, while in gases, this scaling is quadratic. Microscopically, HHG in solids entails a plethora of interesting dynamical phenomena occurring at the attosecond time scale, such as inter-band electron tunneling, Bloch oscillations, and electron-hole (e-h) quasi- particle dynamics.
In this work, we extend the scope of HHG to a distinctly different class of matter, namely, topological materials. Our measurements on the prototypi- cal topological insulator Bi2Se3 reveal an anom- alous laser-ellipticity dependence of the high-har- monic generation process, manifested in a substan- tial enhancement of selected high-harmonic (H) orders for circularly polarized laser fields (see Fig. 1 a). We attribute the latter results to the nontrivial topology of the surface Bloch bands and states, in particular the dipole couplings and Berry connec- tions close to the -point of the Brillouin zone and the influence of the high-order “warping” terms at higher momenta [4]. Our interpretation is supported by a fully quantum-mechanical treatment of the HHG process in the framework of the semiconduc- tor Bloch equations formalism (cp. Fig. 1 b).

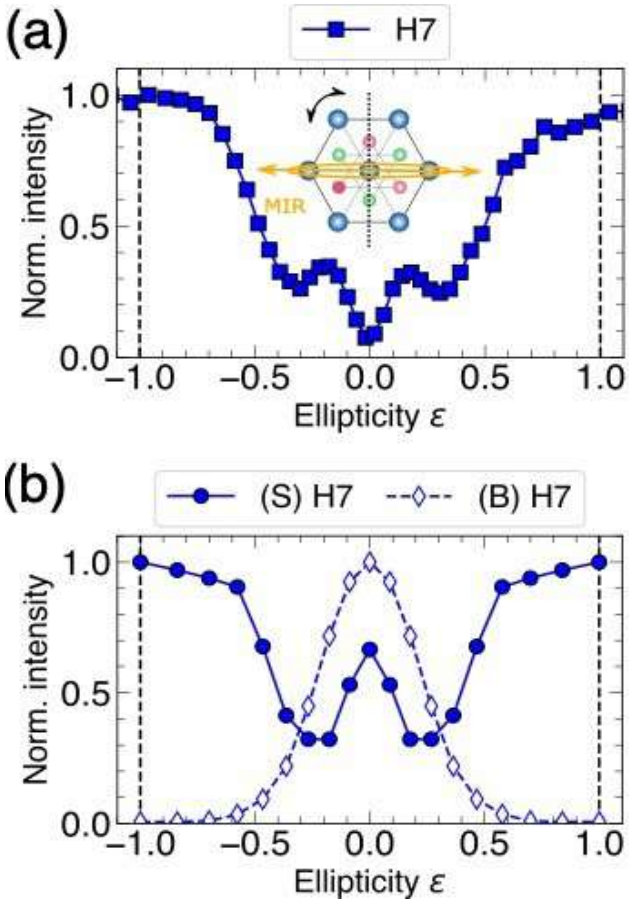

Fig. 1. Observation of anomalous ellipticity behavior. Up- per panel: Experimental yield of H7 as a function of ellipticity. Bottom panel: Theoretical calculation of the surface and bulk contributions to the HHG yield. Reproduced from Ref. [4].

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Influence Of Substrate Properties On Bonding Mechanism Of Coldsprayed Titanium Dioxide Coating

Abstract

The cold spraying of ceramic materials is widely acknowledged as a difficult process because it necessitates the feedstock powder particles experiencing a plastic deformation for deposition on a substrate. The problem arises due to the brittle properties of ceramic powder feedstock such as titanium dioxide (TiO2), combined with a lack of understanding of the bonding mechanisms. In this study, TiO2 coatings were deposited onto copper and aluminum substrates and the adhesion strength was evaluated to investigate the bonding mechanism. The influence of substrate hardness and remaining surface oxide layer was investigated by annealing the substrates with various temperatures. The results showed that the adhesion strength of the coatings on the aluminum substrate was higher than the copper substrate. Furthermore, the adhesion strength was decreased with increasing the annealing temperature on both substrate materials. These results indicate that a softer aluminum substrate was advantageous for adhesion. Annealing led to thermal softening the substrate; however, the thickness of the surface oxide layer was increased. Therefore, bonding occurred between the cold-sprayed TiO2 particle and newly deform substrate surface, which yielded the higher adhesion strength. The main bonding mechanism is metallurgical, similarly to the cold-sprayed metallic coatings.

