Eleventh Annual International Workshop on Advanced Materials (IWAM 2019)

Sunday, February 24 – Tuesday, February 26, 2019

Al Hamra Convention Center
Ras Al Khaimah, United Arab Emirates

Workshop Program

Eleventh Annual International Workshop on Advanced Materials

(IWAM 2019)

Al Hamra Convention Center, Ras Al Khaimah, UAE

Sunday, February 24 – Tuesday, February 26

Saturday 23rd February 2019

14:00 onwards	**Check-in at Hilton Al Hamra Beach & Golf Resort**
18:00-22:00	**IWAM Registration & Reception** ***Hilton Al Hamra*** ***Le Chalet garden (weather permitting)***

Day 1: Sunday 24th February 2019

Session I	Opening Session	Start time: 08:30 End time: 10:00
08:30	**Welcome & Overview of RAK CAM** **Professor Tony Cheetham** Chairman, Ras Al Khaimah Centre for Advanced Materials	
09:00	**Keynote Address** **His Highness Sheikh Saud bin Saqr Al Qasimi** Member of the Supreme Council of UAE and Ruler of Ras Al Khaimah	
09:30	**Our Global Strategy and Philosophy** **Tadaaki Yoshinaga** GSI Creos Corporation Tokyo, Japan	
10:00	**Coffee Break**	

Session II	Materials Physics	Start time: 11:00 End time: 12:20
	Chair: Stuart Parkin	
11:00	**Tuning Properties of Strongly Correlated Oxides using 3D Strain Control** **Judith L. MacManus-Driscoll** Department of Materials Science and Metallurgy University of Cambridge Cambridge, United Kingdom	

11:40	**New Topological Insulators Under High Pressure** **Chandrabhas Narayana** Chemistry and Physics of Materials Unit, School of Advanced Materials Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India
12:20	**Lunch** ***Al-Jazeera Restaurant***

Session III	**Energy Materials**	**Start time: 14:00** **End time: 16:40**
	Chair: Michael Klein	
14:00	**Dresselhaus Memorial Lecture** **Sustainable Energy Materials from First Principles** **Emily A. Carter** School of Engineering and Applied Science Princeton University Princeton, New Jersey, United States of America	
15:00	**High Voltage Phosphate Cathodes for Na-ion Batteries** **Premkumar Senguttuvan** New Chemistry Unit International Centre for Materials Science and School of Advanced Materials Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India	
15:30	**Preparing Organic Electronic Materials under Continuous Flow Conditions** **Andrew Holmes** School of Chemistry and Bio21 Institute University of Melbourne Victoria, Australia	

16:10	**Graphene-based Materials for Applications in Heterogeneous Catalysis, Water Treatment and Solar Water Desalination** **M. Samy El-Shall** Department of Chemistry Virginia Commonwealth University Richmond, Virginia, United States of America
16:40	**Coffee Break** **Free time for informal discussions**

Session IV	**Graduate Student and Post-Doctoral Researcher Talks**	**Start time: 17:30** **End time: 18:30**
	Chair: Chandrabhas Narayana	
17:30	**Discrete Carbon Fractional Order Superapacitors in Flexible Polymer Matrix** **Anis Allagui, Mohammad Abdelkareem, and Halima Alnaqbi** Department of Sustainable & Renewable Energy Engineering University of Sharjah Sharjah, United Arab Emirates	
17:45	**Nonstoichiometry Misfit Calcium Cobalt Oxide as a New Generation Electrocatalyst for Overall Water Splitting** **Kankona Singha Roy and Leela S. Panchakarla** Department of Chemistry Indian Institute of Technology Bombay Mumbai, India	
18:00	**Magnetocaloric Materials based on Binary and Ternary Mn Compounds: Screening and Testing** **Joya A. Cooley, Joshua D. Bocarsly, Matthew Horton, Kristin A. Persson, and Ram Seshadri** Materials Research Laboratory University of California, Santa Barbara Santa Barbara, United States of America	

18:15	**Imaging Assisted Quantitative Colorimetric and Adsorption based Detection of Heavy Metal Ions using Disposable Paper Sensor Strips in Water** **Rishabh Jain, Pahul, Neerja Mittal, Praveen Kumar, and Pooja D.** Material Science Division, Agrionics CSIR-Central Scientific Instruments Organisation Chandigarh, India

Session V	**Poster Session**	**Start time: 18:30** **End time: 20:30**
18:30	**Poster Session I** ***Al Hamra Convention Center***	

End of Day 1

Day 2: Monday 25th February 2019

Session VI	Polymers and Soft Matter	Start time: 09:00 End time: 11:00
	Chair: Susumu Kitagawa	
09:00	**Advanced Design of Self-Healable Materials by Supramolecular Chemistry** **Takuzo Aida** Riken Center for Emergent Matter Science, Saitama, Japan Department of Chemistry and Biotechnology, School of Engineering The University of Tokyo, Tokyo, Japan	
09:40	**Advanced Materials from Metal–Phenolic Networks** **Frank Caruso** ARC Centre of Excellence in Convergent Bio-Nano Science and Technology, and the Department of Chemical Engineering The University of Melbourne, Parkville Victoria, Australia	
10:20	**Self-assembly of Clay/Biopolymer Nano-Composites** **Erika Eiser** Cavendish Laboratory University of Cambridge Cambridge, United Kingdom	
11:00	**Coffee Break**	

Session VII	Computer Simulation	Start time: 11:30 End time: 12:50
	Chair: Emily Carter	
11:30	**Liquids, Crystals, Liquid Crystals, Plastic Crystals, and More ...** **Michael L. Klein** Temple University Philadelphia, Pennsylvania, 19122 USA	
12:10	**Simple yet Successful Descriptors for Self Assembly of Organic Molecules on Surfaces** **Shobhana Narasimhan** Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India	
12:50	**Lunch** ***Al-Jazeera Restaurant***	

Session VIII	Sheikh Saud Award Lecture	Start time: 14:15 End time: 15:15
	Chair: Tony Cheetham	
14:15	**Award of the Sheikh Saud International Prize for Materials Science to Professor C. N. R. Rao, followed by the award lecture** **Glimpses of Materials Highlights, 1958-2019** **C. N. R. Rao** International Centre for Materials Science, New Chemistry Unit, Sheikh Saqr Laboratory and CSIR Centre of Excellence in Chemistry Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India	
15:15	**Coffee Break**	

Session IX	Nanomaterials	Start time: 16:00 End time: 17:00
	Chair: Samy El-Shall	
16:00	**The Next Generation of Robust and Low-Fouling Desalination Reverses Osmosis Membranes based on Carbon Nanotubes-Polyamide Nanocomposite** **Morinobu Endo** COI Aqua Innovation Center and Institute of Carbon Science Shinshu University Nagano, Japan	
16:40	**Carbon Nanotubes Dispersed Super Coating: Its Contribution by our RAK Facility to Oil and Gas Industries in UAE** **Takashi Yanagisawa** Nanotechnology Division GSI Creos Corporation Tokyo, Japan	
17:00	**Coffee Break**	

Session X	Graduate Student and Post-Doctoral Researcher Talks	Start time: 17:30 End time: 18:30
	Chair: Ram Seshadri	
17:30	**Supramolecular Approach to 2D Heterostructures and to the Non-covalent Functionalization of 2-D Materials** **Manjodh Kaur, Navin Kumar Singh, Aritra Sarkar, Subi J George, and C. N. R. Rao** International Centre for Materials Science, Sheikh Saqr Laboratory Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India	

17:45	**Porous Ti Alloys with Non-Cytotoxic Nb and Sn for Body-Implant Applications** **D. Sri Maha Vishnu, Jagadeesh Sure, R. Vasant Kumar,** **and Carsten Schwandt** Department of Materials Science and Metallurgy, University of Nizwa, Oman Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom
18:00	**Mechanically Induced Transition from Indirect to Direct Bandgap in Nanocrystalline Silicon Powder** **Ankit Goyal, P R Soni, and Akhil Garg** Department of Mechatronics Engineering Shantou University Shantou, China
18:15	**From Quasicrystals to Crystals and Superconductors in Ca/Y-Au-Al** **Joyce Pham, Walter Schnelle, Claudia Felser, and Gordon J. Miller** Department of Solid-State Chemistry Max Planck Institute for Chemical Physics of Solids Dresden, Germany

Session XI	**Poster Session**	**Start time: 18:30** **End time: 20:30**
18:30	**Poster Session II** ***Al Hamra Convention Center***	

End of Day 2

Day 3: Tuesday 26th February 2019

Session XII	Inorganic Materials	Start time: 09:00 End time: 10:20
	Chair: Judith Driscoll	
09:00	**Lone Pairs in the Halide Perovskites, Hidden or Otherwise** **Ram Seshadri** Materials Department, and Department of Chemistry & Biochemistry University of California at Santa Barbara Santa Barbara, California, United States of America	
09:40	**Topological Materials Science** **Claudia Felser** Max Planck Institute for Chemical Physics of Solids Dresden, Germany	
10:20	**Coffee Break**	

Session XIII	Semiconductor Devices	Start time: 11:00 End time: 12:10
	Chair: Claudia Felser	
11:00	**Oxide Meso-Structures Formed by Ionic Liquid Gating** **Stuart S. P. Parkin** Max Planck Institute of Microstructure Physics Halle, Germany	
11:40	**Engineering Schottky Barrier Height in Epitaxial TiN/(Al,Sc)N Metal/Semiconductor Superlattices for Thermionic Energy Conversion** **Bivas Saha** International Centre for Materials Science & Chemistry Physics of Materials Unit Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India	

12:10	**Group Photo**
12:30	**Lunch** ***Al-Jazeera Restaurant***

Session XIV	**Metal-Organic Frameworks**	**Start time: 14:30** **End time: 17:00**
	Chair: Shobhana Narasimhan	
14:30	**New Dimensions of Porous Coordination Polymers/Metal-Organic Frameworks** **Susumu Kitagawa** Institute for Integrated Cell-Material Sciences Kyoto University Kyoto, Japan	
15:10	**MOF Design to Applications: Impact of Pore System Control on Gas Separations and Storage** **Mohamed Eddaoudi** Advanced Membranes and Porous Materials Centre, Functional Materials Design, Discovery and development (FMD3) Research Group King Abdullah University of Science and Technology (KAUST) Thuwal, Saudi Arabia.	
15:50	**Hybrid Perovskites and Related Materials with Oxygen-Containing Linkers** **Anthony K. Cheetham** Department of Materials Science and Engineering National University of Singapore Singapore	
16:30	**Closing Remarks** **Tony Cheetham**	
17:00	**Coffee Break**	

19:00	**Dinner Banquet at the Palace hosted by** **His Highness Sheikh Saud bin Saqr Al Qasimi** Member of the Supreme Council of UAE and Ruler of Ras Al Khaimah *All guests must wear nametag to attend banquet

End of Day 3

Sunday, February 24, 2019; 9:30

Our Global Strategy and Philosophy

Tadaaki Yoshinaga

GSI Creos Corporation
Tokyo, Japan

This talk will describe our global strategy that Creos Group as international trading enterprise actively seeks out fresh approaches to world market and “evolution and growth” we look forward to beyond existing frameworks. Further, this talk will also describe our coating facility located in Ras Al Khaimah. This RAK subsidiary offers the world best super coating film contributing to any metallic part in Oil and Gas Plants in region. Our activity in RAK with ultra-high technology also embodies our company’s global philosophy.