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X-Ray Circular Dichroism of a Collinear AntiFerromagnet with a Structural Chirality

Abstract
X-ray magnetic circular dichroism (XMCD) has been widely used to explore the element-specific magnetism of magnets, such as Ferro- or Ferri-magnets with non-zero magnetization [1]. It is generally understood that an antiferromagnet exhibits no XMCD.

In contrast, we will demonstrate that a collinear antiferromagnet Ni3TeO6 with a chiral structure [2,3] does show XMCD but exhibits no net spin moment. The circular dichroism in Ni L3-edge X-ray absorption was observed to show a sign-reversal for crystallographic domains of opposite chirality. We will discuss the coupling between collinear antiferromagnet and chirality based on crystal time-reversal symmetry breaking owing to nonmagnetic atoms at non-centrosymmetric positions [4].

Keywords
Antiferromagnet, XMCD, chirality, time-reversal symmetry breaking

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Nanoresistance Networks Construction Technique in Flexible Sensing Materials

Abstract
Flexible sensors find a wide range of applications in different fields, including human-machine interfaces, electronic devices and robotics.The design and fabrication of these sensors usually have higher demands on the flexibility,miniaturization and easy processing of the sensing materials. Among them, piezoelectric materials occupy a vital position in the design of sensing systems owing to their improved mechanical properties and energy conversion efficiency at the nanoscale level. However, most piezoelectric sensing materials rely on the bottom and top planar electrodes to facilitate the assembly of piezoelectric sensors andrealize the electricity signal conduction.These sandwich-structured piezoelectric sensors with traditional metal electrodes suffer from drawbacks such as rigid, difficulty in miniaturization, disconnections between the functional materials and electrodes.Nevertheless,flexible electrodes require multiple machining, which increases the size, cost and complexity of manufacturing the sensors, limiting their practical application. Here, based on the Wheatstone bridge principle, we propose the nanoresistance networksconstruction techniqueto realize the simultaneous construction of piezoelectric materials and conductive pathwaysvia fabricatingthe flexible electrospun nanofiber integrated sensing materials throughby one-step method. The presented strategy eliminated the constraints of the sandwich structure associated with traditional devices to achieve integrated nanofibers.For the first time, the voltage signal generated by the piezoelectric material is collected and output based on the Wheatstone bridge principle through the nanoresistance network. Meanwhile, the integration of conductive paths and piezoelectric elements was beneficial in improving polarization and collection of the induced charges, contributing to enhanced piezoelectric conversion and output performance.Moreover, the nanoresistance networks can be used as a new feasible alternative material to replace the sensor array and lattice electrodes of traditional devices, and realize force localization by detecting the output voltage distribution. In addition, the multifunctional sensing properties of integrated piezoelectric sensing materials based on nanoresistance networks are also explored.

Keywords
synchronous construction, nanoresistancesnetworks,flexible piezoelectric sensors, Wheatstone bridge, electrospinning

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Tuning Topological Orders by a Conical Magnetic Field in the Kitaev Model

Abstract
We show that a conical magnetic field H=(1,1,1)H can be used to tune the topological order and hence, anyon excitations of the Z_2 quantum spin liquid in the isotropic antiferromagnetic Kitaev model. A novel topological order, featured with Chern number C =4 and Abelian anyon excitations, is induced in a narrow range of intermediate fields $H_{c1} \leq H \leq H_{c2}$. On the other hand, the C =1 Ising-topological order with non-Abelian anyon excitations, as previously known to be present at small fields, is found here to survive up to H_{c1}. The results are obtained by developing and applying a Z_2 mean field theory that works at finite fields and is asymptotically exact in the zero field limit and the associated variational quantum Monte Carlo.

Keywords
Kitaev model; Topological phase transition; topological order; Non-Abelian anyons(Maximum 4).