Sunday, February 24, 2019; 11:00

Tuning Properties of Strongly Correlated Oxides using 3D Strain Control

Judith L. MacManus-Driscoll

Department of Materials Science and Metallurgy
University of Cambridge
United Kingdom

Since the discovery of high temperature superconductivity in, the unearthing of a huge range of physical phenomena in strongly correlated oxides (TMOs) has been remarkable, e.g. new magnetics, ferroelectrics, multiferroics, semiconductors, transparent conductors, calorics, plasmonics, catalysts, etc. The link between lattice structure and properties is very strong and anisotropic (both a benefit and a drawback). To realise the benefits, and hence to dial-in entirely new functionalities, the lattice structure must be engineered in a highly controlled way. In this talk, I show how to 3D strain engineer thin films to enable such new functionalities to be achieved. I show examples in a range of device systems, including superconductors, magnetics, ferroelectrics, and ionics.

Sunday, February 24, 2019; 11:40

New Topological Insulators Under High Pressure

Chandrabhas Narayana

Chemistry and Physics of Materials Unit, School of Advanced Materials
Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)
Bangalore, India

There is a great interest in the new class of materials called Topological Insulators. It has been demonstrated that one of the needs for materials to properties like Dirac Semi-metals, Topological Insulators, Superconductors is a strong spin orbital coupling. Chalcogenides with heavier elements show the strong spin orbit coupling and have been found to be a good candidate for Topological Transitions. Usually by tuning spin orbit coupling one can induce topological transitions. We use pressure to introduce topological transitions. We report the hydrostatic pressure induced multiple topological phase transitions on strong spin-orbit coupling material $TlBiS_2$ at room temperature. Our combined *in situ* high pressure synchrotron XRD and Raman scattering measurements confirms that ambient rhombohedral phase stability up to ~4.0 GPa and a reversible first order structural phase transition has been identified at above ~4.0 GPa. Also, our Raman study shows that first order phonon frequency's (A_{1g} and E_g modes) increases monotonically up to ~4.0 GPa with a small noticeable change at ~1.8 GPa. Interestingly, the phonon linewidths show anomalies at ~0.5 GPa and ~1.8 GPa, which evidence the isostructural electronic transitions associated with this unusual electron-phonon coupling. Further, our first principles density functional theory based electronic band structure and topological invariant Z_2 calculations reveal that the phonon anomalies at ~0.5 GPa and ~1.8 GPa are related to the band inversions at Γ and F points of the Brillouin zone respectively. Hence, this successive band inversions associated with parity change makes the system ($TlBiS_2$) to undergoes into topologically non-trivial (Z_2=1) and trivial (Z_2=0) quantum phase transitions respectively under hydrostatic pressure. Besides, bulk modulus, axial compressibilities and pressure coefficients of phonon modes (A_{1g} and E_g) have been reported and discussed. Finally, based on the pressure evolution of clean semiconducting band structure, we propose that $TlBiS_2$ is a potential and unique candidate for exploring the many exciting physics behind topological effect using multiple high pressure techniques. As another example we have studied $TiSe_2$. High pressure Raman spectroscopy studies on 1T-$TiSe_2$ were carried out up to ~ 20.5 GPa. Based on the anomalies in phonon linewidth (lifetime) and phonon frequency of A_{1g} we observe three transitions at ~2.5 GPa, ~6.0 GPa and ~15 GPa. The transitions at ~2.5 and ~6.0 GPa are the two Topological Quantum Phase Transitions (TQPTs) consistent with the theoretical prediction by Zhu et al. in IT-$TiSe_2$ under pressure, namely, a topological trivial to non-trivial transition (Z_2 =1) and topological non-trivial to trivial transition (Z_2 = 0). The trigonal (1T) phase of $TiSe_2$ is stable up to ~15 GPa beyond which it undergoes structural transition as seen from the appearance of new Raman modes. There is a coexistence of the 1T and the new high pressure phase (monoclinic phase, C2/*m*) up to 19 GPa. The structural transition is completely reversible as seen from the appearance of 1T phase Raman spectra upon release of the pressure.

Sunday, February 24, 2019; 14:00

Sustainable Energy Materials from First Principles

Emily A. Carter

School of Engineering and Applied Science
Princeton University, Princeton, New Jersey 08544-5263, USA
http://carter.princeton.edu

I believe that we scientists and engineers have a responsibility to use our skills to improve life for all Earth's inhabitants. To this end, for the past dozen years, I have used my skills - in developing and applying quantum mechanics simulation methods aimed at complex phenomena difficult to probe experimentally - to help accelerate discovery, understanding, and optimization of materials for sustainable energy conversion processes. These range from materials for converting sunlight and other renewable energy sources to fuels and electricity, to biodiesel fuels, to clean electricity production from solid oxide fuel cells and nuclear fusion reactors, to lightweight metal alloys for fuel-efficient vehicles. During this talk, I will focus on potential technological advances in materials science, nanoscale optics, and electrochemistry that could someday create a virtuous cycle, exploiting energy from sunlight and molecules in air, water, and carbon dioxide to synthesize the fuels and chemicals needed to sustain future generations.

Sunday, February 24, 2019; 15:00

High Voltage Phosphate Cathodes for Na-ion Batteries

Premkumar Senguttuvan

New Chemistry Unit
International Centre for Materials Science and School of Advanced Materials
Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)
Bangalore, India

Electrochemical energy storage is an attractive option to store intermittent energy produced from renewable sources such wind and solar and to deliver it to consumer utilities. Batteries have advantages such as high round trip efficiency and low maintenance.[1] Despite their continuous domination in the portable electronics and electric vehicles market, Li-ion batteries could not be a viable choice for the grid energy storage due to their high cost and limited geographical distribution of the lithium sources. Therefore, to circumvent this issue, researchers have turned their attention towards the development of other cation intercalation chemistries, including Na^+, K^+, Mg^{2+}, Ca^{2+}, Al^{3+} and Zn^{2+}, due to their inexpensive and earth abundant precursors. Sodium-ion Batteries (SIBs) are striking since sodium has similar chemical character and higher electrochemical reduction potential as compared to lithium (-2.71 V vs. NHE).[2] On the cathode side, phosphate compounds are known for high intercalation voltages and structural stabilities.[3] Herein, we will discuss our recent findings on NASICON and other type of phosphate cathodes for their potential application in SIBs.[4]

References:

(1) Dunn, B.; Kamath, H.; Tarascon, J.-M. Electrical Energy Storage for the Grid: A Battery of Choices. *Science* **2011**, *334* (6058), 928–935.

(2) Ellis, B. L.; Nazar, L. F. Sodium and Sodium-Ion Energy Storage Batteries. *Curr. Opin. Solid State Mater. Sci.* **2012**, *16* (4), 168–177.

(3) Masquelier, C.; Croguennec, L. Polyanionic (Phosphates, Silicates, Sulfates) Frameworks as Electrode Materials for Rechargeable Li (or Na) Batteries. *Chem. Rev.* **2013**, *113* (8), 6552–6591.

(4) Zhou, W.; Xue, L.; Lü, X.; Gao, H.; Li, Y.; Xin, S.; Fu, G.; Cui, Z.; Zhu, Y.; Goodenough, J. B. $Na_xMV(PO_4)_3$ (M = Mn, Fe, Ni) Structure and Properties for Sodium Extraction. *Nano Lett.* **2016**, *16* (12), 7836–7841.

Sunday, February 24, 2019; 15:30

Preparing Organic Electronic Materials under Continuous Flow Conditions

Andrew Holmes

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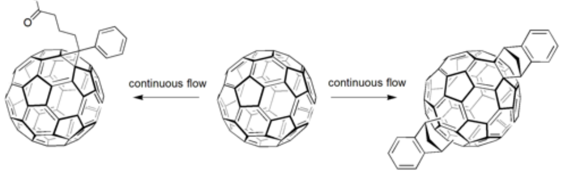
In recent years there has been intense interest in the custom synthesis of organic compounds under continuous flow conditions [1]. The strategies and tactics have become sufficiently sophisticated that a fully integrated manufacturing process has been developed for the production of the renin inhibitor aliskiren [2]. These researchers have gone on to develop a “Plug and Play” integrated combination of flow synthesis hardware, software and analytics [3].

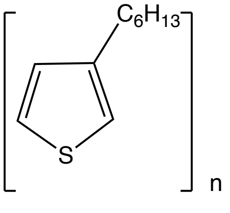
In collaboration with colleagues at CSIRO (Australia) Division of Manufacturing we have developed a continuous flow synthesis of a neurotoxin that is the perhydro derivative of the neurotoxin histrionicotoxin that was iosolated from the poison arrow frog Dendrobates histrionicus [4].

In our research group in Melbourne we also decided to focus on the synthesis of conjugated organic electronic materials, both molecular and polymeric, largely for applications in organic solar (photovoltaic) cells.

Solution-processible fullerenes such as PCBM **1** and ICBA **2** have been the dominant electron accepting component in blends with electron rich light-harvesting compounds [such as poly(3-hexyl)thiophene **3**] in so-called bulk heterojunction organic solar cells. In such devices absorption of photons largely by the electron-rich material results in the production of excitons that separate into electrons and holes at the interface (the heterojunction) with the electron-accepting material. In this talk the synthesis of both compounds **1**, **2** and **3** on a scale suitable for use in the pilot scale fabrication will be illustrated. The potential for the use of flow synthesis for a variety of organic electronic materials will be discussed.



1 **2**



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1. Ley, S. V.; Fitzpatrick, D. E.; Myers, R. M.; Battilocchio, C.; Ingham, R. J. *Angew. Chem. Int. Ed.* **2015**, *54*, 10122.

2. Mascia, S.; Heider, P. L.; Zhang, H.; Lakerveld, R.; Benyahia, B.; Barton, P. I.; Braatz, R. D.; Cooney, C. L.; Evans, J. M. B.; Jamison, T. F.; Jensen, K. F.; Myerson, A. S.; Trout, B. L. *Angew. Chem., Int. Ed.* **2013**, *52*, 12359.
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5. Seyler, H.: Wong, W. W. H.; Jones, D. J.; Holmes, A. B. *J. Org. Chem.*, **2011**, *76*, 3551.
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Sunday, February 24, 2019; 16:10

Graphene-based Materials for Applications in Heterogeneous Catalysis, Water Treatment and Solar Water Desalination

M. Samy El-Shall

Mary Eugenia Kapp Chair in Chemistry
Department of Chemistry, Virginia Commonwealth University
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This talk will address the development of three classes of graphene-based materials as (1) support for metal nanoparticle catalysts in heterogeneous catalysis, (2) sorbent materials for the removal of heavy metal ions from polluted water, and (3) photothermal energy converter materials for efficient solar water desalination.

In heterogeneous catalysis, we will discuss the superior catalytic activity of Pd nanoparticles supported on reduced graphene oxide (RGO) nanosheets for carbon-carbon cross-coupling reactions. Second, the enhanced catalytic activity for the Fe-based nanoparticle catalysts supported on graphene in the *Fischer-Tropsch Synthesis* of liquid transportation fuels will be presented. Finally, the superior catalytic activity and selectivity of Pd nanoparticles supported on a sandwich-type nanocomposite consisting of Metal-Organic Frameworks (MOFs) wrapped with thin RGO nanosheets for the biomass-refining of liquids derived from lignocelluloisc sources will be presented.

For the removal of heavy metals from water, we will discuss the development of chemically modified graphene-based adsorbents containing highly efficient chelating groups such as diamine, imino and thiourea for the effective extraction of the toxic metal ions mercury (II), copper (II), lead(II), chromium (VI), and arsenic (V) from wastewater.

For photothermal energy conversion, we will discuss the development of a new generation of highly efficient, flexible, low weight, highly porous and cost effective *Plasmonic Graphene Polyurethane (PGPU)* nanocomposite materials for solar steam generation through the efficient evaporation of water surface pools. The PGPU nanocomposites contain metallic nanoparticles that exhibit very strong solar absorption. The polyurethane (PU) foam provides a hydrophilic surface with abundant microporous structure, excellent thermal insulation properties, and facile and scalable synthesis. The high solar thermal evaporation efficiency, excellent stability and long-time durability make the PGPU nanocomposites excellent candidates for practical solar-steam-generation applications and seawater desalination.

Sunday, February 24, 2019; 17:30

Discrete Carbon Fractional Order Superapacitors in Flexible Polymer Matrix

Anis Allagui, Mohammad Abdelkareem, and Halima Alnaqbi

Department of Sustainable & Renewable Energy Engineering
University of Sharjah
Sharjah, United Arab Emirates

The Electrical Double Layer Capacitor (EDLC) is the subject of intensive research activity due to its relevance to energy storage, capacitive deionization, and ferroelectric capacitors[1-3]. The behavior of such devices is the collective interfacial electrical charges and ionic charges, which exhibit an intermediary manner between an ideal capacitor and resistor; such property is also referred to as fractional order capacitor, which is usually realized posteriorly[4, 5]. In this work, we propose a fabrication process that controls the resistive, capacitive, and impedance angle anteriorly by sandwiching between two conductive plates an ionically conductive gel polymer impregnated with certain amounts of conductive carbon particles. The overall performance shows that the increase of carbon content shifts the phase angle towards the resistor in a wise controlled manner, which opens up new opportunities for fractional order capacitors.

References:
1. Takahara, E., T. Wakasa, and J. Yamada. A study for electric double layer capacitor (EDLC) application to railway traction energy saving including change over between series and parallel modes. IEEE.
2. Wang, H., et al., Three-dimensional macroporous graphene architectures as high performance electrodes for capacitive deionization. Journal of Materials Chemistry A, 2013. 1(38): p. 11778-11789.
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Sunday, February 24, 2019; 17:45

Nonstoichiometry Misfit Calcium Cobalt Oxide as a New Generation Electrocatalyst for Overall Water Splitting

Kankona Singha Roy and Leela S. Panchakarla

Department of Chemistry
Indian Institute of Technology Bombay
Mumbai, India

Water splitting offers a green alternative to conventional energy such as fossil fuels. The benchmark catalysts for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are Pt-based and Ir/Ru based compounds respectively, which are of high cost and less stable. Hence, the generation of cost-effective with earth abundant materials and highly active electrocatalysts for overall water splitting is immediate thrust and still a big challenge. Herein, we design a highly cost-effective material of misfit calcium cobaltite that shows better catalytic activity just by varying its stoichiometry even in its bulk state. Misfit calcium cobaltite ($Ca_3Co_4O_9$) is moderately catalytically active whereas cobalt rich and calcium rich system of $Ca_3Co_4O_9$ shows excellent performance towards both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) electrocatalysis in alkaline medium at overpotentials of -0.480 V and 0.460 V (with respect to NHE) to produce a current density of 10 mA/cm^2. Consequently, an alkaline electrolyzer constructed using $Ca_{3-x}Co_4O_9$ (non-stoichiometric) as both anode and cathode can produce overall water splitting with the current density of 10 mA/cm^2 at a cell voltage of 2.15 V, suggesting this as a promising bifunctional electrocatalyst for efficient overall water splitting. Most importantly, the catalyst is thermodynamically stable, thus regeneration of the catalyst after electro degradation is possible by thermal annealing.

Sunday, February 24, 2019; 18:00

Magnetocaloric Materials based on Binary and Ternary Mn Compounds: Screening and Testing

Joya A. Cooley, **Joshua D. Bocarsly, Matthew Horton, Kristin A. Persson, and Ram Seshadri**

Materials Research Laboratory
University of California, Santa Barbara
Santa Barbara, United States of America

Magnetic refrigeration is accomplished through the magnetocaloric effect (MCE) associated with a reversible temperature change upon application of a magnetic field. The effect originates from cycling materials between two different magnetic states with high and low entropies. In recent decades, this technology has been proposed as an environmentally friendly alternative to traditional vapor-compression technology, obviating the need for chlorofluorocarbon or hydrochlorofluorocarbon refrigerants, and potentially capable of greater efficiency. The figure of merit for magnetocalorics is the magnetic entropy change, and it has been recently proposed that compounds with high magnetic entropy change can be screened using a density functional theory (DFT) based proxy called the magnetic deformation – a measure of the deformation between relaxed structures with and without spin polarization. Several Mn-containing binary and ternary compounds have been identified as potential magnetocalorics. We will discuss the synthesis, characterization, and magnetic property measurement of some of these candidate materials.

Sunday, February 24, 2019; 18:15

Imaging Assisted Quantitative Colorimetric and Adsorption based Detection of Heavy Metal Ions using Disposable Paper Sensor Strips in Water

Rishabh Jain, Pahul, Neerja Mittal, Praveen Kumar, and Pooja D.

Material Science Division, Agrionics
CSIR-Central Scientific Instruments Organisation
Chandigarh, India

Water is the driving force for the existence of life on earth. The developing nations including India relies upon natural surface and ground water resources such as rivers, lakes, wells, etc. to meet their daily demand. However, in the present scenario, there is an exponential increase in the contamination of these natural resources with various chemical pollutants, such as heavy metals, organic matter, pesticides, and so forth. Zinc is one among the heavy metals, which become toxic when consumed above 3 ppm according to World Health Organization (WHO) guidelines, and leads to various harmful effect on humans such as vomiting, nausea, hypertension, malfunctioning of cellular growth, skin effects (ulcerations and blistering permanent scarring), diarrhoea, etc. The acute exposure of same may leads to pain in chest, dyspnoea, epigastria, and even death. Currently, its presence above permissible limits as high as 5 ppm is observed in several states in India such as Puthwar and Udhampur Districts (Jammu & Kashmir), Hyderabad (Telangana), etc. Therefore, it is of utmost requirement to monitor water resources (including ground and surface water) for Zn (II) ions concentration prior their consumption.

Herein, we report the development of cost-effective, portable, sensitive, and selective paper based colorimetric probe for the Zn (II) ions monitoring for the concentration range of 1-10 ppm. The gold nanoparticles (NPs) were synthesized and modified with cysteamine and dithizone as surfactant and Zn (II) selective receptor, respectively. The synthesized complex is then transferred onto a disposable paper substrate for color based quantification of Zn (II) ions. The fabricated paper sensor showed a color gradient w.r.t. Zn (II) ions concentrations, which is then captured with scanner and smartphone camera as imaging tools. The analysis of images for green channel value was performed with ImageJ computation tool, which is found in strong agreement with color gradient observed. Yet the differentiation is stronger with scanned images over camera captured images. Further, a model is customized fitting the change in colour intensities vs Zn (II) ion concentration and same has been validated with a lab based reference technique i.e. ion chromatography. These findings paves a new path for imaging assisted paper-based sensor for analysis of heavy metals in water at low resources settings meeting the “ASSURED criteria” set by WHO.

Monday, February 25, 2019; 9:00

Advanced Design of Self-Healable Materials by Supramolecular Chemistry

Takuzo Aida

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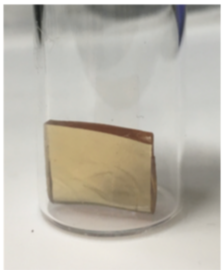
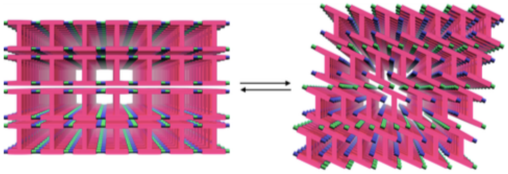


Expanding the range of healable materials is an important challenge for sustainable societies. Noncrystalline, high molecular weight polymers generally form mechanically robust materials, which, however, are difficult to repair once they are fractured. This is because their polymer chains are heavily entangled and diffuse too sluggishly to unite fractured surfaces within reasonable timescales. Here, we report that low molecular weight polymers, when crosslinked by dense hydrogen bonds, give mechanically robust yet readily repairable materials, despite their extremely slow diffusion dynamics [1]. A key was to utilize thiourea, which anomalously forms a zigzag hydrogenbonded array that does not induce unfavorable crystallization. Another key was to incorporate a structural element for activating the exchange of hydrogenbonded pairs, which enables the fractured portions to rejoin readily upon compression.