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Biography
Dr. Wei Chen obtained her Bachelor and Master's degree from Nanjing University, China in 2002 and 2005 respectively, and her PH.D degree in physics in 2011 from University of Washington in Seattle. She then became a postdoc fellow in McGill University in Canada. She joined the IAS in Tsinghua university as an associate fellow in 2014. In 2016, she moved to the department of physics in Nanjing University as an associate professor. Her main research interest is in strongly correlated systems and topological systems, focusing on the electronic, topological and transport properties as well as the phase transitions in such systems. She has published more than twenty research articles on various topics, such as 1D interacting systems, graphene, optomechanics and quantum spin liquid.

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^{75}As NMR Study of the Antiferromagnetic Kondo Lattice CeNiAsO

Abstract
The ZrCuSiAs-structured rare-earth oxypnictides notonly boosted a new wave of research boom on high-Tcsuperconductors, but also provided a novel playground for investigating strongly correlated electronic effects and quantum critical phenomena. Our previous works have manifested that CeNiAsO is an ideal candidate explore theheavy-fermi on properties of the 4f electrons. Here we revisit the magnetic properties of the antiferromagnetic Kondo lattice CeNiAsO by 75Asnuclear magnetic resonance measurements. Our results confirm two successive antiferromagnetic transitions of Ce moments at TN1 = 9.0(3) K and TN2 = 7.0(3) K. A Knight shift anomaly, characterized by the failure of K(T) - χ(T) scaling, is observed below T* 15 K, which gives a measure of the onset of coherent c-f correlations. This energy scale is further confirmed by the spin-lattice relaxation rate (1/T1). The analysis of spin dynamics also reveals a quasi-two-dimensional character of spin fluctuations in CeNiAsO. This work paves the way for further 75Asnuclear magnetic resonance studies under pressure.

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Biography
Yongkang Luo is a Professor in the department of Wuhan High Magnetic Field Center, Huazhong University of Science and Technology, China. He has received Awards, Patents and Honors: 2008: Excellent Graduate of Zhejiang Province, for B.S.; 2009: Excellent Thesis Award of the 12th Chinese Low Temperature Physics Society Conference; 2012: Chinese National Scholarship, for Ph.D.; 2018: 1000 Youth Talents Plan of China. He has given 20+ participations and has 75+ publications. Research Interests: Condensed matter physics, Experimental physics. Superconductivity, Magnetism, Strongly correlated systems, Topological materials, Quantum matters. Transport measurements, Resonant Ultrasonic Spectroscopy, Magnetic Resonance.

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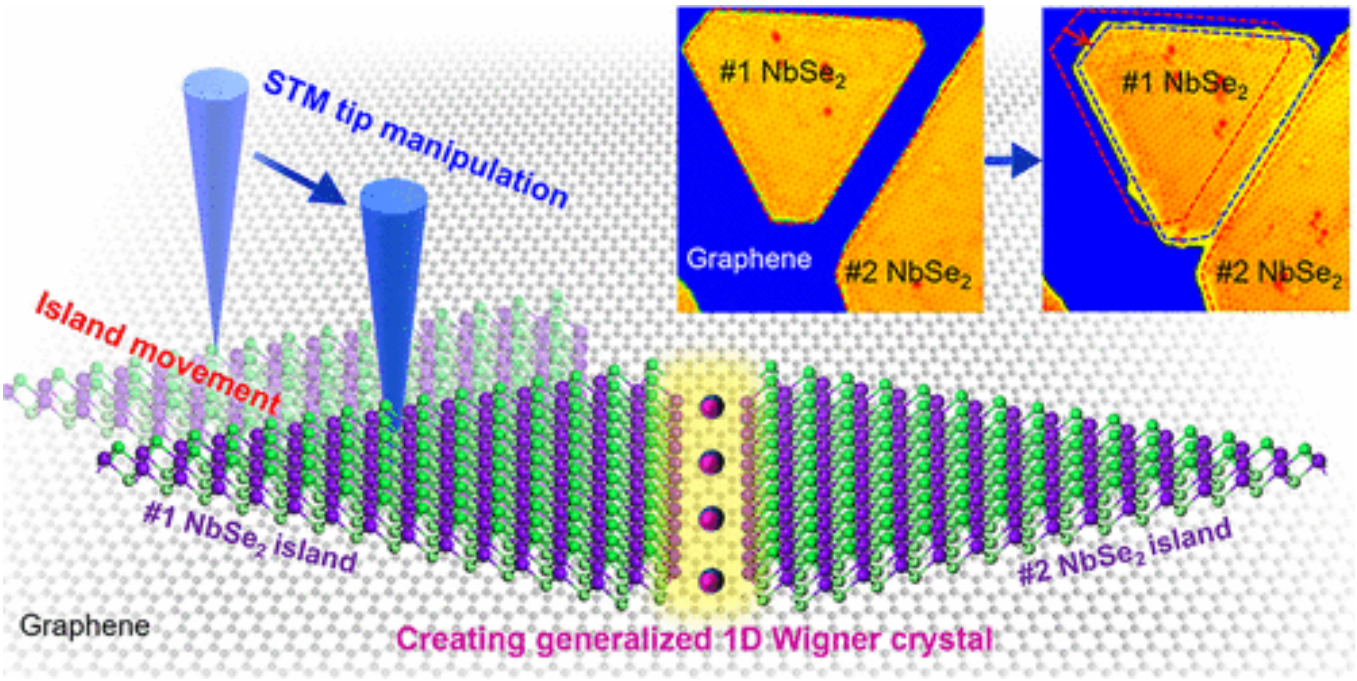
Nanoscale Control of One-Dimensional Confined States