We also report here heat-resistance, self-healable porous organic crystal. This crystal is an anomalous porous molecular crystal built up of 'C–H···N-bonded double-layered roof/floor components' and 'wall components consisting of a segregatively interdigitated architecture' [2]. This complicated porous structure is given by only one type of C3- symmetric fully aromatic multi-joint molecule carrying three identical dipyridylphenyl wedges. Despite its high symmetry, this molecule accomplishes difficult tasks by employing two of its three wedges for constructing the roof/floor components, while employing the residual one wedge for constructing the wall components. Although a C–H···N bond is extremely labile, the porous crystal maintains its porosity until thermal breakdown of the C– H···N bonded roof/floor components as "selectively crushable zones" at 202 °C, affording a non-porous crystal. While this non-porous structure survives even up to 325 °C, it can retrieve the original porous structure upon exposure to acetonitrile vapor. C–H···N bonds have never been utilized for the formation of porous crystals. These findings demonstrate how one can construct selfhealable porous crystals using extremely labile noncovalent bonds and also how one can translate structural simplicity into ultrahigh geometrical complexity.



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Monday, February 25, 2019; 9:40

Advanced Materials from Metal–Phenolic Networks

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The development of rapid and versatile coating strategies for interface and particle engineering is of immense scientific interest [1]. This presentation will focus on our studies on the rapid formation of thin films constituted of metal–phenolic networks (MPNs), a unique class of metal–organic materials. MPNs can be formed on various substrates by simply mixing natural polyphenols and metal ions [2,3]. This coating technique is substrate independent (covering organic, inorganic and biological substrates) and has been used for the assembly of capsules by coating particles and then removing the coated templates. It will be shown that a range of polyphenols and a library of metal ions are suitable for forming MPNs for film and capsule engineering. The MPN films and capsules are stable at physiological pH but degrade at acidic pH, thus making them of interest for intracellular release of therapeutics. By altering the metal ion, different functions can be incorporated in the MPN materials, ranging from fluorescence to MRI and catalytic capabilities. Furthermore, synthetic polymer–phenol conjugates have been used as building materials to control the biofouling properties of the MPN materials. Examples of self-healing MPN gel materials will also be highlighted. The ease and scalability of the assembly process, combined with the tunable properties of MPNs, provide a new avenue for functional interface engineering and make MPNs potential candidates for biomedical, environmental, and advanced materials applications.

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Monday, February 25, 2019; 10:20

Self-Assembly of Clay/Biopolymer Nano-Composites

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Inspired by the relationship between the 3-dimensional structure found in natural *mother-of-pearl* we present a simple self-assembly strategy to obtain large-scale organic/inorganic coatings by connecting Laponite-nanoclays to each other using naturally abundant cellulose [1]. By simple evaporation of the initially dilute, aqueous clay-polymer suspensions we create thin, flexible films, as shown in the figure below, with a local *brick-and-mortar* architecture that resembles that found in mother-of-pearl. However, our building blocks are on much smaller scale. While the aqueous solutions have weak viscoelasticity, the dried films show a Young's modulus ranging in GPa. Moreover, the films show glass-like transparency along with exceptional shape-persistent flame shielding.

The films stability against dissolution in water can be also tuned by metal ion-coordination, which further strengthen the interactions between the polymers and the nanoclays. This ion-coordination also leads to a further strengthening of the dry films. We believe that our simple pathway to fabricate such versatile polymer/clay nanocomposites can open avenues for inexpensive production of environmentally friendly, biomimetic materials in various industries.

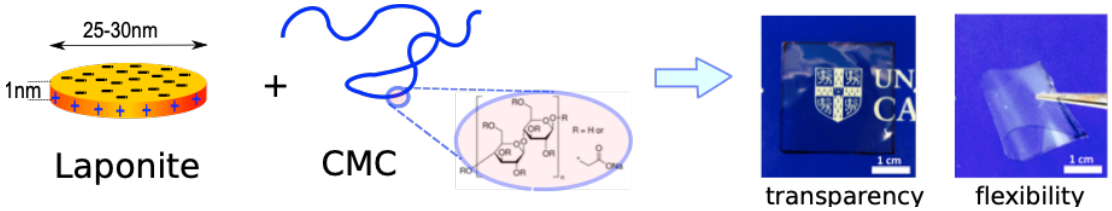

Figure: (*Left*) Cartoon of the charging state of Laponite clay-platelets in water and a schematic of the cellulose polymer, denoted as sodium carboxymethyl cellulose or CMC. (*Right*) Photographs of Laponite-clay composite films demonstrating their transparency and flexibility.

[1] P Xu, T Erdem, E Eiser '*A Facile Approach to Prepare Self-Assembled, Nacre-Inspired Clay/Polymer Nano-Composites*' arXiv:1808.03972 (2018)

Work done in collaboration with Peicheng Xu and Talha Erdem.

Monday, February 25, 2019; 11:30

Liquids, Crystals, Liquid Crystals, Plastic Crystals, and More ...

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My talk will review the states of matter accessible to condensed phase systems. Atomic solids typically exhibit three phases: long-range center-of-mass order (conventional solid) plus disordered liquid or glass phases. Molecular systems, on the other hand, have orientational (and internal) degrees of freedom, which introduce additional possibilities, even for small rigid molecules such as, CCl_4, and O_2. Macromolecules with internal degrees of freedom and/or flexibility, such as, surfactants, lipids, and dendrimers, self-assemble into an array of distinct condensed phases. Using selective examples, the talk will survey some of the intriguing phases exhibited by Nature.

Monday, February 25, 2019; 12:10

Simple yet Successful Descriptors for Self Assembly of Organic Molecules on Surfaces

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Self-assembly is probably the most promising route to constructing devices at the nanoscale. The challenge is to predict the geometries of self-assembled architectures by utilizing only the properties of the individual molecular components. Working jointly with experimentalists, we have explored the feasibility of such an approach for a model set consisting of three host molecules (carboxylic acid derivatives of phenyleneethynylene) and five guest molecules (napthalene, phenanthrene, benzo-c-phenanthrene, benzo-ghi-perylene and coronene), self-assembled on graphene.

Using insights gained from scanning tunneling microscopy experiments and density functional theory calculations, we have formulated simple descriptors that can successfully predict the geometries of the host-guest architectures self-assembled from our palette of organic molecules. A structure map can be constructed using host and guest descriptors, with structures of the same type clustering in descriptor space. Though these descriptors can be evaluated at essentially zero computational cost, they correctly reproduce experimental observations, including the structural transitions exhibited by host assemblies upon introducing certain guest molecules. The descriptors are validated by their success in predicting not just the ground state geometry but also the energetic difference between competing structures for molecules that did not form part of of the training set used when formulating the descriptors. This work suggests a novel approach toward the rational design of self-assembled nanostructures.

Work done in collaboration with Sukanya Ghosh at JNCASR, and Pratap Zalake and K. George Thomas at IISER Thiruvananthapuram.

Monday, February 25, 2019; 14:15

Glimpses of Materials Highlights, 1958-2019

C. N. R. Rao

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Materials chemistry was in its infancy when I started my independent research efforts in India in the late 1950s. India was very poor, and we had no modern facilities then. I investigated phase transformations of TiO_2 and alkali halides and also carried out defect calculations. While working on rare-earth oxides, I made TbO_2 and PrO_2 by a simple solution route, an early example of chimie douce. In the sixties, I started working on transition metal oxides specially pervoksites by building simple instruments. Oxides have been of great interest to me because of the variety of structures and phenomena exhibited by them. In 1987, we were able to characterize the first liquid N_2 superconductor ($YBa_2Cu_3O_7$) with the aid of a home-built AC susceptometer. I have studied many aspects of transition-metal oxides, including metal-insulator transitions, colossal magnetoresistance, and multiferroics. The last two decades have been prosperous and allowed research on synthesis, characterization, and properties of various nanomaterials, and in particular, two-dimensional materials (graphene and its inorganic analogues). Two-dimensional sheets have been covalently cross-linked to derive new materials with novel properties. Studies on water splitting and reduction of CO_2, besides using aliovalent anion substitution to generate novel inorganics (e.g., TiNF in place of TiO_2) are other areas of interest.

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Monday, February 25, 2019; 16:00

The Next Generation of Robust and Low-Fouling Desalination Reverses Osmosis Membranes based on Carbon Nanotubes-Polyamide Nanocomposite

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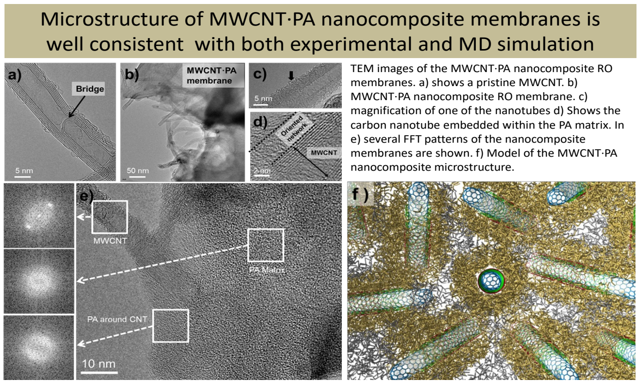
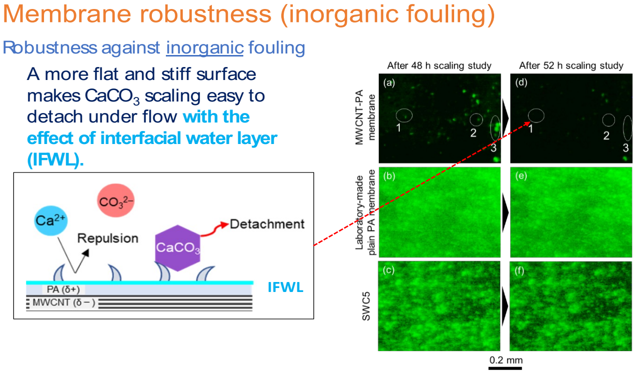
Nanocomposite reverse osmosis membranes made of carbon nanotubes (CNTs) and aromatic polyamide (PA) have attracted great attention in the last years due to their easy preparation, high salt rejection rate and high permeation. We have developed an easy and scalable method of synthesis to prepare these composite membranes through interfacial polymerization over porous polysulfone support membranes (Figure 1).[1] The present nanocomposite membranes have an excellent chlorine resistance and anti-fouling performances than the typical plain PA membranes. The chlorine resistance seems to increase as a combination of several factors, including the lower chlorine diffusion and an electronic effect of the CNTs on the activation energy of the polyamide chlorination reaction.[2] We carried out molecular dynamics simulations to understand not only the effect of the CNTs on the polymerization but also on the diffusion and the fouling of these novel membranes. Our results showed that carbon nanotubes provide a low energy path for the diffusion of water molecules across the membrane.[3-5] The fouling of the membrane was also reduced due to several factors, including the formation of an interfacial water layer given rise to the charge transfer from matrix PA to CNTs.[6,7] (Figure 2) These results indicate that CNTs-PA nanocomposite membranes can become a next generation of desalination RO membranes because of their outstanding performances.



Microstructure of MWCNT·PA nanocomposite membranes is well consistent with both experimental and MD simulation

TEM images of the MWCNT·PA nanocomposite RO membranes. a) shows a pristine MWCNT. b) MWCNT·PA nanocomposite RO membrane. c) magnification of one of the nanotubes d) Shows the carbon nanotube embedded within the PA matrix. In e) several FFT patterns of the nanocomposite membranes are shown. f) Model of the MWCNT·PA nanocomposite microstructure.

Fig.1 TEM images of the CNTs-PA nanocomposite RO membranes, and model of the CNTs-PA nanocomposite microstructure.



Membrane robustness (inorganic fouling)

Robustness against inorganic fouling

A more flat and stiff surface makes $CaCO_3$ scaling easy to detach under flow **with the effect of interfacial water layer (IFWL).**

Fig.2 FM snapshots of the membranes after 48 h and 52 h of scaling. The $CaCO_3$ deposited on the membrane surface was confirmed on all membranes, by Calcein which was stained for fluorescent microscope observation.

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Work done in collaboration with Jun Maeda, Isamu Ito, Rodolfo Cruz-Silva, and Kenji Takeuchi.

Monday, February 25, 2019; 16:40

Carbon Nanotubes Dispersed Super Coating: Its Contribution by our RAK Facility to Oil and Gas Industries in UAE

Takashi Yanagisawa[†‡] **and Shoji Kuroyama**[‡]

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Corrosion has huge impacts on social economy and safety, and many kinds of surface treatments were developed in order to reduce the costs of corrosion in its history. Recently, polymer coating has become one of the most important surface treatments for anti-corrosion applications. To obtain high-performance polymer coatings, several factors are required, such as strong adhesion between metal and polymer with appropriate chemical and physicochemical properties. These factors mainly depend on the selection of polymers and coating technologies. But the hardness of polymer-based coatings is fundamentally not enough against mechanically severe conditions. We have learned that some cracks in polymer layers caused by static and/or dynamic force applied by fastening nuts and bolts induce invasion of corrosion factors into the surface of metallic parts.

We have developed and commercialized high-performance thermo-setting resin (TSR) based paint system having extraordinary mechanical properties as well as anti-corrosion performance reinforced by our carbon nanotubes (CNT) to solve present problems mentioned above. This novel coating will drastically increase lifetimes of metallic parts even in harsh environment, chemically and mechanically, thus reducing their life cycle costs, sufficiently.

This talk describes our CNT reinforced paint system and superior coating facility, TME (TAKENAKA MIDDLE EAST LLC), located in Ras Al Khaimah, and our recent progress and contribution to national oil & gas plant in region.

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Applied Physics Letters 2002; 80(7)

Monday, February 25, 2019; 17:30

Supramolecular Approach to 2D Heterostructures and to the Non-covalent Functionalization of 2D Materials

Manjodh Kaur, Navin Kumar Singh, Aritra Sarkar, Subi J. George, and C. N. R. Rao

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Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)
Bengaluru, India

Synthesis of 2D heterostructures by van der Waals vertical stacking to modulate their properties has gained interest over the past few years. Van der Waals stabilization is an efficient synthetic strategy to obtain 2D heterostructures, although precise sequence and composition of the components still remains a challenge. A new synthetic strategy of covalent cross linking of different 2D materials has been extensively explored by Rao *et al.*[1] This novel class of covalently cross-linked 2D materials are different from van der Waals heterostructures and show exciting properties. Although, cross-linked heterostructures show exceptional properties, further advancement to obtain the heterostructures of higher complexity with multiple components and precise sequences is appealing to explore novel applications. Therefore, for the first time successfully, supramolecular non-covalent synthetic strategy has been utilised to obtain reversible non-covalent heterostructure assemblies with self-organising components.[2] Wherein, Kumar *et al* reported the novel, stable and reversible multi-component heterostructures of graphene:BN and MoS_2:graphene. The 2D-materials have been covalently functionalized by organic coupling reactions between surface functional groups and organic molecules. Thereafter, the covalently functionalized 2D sheets have been noncovalently attached in the presence of cucurbit[8]uril to obtain supramolecular heterostructures. The work has been extended to synthesise supramolecular heterostructures of MoS_2:g-C_3N_4 and MoS_2:BC_7N. The supramolecular heterostructures have been investigated for their potential application in visible-light assisted photochemical H_2 evolution studies and gas adsorption properties. These results for H_2 evolution were found to be in good agreement with current literature reports and these results will be presented.[3]

In order to tailor the electronic properties of 2D materials like MoS_2, which unlike graphene cannot be functionalized by π-π stacking or CT interactions, new strategy for non-covalent functionalization of MoS_2 with organic chromophores based on host-guest ternary complexation has been achieved.[4] This strategy can be utilised to tune the electronic properties of other 2D materials.

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Monday, February 25, 2019; 17:45

Porous Ti Alloys with Non-Cytotoxic Nb and Sn for Body-Implant Applications

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Ti-based alloys are becoming increasingly attractive in the medical field as implant materials due to their excellent biocompatible, non-corrosive and mechanical properties [1]. However, the elastic modulus of Ti alloys synthesised by melting methods is relatively high (50-120 GPa) in comparison with that of bone (0.1-20 GPa), and this will lead to loosening of the implant from the bone over time owing to non-uniform load transfer at their junction. Porous Ti alloys would be desirable as implant materials due to their more suitable mechanical properties and the possibility of tissue in-growth (osseointegration). Therefore, porous Ti alloys with non-cytotoxic elements such as Nb, Zr, Ta and Mo are currently being developed. Recent studies with arc-melted Ti-Nb-Sn alloys have furthermore shown that the presence of Sn leads to a significant decrease of the elastic modulus [2].

In the present study, Ti_xNb_ySn alloys with different Nb and Sn contents ($x = 24, 35, 42$ and $y = 4.0, 7.9$ mass%) have been synthesised directly from TiO_2, Nb_2O_5 and SnO_2 oxides. The mixed oxide discs were converted into the corresponding alloys by employing them as the cathode against a graphite anode in CaCl2 molten electrolyte at 1173 K. In the alloys, Nb and Sn acted as β-stabilising and neutral elements, and the alloys with the lowest Nb content were dual α/β-phase while the other alloys were single β-phase. Microstructural studies revealed that all alloys were quite porous and that the particle size decreased with increasing Nb and Sn contents. EDX analysis confirmed that the compositions of the synthesised alloys were close to the target values. SEM-EDX and XPS studies on the surfaces of the alloys subjected to long-term immersion of 7 and 15 days in Hanks' simulated body fluid solution at 310 K evidenced the formation of a passive film consisting of mixture of Ti, Nb and Sn oxides upon which a hydroxyapatite layer had grown.

Polarisation studies of the alloys in Hanks' solution demonstrated superior corrosion resistance with corrosion current densities in the range of 2-9 $\mu A/cm^2$ despite their high open porosities. The alloys were heat treated at 1473 K in vacuum, and the mechanical properties of as-synthesised and heat-treated alloys were compared. The as-synthesised alloys had lower elastic modulus and hardness than the heat-treated ones, with values of 5.0-10.1 and 7.4-23.7 GPa, and 28-125 and 185-335 HV, respectively. The mechanical properties of all alloys were in the range of that of human bone and the corrosion properties were adequate. From comparison of all properties, it has been concluded that phase-pure β-$Ti_{35}Nb_4Sn$ should be a promising candidate as an implant material, and further studies regarding its potential application are in progress.

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Monday, February 25, 2019; 18:00

Mechanically Induced Transition from Indirect to Direct Bandgap in Nanocrystalline Silicon Powder

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In this work, we report the synthesis of direct bandgap Si nanocrystallites by mechanically induced transition. Si powder was ball milled in an attrition mill for 4 hours in argon gas atmosphere. Optical properties of the milled and as received powders were investigated by UV-Vis–IR spectroscopy and photoluminescence (PL) spectroscopy. Bandgap determination by Tauc method suggested the presence of direct nature of bandgap in milled powder than indirect as in as-received Si powder. Visible range PL emission was recorded for the milled powder. The samples of as received and milled Si powders were then dispersed in the toluene and illuminated under the UV light. The milled powder sample has shown green fluorescence while as received powder sample didn't show any fluorescence, confirming the direct bandgap in milled Si powder. Raman spectroscopy confirmed 100% crystalline nature of both the powders. The presence of high tensile strains and nanocrystallites in milled powder than as received powder suggested combine effect of the tensile strain and quantum confinement responsible for transition to direct bandgap silicon. X-ray diffraction studies were done to approximate strain % and crystallite size in both the powders. The crystallite size in as received and milled powder was found to be 98 and 52 nm, respectively. No change in phase or new phase was observed in the milled powder. Transmission electron micrographs confirmed the presence of nanocrystallites in the milled powder. Selected area electron diffraction patterns confirmed the results of the X-ray diffraction. The transition from indirect to direct bandgap in Si powder took place under the combine effect of tensile strain and quantum confinement.

Monday, February 25, 2019; 18:15

From Quasicrystals to Crystals and Superconductors in Ca/Y-Au-Al

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In the Au-rich region of the Ca–Au–Al system, an icosahedral quasicrystal (i-QC) $CaAu_{4.5-x}Al_{1.5+x}$ was discovered and shown to irreversibly transform into the cubic 2/1 crystalline approximant (CA) $Ca_{13}Au_{56.79(6)}Al_{21.20}$ (space group $Pa\bar{3}$ (no. 205); Pearson symbol: cP728; a = 23.8918(2) Å), via *in-situ*, high-energy, variable-temperature powder X-ray diffraction, which thereby provides direct experimental evidence for the relationship between QCs and their associated CAs. The 2/1 CA crystallizes in a Tsai-type structure and, following the polar intermetallic depiction, the atoms of different electronegativities, viz., electronegative Au+Al vs. formally electropositive Ca, are arranged in concentric shells. As part of an overarching chemical pressure and valence electron count investigation, the cubic 1/1 CA $Y_3Au_{14.08(2)}Al_{4.49(1)}$ (space group $Im\bar{3}$ (no. 204); Pearson symbol: cI192; a = 14.662(2) Å) was discovered to also crystallize in the Tsai-type, and exhibit superconductivity behavior below Tc around 0.4 K. The QC-CA transformation, crystallographic structure, and atomic site preference analysis of Ca–Au–Al, along with the crystal and electronic structures, and transport properties, including resistivity and specific heat, of the 1/1 CA $Y_3Au_{14.08(2)}Al_{4.49(1)}$ will be presented for discussion.