Abstract

Construction of lateral junctions is essential togenerate one-dimensional (1D) confined potentials that caneffectively trap quasiparticles. A series of remarkable electronicphases in one dimension, such as Wigner crystallization, areexpected to be realized in such junctions. Here, we demonstratethat we can precisely tune the 1D-confined potential with an in situmanipulation technique, thus providing a dynamic way to modifythe correlated electronic states at the junctions. We confirm theexistence of 1D-confined potential at the homojunction of twosingle-layer 1T-NbSe2 islands. Such potential is structurallysensitive and shows a nonmonotonic function of their interspacing. Moreover, there is a change of electronic properties from thecorrelated insulator to the generalized 1D Wigner crystallization while the confinement becomes strong [1]. Our findings not onlyestablish the capability to fabricate structures with dynamically tunable properties, but also pave the way toward more exoticcorrelated systems in low dimensions.



Keywords

Confined Potential, Homojunction, Manipulation, Correlated Insulator

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Biography

Yu Zhang is an associate professor in Beijing Institute of Technology, China. She completed her Ph.D. in physics at Beijing Normal University. Since the year 2016, she has been focusing on the construction and manipulation of the novel electronic states in two-dimensional materials.

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Optimization of Mxene Photoelectrodes for Energy Conversion and Storage Purposes

Abstract
This study significantly reveals the basic insights into utilizing Mxene functionalized mesoporous TiO2 as a photoelectrode. This novel composite based upon Mxene functionalized TiO2 electrodes with and without TiCl4 treatment is fabricated to achieve efficient photon absorption; charge separation and photocurrent; causing superior photoelectrode performance. Here-in, Mxene was prepared through selective etching of Ti3AlC2 powder in HF solution. Furthermore, the seed solution for TiO2: Mxene layers was prepared by adding Mxene dispersion into titanium disopropoxide bis (acetylacetonate) and dropped onto FTO substrates in a specific amount. These films were further chemically modified in multi steps such as Mxene-added TiCl4 treatment and then by Mxene- mesoporous layer. The enhanced photocurrent values were recorded in the prepared samples upon increased contents of Mxene due to higher absorption efficiency within the visible region; as verified by UV-Vis absorption spectroscopy. The anatase phase of TiO2 is clearly prominent due to increased amount of Mxene and postdeposition thermal exposure; as revealed by structural analysis. Moreover, a good coverage of well-developed grains on the FTO surface was observed in SEM images. Therefore; these newly developed conductive mesoporous TiO2 photoelectrodes are potential candidates for photoinduced energy conversion and storage applications.