Tuesday, February 26, 2019; 9:00

Lone Pairs in the Halide Perovskites, Hidden or Otherwise

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The ABX_3 halide perovskites that have attracted so much renewed attention mostly possess B = Sn^{2+} or Pb^{2+}, with ns^2 lone pairs of electrons. These lone pairs are frequently hidden, in the sense that the crystal structures are not consistent with the presence of a stereochemically active lone pair, that would for example result in certain characteristic distortions of MX_6 polyhedra in the structure. Such hidden lone pairs can be seen in many of the perovskites including the hybrids with methylammonium [A = $CH_3NH_3^+$] and formamidinium [A = $CH(NH_2)_2^+$], where the lone pairs are associated with proximal instabilities that can profoundly influence materials properties. We will discuss the understanding that we have developed from extensive real and k-space studies of local and average structure in these materials using synchrotron and neutron scattering. DFT calculations and NMR studies complement the structural studies to obtain a coherent picture of what is happening, and where all the red herrings are.

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Tuesday, February 26, 2019; 9:40

Topological Materials Science

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Topology, a mathematical concept, recently became a hot and truly transdisciplinary topic in condensed matter physics, solid state chemistry and materials science. Since there is a direct connection between real space: atoms, valence electrons, bonds and orbitals, and reciprocal space: bands, Fermi surfaces and Berry curvature, a simple classification of topological materials in a single particle picture should be possible. One important criterion for the identification of the topological material is, in the language of chemistry, the inert pair effect of the s-electrons in heavy elements, and the symmetry of the crystal structure [1]. Beyond Weyl and Dirac, new fermions can be identified in compounds that have linear and quadratic 3-, 6- and 8- band crossings that are stabilized by space group symmetries [2]. Binary phosphides are an ideal material class for a systematic study of Dirac, Weyl and new Fermion physics, since these compounds can be grown as high-quality single crystals. A new class of topological phases that have Weyl points was also predicted in the family that includes NbP, NbAs. TaP, MoP and WP_2. [3-8]. In magnetic materials the Berry curvature and the classical anomalous Hall (AHE) and spin Hall effect (SHE) helps to identify potentially interesting candidates. As a consequence, the magnetic Heusler compounds have already been identified as Weyl semimetals: for example, Co_2YZ [10-12], Mn_3Sn [13-15] and $Co_3Sn_2S_2$ [16]. The Anomalous Hall angle also helps to identify materials in which a QAHE should be possible in thin films. Even beyond this reciprocal Berry curvature, Heusler compounds with non-collinear magnetic structures also possess real-space topological states in the form of magnetic antiskyrmions, which have not yet been observed in other materials [17].

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Tuesday, February 26, 2019; 11:00

Oxide Meso-Structures Formed by Ionic Liquid Gating

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Ionic liquid gate induced migration of oxygen ions at the surface of oxide thin films has been shown recently to be a powerful tool for manipulating their bulk properties and structures(*1-5*). Here we directly image these processes, using in-situ ionic liquid gating within a high-resolution transmission electron microscopy, as we induce the reversible transformation between brownmillerite $SrCoO_{2.5}$ and perovskite $SrCoO_3$. A massive quantity of ~0.5 oxygen per formula unit is observed to be reversibly extracted or injected over several minutes. The film structure is transformed throughout its volume but the phase transformation boundary velocity is highly anisotropic, traveling at speeds ~30 times faster laterally than through the thickness of the film. Furthermore, by taking advantage of ionic liquid gating through lithographically patterned orifices at the surfaces of oxide films with distinctly different anisotropies in oxygen transport, we show that a range of three-dimensional metallic structures such as cylinders and rings can be realized. Our results provide a roadmap to the construction of complex meso-structures in ion-transporting materials from their exterior surfaces (*6*).

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Tuesday, February 26, 2019; 11:40

Engineering Schottky Barrier Height in Epitaxial TiN/(Al,Sc)N Metal/Semiconductor Superlattices for Thermionic Energy Conversion

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Since the 1960s, researchers exploring the potential of artificially-structured materials for applications in quantum electronic devices have sought combinations of metals and dielectrics that could be combined on the nanoscale with atomically-sharp interfaces. Early work with multilayers of polycrystalline elemental metals and amorphous dielectrics showed promise in tunneling devices. More recently, similar metal/dielectric multilayers have been utilized to demonstrate novel optical metamaterials. These metal/dielectric multilayers, however, are not amenable to atomic-scale control of interfaces. We developed the first epitaxial nominally single crystalline metal/semiconductor superlattices that are free of extended defects. These rocksalt nitride superlattices have atomically sharp interfaces and properties that are tunable by alloying, doping and quantum size effects. Furthermore, these nitride superlattices exhibit exceptional mechanical hardness, chemical stability and thermal stability up to ~1000 °C.

In this presentation, I will describe growth, structural characterization and transport properties of epitaxial TiN/(Al,Sc)N metal/semiconductor superlattices for their thermionic energy conversion and optical metamaterial applications. Since Schottky barrier height at metal/semiconductor interfaces control current flow across cross-plane (growth) directions in superlattices, synchrotron based X-ray photoemission spectroscopic measurements, along with first-principles modeling analysis are performed to determine valence band offset, band alignments and the Schottky barrier height. Moreover, the carrier concentration of semiconducting layers are tuned with dopants to control the depletion width and semiconductor band bending at the interfaces. The effects of dopants on the energy band structure of the semiconductor are also analyzed to gain insights into the Schottky barrier formation and its experimental determination.

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2. S. Nayak, S. Acharya, B, Baral, M. Garbrecht, T. Ganguli and B. Saha, "Valence Band Offset in Epitaxial Lattice-matched TiN/AlScN Metal/Semiconductor Superlattice Interfaces for Thermionic Energy Conversion. *(In-review, 2019).*
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Tuesday, February 26, 2019; 14:30

New Dimensions of Porous Coordination Polymers/Metal-Organic Frameworks

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We have found unique porous properties of porous coordination polymers (PCPs) or metal-organic frameworks (MOFs), which respond to specific guests, dissimilar to the conventional porous materials.[1] The third generation MOFs[2] possess flexible or dynamic porous frameworks, which reversibly respond to external stimuli, not only chemical but also physical, unlike the previous generations. They were developed in an effort to realize dynamic porous and collective functionality not found in conventional materials. Their compositions of metal ions and organic molecules have achieved diversity in the electronic states. That is, the spatial and electronic structures can be altered, realizing magnetic and dielectric properties as well as oxidation−reduction functions. Besides normal storage, dynamic MOFs have vast potential for separation with an extremely high selectivity, high-efficiency storage, and catalysis, as well as sensing and actuator functions. For these reasons, many studies investigate these materials. Here, I discuss porous materials with capabilities that exceed current ones (i.e., the fourth generation MOFs) and the future research direction.[3,4] It would be fabulous if novel porous materials possessed more features than just the third generation's excellent characteristics (flexibility, collectivity, and diversity). These additional features include 1) Hierarchy and Hybrid (double-H), which means to combine different functions and pursue the dynamic development of combined functions, (2) Anisotropy and Asymmetry (double-A), which means to learn from living organisms and then go beyond such organisms' capabilities, and (3) Disorder and Defect (double-D), which may lead to excellent catalytic reactivities and electronic functions. Hereinafter these three characteristics are referred to collectively as " HAD" characteristics.

References:
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Tuesday, February 26, 2019; 15:10

MOF Design to Applications: Impact of Pore System Control on Gas Separations and Storage

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Metal-organic frameworks (MOFs) burgeoned in recent years due to effective design strategies (i.e. reticular chemistry) for their synthesis and their inherent [and readily interchangeable] hybrid, functional character.

Markedly, MOFs are amenable to design and manipulation for desired function and application. Several design strategies have been utilized and developed to target viable MOF platforms based on edge transitive nets, minimal edge transitive nets, and our recently introduced merged nets: molecular building block (MBB) approach, hierarchical supermolecular building block, supermolecular building layer approaches (SBB and SBL, respectively).

Various key gas/vapors separations are accomplished using energy intensive processes as exemplified by the olefin/paraffin separation, an essential separation in chemical industry.

Here we present our progress in the development of functional MOFs to address some energy-intensive separations. Successful practice of reticular chemistry had afforded the fabrication of various chemically stable fluorinated MOF adsorbent materials (**NbOFFIVE**-1-Ni, also referred to as **KAUST**-7 and **AlFFIVE**-1-Ni, also referred to as **KAUST**-8). The restricted MOF window resulted in the selective molecular exclusion of propane from propylene at atmospheric pressure, as evidenced by multiple cyclic mixed-gas adsorption and calorimetric studies. Remarkably, **KAUST**-7 maintains its distinctive separation properties in the presence of water as a result of its high chemical and hydrolytic stability.[1]

The development of suitable storage and refining processes makes natural gas an excellent alternative fuel, but before its transport and use, natural gas must first be dehydrated. Conventional dehydration agents are energy intensive. **KAUST**-8 selectively removes water and requires just 105 °C for regeneration of the dehydrating agent.[2]

The deliberate control of the pore aperture-size of various selected MOFs and its impact on various separations will be discussed.

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Tuesday, February 26, 2019; 15:50

Hybrid Perovskites and Related Materials with Oxygen-Containing Linkers

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Hybrid organic-inorganic perovskites are found in a number of important families, including the lead-based halides (e.g. $[CH_3NH_3]PbI_3$) and the formates (e.g. $[(CH_3)_2NH_2]Zn(HCOO)_3$) [1]. The focus of the talk will be on perovskite systems in which the bridging between the B-cations is via oxygen-containing linkers. We shall discuss two important classes - the formates [2] and the closely-related hypophosphites, $[AmineH]M(H_2POO)_3$ [3]. These show a range of very interesting properties, including multiferroic behaviour in the case of the formates. We shall also examine a number of systems that adopt the ReO_3 structure, including a recently discovered family of hypophosphites of general composition $M(H_2POO)_3$, M = Al, Ga, V [4].