Keywords
Mxene; Energy storage; Surface Plasmon Resonance (SPR); nano structuring; photocatalyst; mesoporous Titania

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Guodong (David)
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A New Way to Convert Opaque CVD Diamond into Transparency

Abstract
Diamond's unique combination of excellent optical, thermal and mechanical properties, as well as other properties such as low coefficient of friction, make it an ideal material for many applications, such as "industrial teeth" in the oil and gas industry and/or optical windows for harsh and extreme environments.Despite the large intrinsic band gap (5.5 eV) of diamond, most natural diamonds absorb light from the ultraviolet, visible, and infrared spectral regions due to microstructural defects and/or internal stresses/strains.In recent years, the synthesis of free-standing diamond films by chemical vapor deposition (CVD) has attracted considerable academic and industrial interest. However, when the thickness of the diamond film reaches the millimeter level, it is difficult to meet the requirements of transparent materials due to more internal defects at larger sizes. The optical properties of CVD diamond are enhanced by low-pressure/high-temperature annealing. However, polycrystalline CVD diamond films have poor stability under heat treatment at high temperatures and have significant optical degradation.High Pressure/High Temperature (HPHT) annealing has been shown to significantly alter the optical properties of diamond, especially by reducing UV/VIS absorption, thereby increasing the potential use of the material in a variety of applications. High-pressure/high-temperature annealing has become a commercial process that changes the optical properties of natural diamonds.The process requires a temperature range of 1800-2500°C and typically uses a pressure of ~5 GPa to prevent diamond graphitization. However, the variation in the optical properties of natural diamonds and CVD diamonds and the origin of the annealing mechanism are unclear.In this report, for the first time, we will propose a new method for transforming opaque CVD diamonds into transparent ones with enhanced optical and mechanical properties. The new reinforced transparent CVD diamond will broaden the range of applications.

Biography
Dr. Guodong (David) Zhan is currently a Science Specialist and the Team Leader of Drilling Technology Team at the Exploration & Petroleum Engineering Center - Advanced Research Center, Saudi Aramco. Dr. Zhan is a world-renowned materials scientist and expert in advanced drilling tools/technology. He has over 29 years of experience in industrial R&D and managerial positions, including positions as Chief Engineer and R&D Manager at top oil/gas and semiconductor global companies such as Schlumberger and Applied Materials. Additionally Dr. Zhan has held academic positions at the University of London and the University of Colorado at Boulder, and staff scientist

positions at the Japan National Institute for Materials Science and Shanghai Institute of Ceramics, Chinese Academy of Science.

Dr. Zhan is an active member of the Society of Petroleum Engineer (SPE), where he serves on several conferences as co-chair and technical committee member. He received many prestigious academic and industrial awards such as E&P Hart Energy Award, IoT World Award and World Oil Award. Dr. Zhan is also serving as an editorial board member and reviewer for a number of international scientific journals. Dr. Zhan has published in 98+ peer-reviewed journals such as Nature Materials and Scientific Reports, 100+ conference proceedings, and holds more than 120 filed/granted US patents with citations of 5,000+ and an H-index of 37.

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Superconductivity of Organometallic Fullerides Intercalated with Methyl Me, Ethyl Et, Butyl Bu and Ammonium NH4

Abstract
In this work, for the first time, the superconducting and structural properties of heterofullerides intercalated with ammonium and ammonium bases: ammonium, tetramethylammonium, tetraethylammonium, tetrabutylammonium, synthesized by exchange reactions of fullerides of alkali metals with halides of ammonium bases in an organic solvent are investigated. Taking into account the size and properties of the NH4 + cation, the existence of a superconducting fulleride of the composition (NH4+)3C60 3- was predicted in [1]. Previously we found superconductivity in heterofullerides of alkali and transition metals [2-5]. We also investigated the isotopic effect in homofullerides with ammonium compositions K1-n(NR4)xC60 and Rb1-n(NR4)nC60 (R=H, D; n=1, 2, 3). The superconductor (NH4)3C60 has Tc=16.4 K. All superconductors crystallize in fcc crystallattices with increased crystal lattice parameters “a” in comparison with the initial known superconductors K3C60 and R3C60. However, despite this, the superconducting transition temperatures of these substances turned out to be lower than those of the initial fullerides (18.5 K for K3C60 and 29 K for Rb3C60): Tc=14-16 K for fullerides with potassium and Tc=19-20 K for fullerides with rubidium. The superconducting transition temperature did not change when H was replaced by D within the measurement accuracy. From this we can conclude that the main role in superconductivity is played by phonons bound to the C60 molecule.

Keywords
Superconductivity, fulleride, isotope effect

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Biography
Vladimir A. Kulbachinskii graduated from Lomonosov Moscow State University, Physics Faculty and was awarded a PhD degree in 1978. In 1991 was awarded a Dr. of Science degree. His

research interests include low temperature physics, superconductivity, graphite intercalation compounds, high pressure, thermoelectricity, magnetism, fullerenes and fullerides, etc. Current status is a distinguished professor of Lomonosov Moscow State University, Low Temperature and Superconductivity department, co-author of more than 400 scientific papers. He is a Laureate of the Russian Federation Government award for his pedagogical activity.

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Metal-Insulator Transition and Robust Thermoelectricity via Strain-Tuned Interplay Between Structural and Electronic Properties in (SrVO3)1/(SrTiO3)1(001) Super Lattices

Abstract
Exploring the origin of the metal-to-insulator transition (MIT) in transition metal oxide heterostructures is of high interest in current condensed matter physics research. Based on the density functional theory calculations combined with an on-site Coulomb repulsion term U for (SrXO3)1/(SrTiO3)1(001) superlattice (SL), X = V and Ru, a general recipe has been outlined to address the electronic and magnetic properties using the correct ground state structural symmetry, at a given in-plane lattice constant. This work demonstrates that the meta GGA SCAN functional correctly describes the structural properties and is already sufficient to address the electronic and magnetic properties of the weakly correlated (SrRuO3)1/(SrTiO3)1(001) SL and its bulk constituent by minimizing the self-interaction error. In contrast, an additional on-site Coulomb repulsion term is necessary to describe the electronic and magnetic properties of the correlated bulk SrVO3 as well as in (SrVO3)1/(SrTiO3)1(001) SLs. Based on the structural symmetries of (SrVO3)1/(SrTiO3)1(001) Sls at the in-plane lattice constants of bulk STO and YAO, respectively, determined by SCAN functional, this work reports distinct mechanisms of the metal-to-insulator transition in the (SrVO3)1/(SrTiO3)1(001) Sls. Using the Boltzmann transport theory within the constant relaxation time approximation for (SrVO3)1/(SrTiO3)1(001) SL at the in-plane lattice constant of bulk STO, a robust thermoelectric response was obtained, categorizing it among the prominent oxide thermoelectric materials. These results might be instructive for studying the strongly correlated quantum phases by incorporating realistic structural degrees of freedom in other, not limited to SrTiO3, based SLs.

Biography
Manish Verma started his PhD in 2017 in the group of Prof. Dr. Rossitza Pentcheva at the University of Duisburg-Essen, Duisburg, Germany, and is awaiting his defense. He earned his M.Sc. in physics from Thapar University, India in 2015. In 2016, he worked as a pre-PhD researcher at Thapar University in collaboration with Dr. Volker Eyert at Materials Design, S.A.R.L., France. His research focuses mainly on the electronic, magnetic, and thermoelectric properties of transition metal oxide super lattices and surfaces using state-of-the-art density functional theory and beyond.

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Two-Dimensional Material Confined Water

The interface between water and solid materials under ambient conditions are of fundamental importance due to their relevance in daily life and a broad range of scientific research. The structural and dynamic properties of water at an interface have been proven to be a significant difference from those of bulk water. However, the exact nature of these interfacial water adlayers at ambient conditions is still under debate. Recent scanning probe microscopy (SPM) experiments, where two-dimensional (2D) materials such as ultrathin coatings are utilized to assist the visualization of interfacial water adlayers, have made remarkable progress on interfacial water and started to clarify some of these fundamental scientific questions. In this talk, we review the recently conducted research exploring the properties of confined water between 2D materials and various surfaces under ambient conditions. We focus on the studies of water ad layer growth at both hydrophilic and hydrophobic substrates in the presence of 2D coating materials. Ice like water adlayers confined between hydrophobic graphene and hydrophilic substrates can be directly observed in detail by SPM. It was found that the packing structure of the water adlayer was determined by the hydrophilic substrates, while the orientation of intercalation water domains was directed by the graphene coating. In contrast to hydrophilic substrates, liquid-like nanodroplets confined between hydrophobic graphene and hydrophobic substrates appear close to stepping edges and atomic-scale surface defects, indicating that atomic-scale surface defects play significant roles in determining the adsorption of water on hydrophobic substrates. In addition, we also review the phenomena of confined water between 2D hydrophilic surfaces and the hydrophilic substrate. Finally, we further discuss researchers taking advantage of 2D coatings to stabilize confined water nanodroplets to manipulate nanofluidics by applying an external force by using novel SPM techniques. These new findings potentially can be utilized to understand the boundary condition for water structures and dynamic behaviors at interfaces, and the aqueous interfacial chemistry