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Poster Session I

Al Hamra Convention Center

Sunday, February 24, 2019 18:30-20:30

I.1 Selective-Jet Electrodeposition for Low-Cost Additive Manufacturing of Metallic Components at Room-Temperature

Wael Othman, Omar Almelhi, Lütfiye Y. Ozer, Marco Stefancich, and Matteo Chiesa
Department of Materials Science and Engineering
Khalifa University, Abu Dhabi, United Arab Emirates

I.2 Potassium Levels on Gladiolus Corms Production in Open Field and Intercropping Conditions

Farooq Abdul Sattar, Ashfaq Alam, Abdul Rauf, and Baghet T H
Department of Arid Land Agriculture
King Abdul Aziz University, Jeddah, Kingdom of Saudi Arabia

I.3 Optimization of Injection Molding Parameters of UHMWPE for Production of UHMWPE/Nano-filler Composites for Biomedical Applications

Omar G. Ayad, Abdel-Hamid I. Mourad, and Yaser E. Greish
Department of Mechanical Engineering
United Arab Emirates University, Al Ain, United Arab Emirates

I.4 Synthesis, Characterization, Crystal Structure, DNA-binding and Antimicrobial Activities of Co(III) and VO(IV) Schiff-base Complexes

Disha Sharma and H. D. Revanasiddappa
Department of Studies in Chemistry
University of Mysore, Mysuru, India

I.5 Quantitative Investigation of the Swelling Behavior of Alginate and Alginate/Clay Beads Cross-Linked with Ca^{2+}

Berraaouan Doha, El Miz Mohammed, Essifi Kamal, and Tahani Abdesselam
Department of Chemistry
Mohamed First University, Oujda, Morocco

I.6 Fabrication of Metalosomes (Metal Containing Cationic Liposomes) using Single Chain Surfactant as Precursor via Formation of Inorganic Organic Hybrids

Preeti Garg, Gurpreet Kaur, and Ganga Ram Chaudhary
Department of Chemistry
Panjab University, Chandigarh, India

I.7 Modification of Gold Nanoplates into Gold Nanosquares to Increase Sensitivity of Plasmonic Sensors

Nur Liyana Razali, Marlia Morsin, Suratun Nafisah, and Nur Zehan An'nisa Md Shah
Department of Electronic Engineering
Universiti Tun Hussein Onn Malaysia, Batu Pahat, Malaysia

I.8 Evaluating the Potential Use of Waste Eggshells in Lead Adsorption Using Response Surface Methodology

Haliemeh Sweidan, Mohamed Hamouda, and Hilal El-Hassan
Department of Civil and Environmental Engineering
United Arab Emirates University, Al Ain, United Arab Emirates

I.9 Synthesis of Curcumin Based Novel Nano Hybrid Composite with ZnO and its Application for Biological Activity

Sushma and S. Ananda
Department of Chemistry
University of Mysore, Mysore, India

I.10 Characterization of Bioactive 3D-Printed Biodegradable Bone and Dental Fixation Prosthetics

Hessa N. Alnuaimi, Alya M. Almehrezi , and Yaser E. Greish
Department of Chemistry
United Arab Emirates University, Al Ain, United Arab Emirates

I.11 Characterization of Hydroxyapatite-containing Zinc Polycarboxylate Cement for the Treatment of Bone Fracture

Heba Al-Amoudi and Yaser E. Greish
Department of Chemistry
United Arab Emirates University, Al Ain, United Arab Emirates

I.12 Comparative Study of CTS-nHA and CTS-nBG Composite based Scaffolds for Hard Tissue Engineering Applications

Pawan Kumar, Brijnandan S Dehiya and Anil Sindhu
Department of Materials Science and Nanotechnology
Deenbandhu Chhotu Ram University of Science and Technology, Sonipat, India

I.13 Green Silver Nanoparticles by and Against the Two-spotted Spider Mite, *Tetranychus urticae*

Rania Ahmed Abd El-Wahab
Department of Biological Control
Plant Protection Research Institute, Agricultural Research Center, Giza, Egypt

I.14 Development of Metal-Organic Frameworks based Nanocomposites for Impedimetric Sensing of *Staphylococcus arlettae*

Arushi Gupta, Amit L. Sharma, and Akash Deep
Department of Advance Material and Sciences
Central Scientific Instrument Organization(CSIR-CSIO), Chandigarh, India

I.15 Green Silylation of Cellulose Fibers for Oil Spill Remediation

Khalid Jarrah, Mohammad H. Al-Sayah, and Soleiman Hisaindee

Department of Chemistry
United Arab Emirates University, Al Ain, United Arab Emirates

I.16 Enhanced Structural Stability and Catalytic Activity of Sol-gel Prepared Ti(IV)-doped-Fe_2O_3 Nanoparticles and Ti(IV)-Fe(III) Mixed Oxides

Abbas Khaleel, Maliha Parvin, and Ahmed Alzamly, and Mohamed Al Tabaji

Department of Chemistry
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I.17 Tuning of the Dopant Size and Valance State in TiO_2 Thin Films for Efficient Photocatalysis

A. Ali, M. M. Alam, S. Naseer, and A. S. Bhatti

Department of Physics
COMSATS University Islamabad (CUI), Islamabad, Pakistan

I.18 Magnetic Framework Composites as New Catalysts for Biodiesel Production through Esterification Reaction

Ghewa Sabeh and Mohamad Hmadeh

Department of Chemistry
American University of Beirut, Beirut, Lebanon

I.19 Carbon doped TiO_2 Photocatalysts for Visible Light Photodegradation of Methylene Blue

Ines Bouzaiene, Semy Ben Chaabene, Rym Akkari, and Mongia Saïd Zina

Department of Chemistry
University of Tunis El Manar, Tunis, Tunisia

I.20 Hydrothermal Synthesis of $BiVO_4/TiO_2$ Hetero-Nanojunction for Methylene Blue Degradation under Solar Light Irradiation

Sahar Mansour, Rym Akkari, Semy Ben Chaabene, and Mongia Saïd Zina

Department of Chemistry
Faculty of Sciences of Tunisia, Tunis, Tunisia

I.21 Synthesis and Characterization of TiO_2 Photocatalysts Doped with Transition Metals: Application in Wastewater Treatment

Jamila Sakfali, Semy Ben Chaabene, Rym Akkari, Mongia Said Zina

Department of Chemistry
Faculty of Sciences Tunis, University of Tunis El Manar, Tunis, Tunisia

I.22 Synthesis of CuO-GO/TiO_2 Visible Light Photocatalyst for 2-Chlorophenol Degradation, Pretreatment of Dairy Wastewater and Aerobic Digestion

Ziad Omar Ahmad AlAfif, Muzammil Anjum, Rajeev Kumar, S. M. Abdelbasir, and M. A. Barakat
Department of Environmental Sciences
King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

I.23 Organic Waste as a Feedstock to Sustainable Hydrogen Fuel: A Solar Driven Quantum Leaf

Anupma Thakur, Praveen Kumar, Rishabh Jain, R. K. Sinha, and Pooja D.
Material Science Division, V1(A), Agrionics
CSIR-Central Scientific Instruments Organisation, Chandigarh, India

I.24 Enhancement of Visible Light Photocatalysis and Anaerobic Digestion of Wastewater Sludge

Muzammil Anjum, Rajeev Kumar, and M. A. Barakat
Department of Environmental Sciences, Faculty of Meteorology, Environment
KAU University, Jeddah, Kingdom of Saudi Arabia

I.25 Synthesis and Catalytic Properties of Metal Nanoparticles in Biodegradable Polymers Coated Polyurethane Sponge Substrate

May Alruwaili[†], Ali Alhasan[‡], and Edreese Alsharaeh[†]
[†]College of Science and General Studies, Alfaisal University
[‡]Nanomedicine Lab, King Abdulaziz Center for Science and Technology (KACST)

I.26 Synthesis of a Novel Mixed-Shape ZnO with Metal Nanoparticles Embedded in Graphene Oxide with a Powerful Photoactivity for Degradation of Methylene Blue

Nathir A. F. Al-Rawashdeh, Mohannad Theeb Al-Jarrah, and Odai Monzer Allabadi
Department of Math & Natural Science (Chemistry)
Higher Colleges of Technology, Ras Al Khaimah, United Arab Emirates

I.27 Nanocomposite Fibers of Chitosan-Graphene Oxide Supported Copper Nanoparticles Based Perceptive Sensor and Active Catalyst for Nitrophenol in Real Water

Fayaz Ali and Sher Bahadar Khan
Department of Chemistry
King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

I.28 Effect of Light Irradiance on Electrical Performance of GaInNAs Multiple Quantum Well (MQW) p-i-n Diode

Muhammad Izzuddin Bin Abd Samad[†], **Khairul Anuar Mohamad**[†], **Mohammad Syahmi Nordin**[‡], **Nafarizal Nayan**[†], **Afishah Alias**[§], **Adrian Boland-Thoms**[‡] **and Anthony John Vickers**[‡]
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[‡]School of Computer Science and Electronic Engineering, University of Essex, United Kingdom
[§]Faculty of Applied Science and Technology, Universiti Tun Hussein Onn Malaysia, Malaysia

I.29 Transparent Conducting p-Type Nickel Oxide Fabricated by Annealing of Phosphorous Doped Electroless Nickel

Anirban Chakraborty, Prahalad Murali, and P. Swaminathan
Department of Metallurgical & Materials Engineering
Indian Institute of Technology Madras, Chennai, India

I.30 Observation of Large Topological Hall Effect in Antiskyrmion Hosting Compound $Mn_{1.4}PtSn$

Praveen Vir
Solid State Chemistry
Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

I.31 The Effect of h-BN/Graphene on the Efficiency of DSSCs

Khalil Guizani, Mahmoud Hezam, and Edreese Alsharaeh
Department of Science and General Studies
Alfaisal University, Riyadh, Kingdom of Saudi Arabia

I.32 Multifunctional Hybrid Diode: Study of Photoresponse, High Responsivity, and Charge Injection Mechanisms

Jitendra Singh, R G Singh, Subodh K. Gautam, and Fouran Singh
Department of Physics
Inter-University Accelerator Centre (IUAC), New Delhi, India

I.33 Effect of Deposition Angle on Morphological and Optical Properties of Sputtered Tin Nitride Thin Films

Teena Jangid and G. Mohan Rao
Department of Instrumentation and Applied Physics
Indian Institute of Science, Bangalore, India