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Advances in Complex Functional Materials through Templating

Abstract

Templating methods employing soft templates (e.g., surfactants, block co-polymers, emulsions), hard templates (e.g., colloidal particles, colloidal crystals), or both together, are powerful approaches for controlling structure of materials, in particular porous materials, on multiple length scales to effect specific functions. Many applications require materials with complexity in both structure and composition. During synthesis and processing of complex materials, multiple interactions between templates and precursors can provide a richness in structure, but can also be exploited to influence the arrangement and distribution of separate components in a complex material. This tutorial review will highlight methods of controlling parameters of importance for functional materials, including surface area; pore geometry and shape; pore hierarchy, interconnectivity and accessibility; transport path length; material composition and component distribution in multicomponent systems; surface functionality; site isolation; and stability. The impact of these parameters on functional materials for energy storage and conversion, catalysis, sensing, and optical/photonic materials will be discussed with specific examples from our research in this area.

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Some Challenges in Understanding the Corrosion of Copper

Abstract

Although copper and its alloys are among the most studied systems from a corrosion perspective, manychallenges remain to be explored in order to fully understand the physico-electrochemistry of the corrosion process as related, for example, to the disposal of high-level nuclear waste and the corrosion of electronic microcircuits. For instance, it is known that sulfur-containing species, such as bisulfide (HS-), induce the rapid corrosion of copper by enabling hydrogen evolution to become a viable partial cathodic reaction thereby leading to the rapid destruction of the metal substrate. Furthermore, it has also been reported that oxygen-free, phosphorous copper (OFP-Cu) does not pit in sulfide-containing geological brine that is of interest in the disposal of HLNW in granitic rock repositories, whereas pure Cu does and yet the nominal difference in composition is only 40 - 60 ppm P in OFP-Cu. The mechanism by which phosphorous at such low concentrations induces pitting resistance on copper is currently unknown. However, a promising approach to resolving this issue is contained within the Solute-Vacancy Interaction Model (SVIM), which postulates that the phosphorous segregates from the metal into the Cu2S barrier layer substitutionally onto the cation sublattice to yield highly, positively charged local centers () that interact with the mobile, negatively charged cation vacancies (), which leads to passivity breakdown. Thus,this electrostatic interaction impedes the movement of cation vacancies, such that a higher voltage must be applied to achieve cation vacancy condensation at the metal/barrier layer interface resulting in a higher passivity breakdown potential. In this talk, I will review the corrosion chemistry of copper in a variety of environments and indicate the current directions of research.

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Kondo Effect at Nanoscale In Ytterbium Organometallic Molecule Cp*2Yb(4,4'-Me2-Bipy) Under High Pressure

Abstract
Analogous to the Kondo effect in bulk 4f intermetallic systems, a group of ytterbium organometallic molecules, Cp*2Yb(L) [Cp* is pentamethylcyclopentadienyl, L is various 2,2' - bipyridine related ligand] is reported to show Kondo effect at nanoscale. Similar to canonical compounds like cerocene [Ce(C8H8)2] and ytterbocene Cp*2Yb(bipy) [Cp*=pentamethylcyclopentadienyl, bipy=bipyridine), these group of compounds also show coupling between magnetic ions and the aromatic ring through Kondo effect. Cp*2Yb(4,4'-Me2-bipy) molecule belongs to this class of compounds and is an intermediate valance system. Complete Active Space Self-Consistent Field (CASSCF) calculations for this compound shows that it is an intermediate valence system due to the configuration interaction between open shell [4f↑13π↓*1] and closed shell [4f↑↓14π*0] spin singlet states. This is analogous to the Kondo effect in intermetallic systems where the system contains mixture of energetically close different valences like Yb2+ [(5d6s)24f14] and Yb3+ [(5d6s)34f13]. Our previous work shows a valance transition at 200 K observed through magnetic susceptibility and x-ray absorption measurements. Here, we report on the room temperature high pressure (0 - 15 GPa) x-ray absorption measurements in partial fluorescence yield mode (XAS- PFY) on Cp*2Yb(4,4'-Me2-bipy) molecule at the Yb L3 absorption edge. Our analysis shows that with the increase in pressure the mean valency of the Yb atom shows an overall increase from 2.77 at 2.78 GPa to 2.97at 15.39 GPa. Compare to the overall change in the mean valency, the change in the pressure region ~ 3.26 GPa is very drastic due to change in the slope.

Biography
Farzana Nasreen received her MSc in Physics from University of Hyderabad, India in 2003. She finished her PhD in physics from New Mexico State University in 2010. During her Ph. D, she worked at National High Magnetic Field Laboratory (NHMFL) at Los Alamos as a visiting graduate student and studied different kinds of uranium intermetallic compounds and organometallic compounds which exhibit strongly correlated electron behavior such as quantum criticality, superconductivity, heavy fermion, non-Fermi liquid behavior and multiferroic behavior. In her last year of PhD, she was awarded Seaborg Fellowship from G. T. Seaborg Institute for Transactinium Science. Afterwards, she worked as a postdoctoral research associate at High Pressure Science and Engineering Center (HiPSEC) at the University of Nevada, Las Vegas from 2012 to 2014. In her postdoctoral work, she

studied different rare earth and uranium intermetallic and organometallic compounds under very high pressure (up to 50 GPa) to investigate their valence fluctuation phenomena using synchrotron x-ray absorption spectroscopy and x-ray scattering technique at high pressure beamline at Advance Photon Source in Argonne National Laboratory. Currently, she is working as a postdoctoral fellow in Physics and Astronomy Department at Colgate University. Her research work is in the area of superconducting neuromorphic computing.

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Flexible & Stretchable Random Lasers and Random Fiber Lasers

Abstract
Random Lasers (RLs) and Random Fiber Lasers (RFLs)have attracted a great deal of interest in the last 3 decades. They are coherent optical sources and differ from conventional laserdue to the optical feedback mechanism: in RLs (RFLs),the oscillation in the gain material comes from scattering in a disordered media, rather than from two static mirrors.Therefore, RLs (RFLs) are cavityless, but they are not modeless, and behave as multimode lasers. The subject was first theoretically introduced in 1967, has been recently reviewed [1].
In this talk, I willinitially review the state-of-the-art in RLs and RFLs. Then, we shall focus on one of the modernadvantagesof this photonic device, which is their ability to be flexible and stretchable, yet emitting coherent radiation. Examples for biomaterials host for RLs will be emphasized.

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Granular Superconductivity at Room Temperature at the Stacking Faults of Graphite

Abstract

While early reports assumed graphite samples as a semimetal based on galvanomagnetic and magnetization results, recent studies reveal that the ideal graphite structure with Bernal or rhombohedral stacking orders is a narrow gap semiconductor. The metallic as well as superconducting properties are localized mainly on the stacking faults (SFs) one can recognized through TEM measurements with the electron beam parallel to the graphene layers. After showing this evidence I will discuss the magnetotransport studies on several TEM lamellae and bulk samples of natural graphite that provide evidence for the existence of granular superconductivity to temperatures as ~350K. Current-voltage curves obtained in superconducting TEM graphite lamellae are quantitatively identical to the years-later published results on twisted bilayers graphene, confirming a common origin for the superconductivity in bulk graphite samples reported in the last 50 years. As a further proof for the granular nature of the superconductivity in the SFs of graphite, I will show magnetic force microscopy (MFM) measurements of permanent current lines in remanent state of the samples, obtained after removing an applied magnetic field at room temperature. Several experimental and theoretical works of the last years suggest that the SFs between Bernal and rhombohedral stacking orders are probably the ones with the highest superconducting critical temperature.

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