I.34 Emergence of Two Dimensional Spin Polarized Electron Gas at the Surface of Polar Insulators

Arpita Sen[†], **Umesh V. Waghmare**[‡], **and Prasenjit Sen**[†]
[†]Department of Physics, Harish Chandra Research Institute, Allahabad
[‡]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

I.35 Insights into the Characteristic Gap Level and n-Type Conductivity of Rutile TiO_2

Xiaoping Han, Noureddine Amrane, and Maamar Benkraouda
Department of Physics, United Arab Emirates University, Al Ain, United Arab Emirates

I.36 Efficiency Improvement of Organic Solar Cells by Using solvent Vapor Annealing and Thermal Vapor Annealing

Arsalan Haider and Thomas Zeh
Department of Electrical Engineering
University of Applied Sciences Kempten, Kempten, Germany

I.37 Performance Improvement of Supercapacitors by using h-BN/RGO as Material Electrodes

Nada Althubaiti, Edreese Alsharaeh, and Yasmin Mussa
Department of Chemistry
Alfaisal University, Riyadh, Saudi Arabia

I.38 Vertically Aligned Tree-like Carbon Nanostructures as Electrode for Electrochemical Capacitors

Monalisa Ghosh and G. Mohan Rao
Department of Instrumentation and Applied Physics
Indian Institute of Science, Bangalore, India

I.39 TiO_2/g-C_3N_4 based Biodegradable Nanolubricant towards Improving Tribological Properties

Nisha Ranjan, M Kamaraj, and S Ramaprabhu
Departments of Physics and Metallurgical and Materials Engineering
Indian Institute of Technology Madras, Chennai, India

I.40 Synthesis of Nano-Sized High-Entropy Carbide Powder by Electrochemical Deoxidation for Possible Application in Supercapacitors

Jagadeesh Sure, D. Sri Maha Vishnu, Hyun-Kyung Kim, R. Vasant Kumar, and Carsten Schwandt
Department of Materials Science and Metallurgy
University of Cambridge, Cambridge, United Kingdom

I.41 Feasibility of Quantum Dot Based Lasers in Blue and Green Region

Aparna Shinde, Amruta Lohar, Richa Gahlaut, and Shailaja Mahamuni
Department of Physics
Savitribai Phule Pune University, Pune, India

I.42 Microwave-Assisted Synthesis of Some Potential Bioactive Imidazolium-Based Room-Temperature Ionic Liquids

Ahmed H. Albalawi and Mouslim Messali
Department of Chemistry
Taibah University, Madinah, Kingdom of Saudi Arabia

I.43 Design, Microwave Synthesis and Characterization of Some New Bioactive Functionalized Imidazolium-based Ionic Liquids

Anas R. Al Johani and Mouslim Messali
Department of Chemistry
King Abdullah Air Defense College, Taif, Kingdom of Saudi Arabia

I.44 Microwave-Assisted Synthesis of Novel Imidazolium, Pyridinium and Pyridazinium-based Ionic Liquids and/or Salts and Prediction of Physico-Chemical Properties for their Toxicity and Antibacterial Activity

Mouslim Messali
Department of Chemistry
Taibah University, Madina, Kingdom of Saudi Arabia

I.45 Preparation of $CaCO_3$-HDPE Composite Sheets and their Physiochemical Characterization

Sidra Siraj Ahmed, Ali H. Al-Marzouqi, and Muhammad Z. Iqbal
Department of Chemical Engineering
United Arab Emirates University, Al Ain, United Arab Emirates

I.46 Thermally Reduced Graphene/Polyethylene Nanocomposites: Study of Melt Crystallization

Ahmed Z. A. Abuibaid and Muhammad Z. Iqbal
Department of Chemical Engineering
United Arab Emirates University, Al Ain, United Arab Emirates

I.47 Synthesis of Multivariate Metal-Organic Frameworks

Fayrouz Abou Ibrahim, Mazen Al Ghoul and Mohamad Hmadeh
Department of Chemistry
American University of Beirut, Beirut, Lebanon

I.48 Fabrication of Multiferroics and High Refractive Index Glasses by Containerless Process

Malahalli Vijaya Kumar, Sannaiah Ananda, Takehiko Ishikawa, and Kuribayashi
Departments of Chemistry and Space Biology and Microgravity Sciences
University of Mysore, Japan Aerospace Exploration Agency, Mysuru, India

I.49 Giant Room Temperature Ferroelectricity in Ferromagnetic $SmMnO_3$

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I.50 Photocatalytic Degradation of Nizatidine in Aqueous Solution by $BiVO_4$ Catalyst Under Ultraviolet Radiation

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Poster I.1

Selective-Jet Electrodeposition for Low-Cost Additive Manufacturing of Metallic Components at Room-Temperature

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Additive manufacturing (AM) techniques have improved to a level that allows diversifying our manufacturing capabilities. In this context, Selective-Jet Electrodeposition (SJE) has emerged as a novel technique to manufacture metallic components at room temperatures with low cost. Due to the high resolution and material quality, this can be applied to high-performance small-scale heat exchangers for high-density fluxes. This directly impacts energy requirements for computation activities and energy harvesting in micro-scale devices. The technique consists of reducing ions of different metals into a specific location on a conductive substrate. The deposition is controlled in the 3-dimensions, which allows layer-by-layer structure build-up. So far, most of the focus has been on the deposition phenomena, and on the chemical composition of the electrolyte, while less attention has been focused towards the deposition rate. One of the key characteristics is the capability of adding or subtracting material simply by reversing the polarity applied during the process. One of the remaining drawbacks of this technique is the slow deposition rate that needs to be enhanced in order to achieve fully the promises of SJE. In this work, the deposition (addition) and etching (subtraction) of copper were monitored by using various polymer-printed nozzles diameters, along with varying current densities and process time. More specifically, relations of the dimensions, density and electrical conductivity of the deposited/etched materials to the mentioned parameters are investigated. These observations provide the critical parameter space to be optimized in order to achieve a speedy deposition and obtain the desired density. The nature of the deposited material is poly-crystalline, with a density that varies with the changing current density, due to the formation of porous regions in the structure. Our results show that the deposition area of the copper is around 60% of the used nozzle diameter, while the deposition rate keeps constant with the chosen current.

Poster I.2

Potassium Levels on Gladiolus Corms Production in Open Field and Intercropping Conditions

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The influence of potassium levels on gladiolus corm (Gladiolus grandiflorus) production under two growing conditions were studied at Agriculture Research Institute, Mingora Swat. The two growing conditions (open field and intercropping) and potassium levels (0, 30, 60 and 90 kg ha^{-1}) were studied during the experiment. The experiment was planned in randomized complete block design having split plot arrangement with three replications. Light intensity and soil humidity were also recorded in both conditions. Data was recorded on various growth attributes, which showed that both growing conditions and potassium levels had significantly affected most of the attributes. The maximum sprouting percentage (93.7%), diameter of corms (5.3 cm), corms weight (69.9 g), number of cormels plant-1 (19.0) and survival percentage (88.8%) were recorded in open field, while maximum plant height (120.2 cm) was observed in intercropping. Moreover, maximum number of leaves plant-1 (6.5), plant height (120.4 cm), diameter of corms (4.3 cm), corms weight (47.9 g), number of cormels plant-1 (16.9) and survival percentage (88.8%) were recorded in plots applied with 90 kg potassium ha-1. Hence, it was concluded that gladiolus could be grown in open field condition with application of potassium at 90 kg ha^{-1} for better growth and production of corms under the agro-climatic conditions of Swat valley.

Poster I.3

Optimization of Injection Molding Parameters of UHMWPE for Production of UHMWPE/Nano-Filler Composites for Biomedical Applications

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Pure Ultra-High Molecular Weight Polyethylene (UHMWPE) and its Nano-filler composites have a broad range of applications in biomedical engineering field due to their superior properties. In spite of the verity that extremely long chains and high molecular weight of UHMWPE determines its superior properties, it simultaneously imposes restrictions on processing. It has been deep-dyed that the extremely high melt viscosity of UHMWPE polymer originates from the immense entanglement density of the long polymeric chains which hinder the molecular chain mobility. In that vein, decreasing entanglement density is anticipated as a feasible method to improve processability of UHMWPE using injection molding which represents the gold standard among other manufacturing techniques. This work targets optimizing injection molding processing parameters with the aim of improving self-diffusion of molecular chains. Groups of UHMWPE samples were prepared at different processing parameters including barrel temperature, injection pressure, mold temperature, and holding time in both barrel and mold. Mechanical properties including the tensile test yield stress, fracture stress and elongation at break were selected as the response variables. Scanning Electron Microscope (SEM) was utilized to investigate the effect of different processing parameters on the microstructure and morphology. Additionally, thermal stability was studied using Differential Scanning Calorimetry (DSC), and Thermogravimetric Analysis (TGA). Fourier Transform Infrared Spectroscopy (FTIR) was used to identify the presence of various bonds, and study both oxidation and degradation behavior of the injection molded UHMWPE specimens, if any. Moreover, the optimally prepared UHMWPE samples were subjected to *in vitro* evaluation using dental stem cells to evaluate their potential as hard tissue partial and total replacements. Based on the results of this study, optimum injection molding process parameters were specified to produce quality UHMWPE samples. These optimum parameters will be used to produce UHMWPE/nano-filler composites.

Poster I.4

Synthesis, Characterization, Crystal Structure, DNA-binding and Antimicrobial Activities of Co(III) and VO(IV) Schiff-base Complexes

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A series of metal complexes of Co(III) and VO(IV) having the general composition $[M(L)_2]Cl_2$ and $[M(phen)(L)]Cl_2$ [where L=(E)-2-((3-(benzyloxypyridinylimino)methyl)-4-bromophenol; (phen=1,10-phenanthroline); M=Co(III) and VO(IV)] have been prepared and characterized by elemental analysis, spectroscopy (IR and UV-visible) studies, molar conductance and magnetic susceptibility measurements. The structure of ligand was authenticated by X-ray single-crystal analysis. On the basis of above studies, a square pyramidal geometry for VO(IV) complexes whereas octahedral geometry for Co(III) complexes has been assigned respectively. Free ligand and its metal complexes have been tested *in vitro* against a number of microorganisms. The tested compounds exhibited significant activity. In addition, the DNA-binding properties of the ligand and its complexes have been investigated by absorption, fluorescence and viscosity measurements. The results obtained indicate that these complexes bind to DNA via an intercalation binding mode.

Poster I.5

Quantitative Investigation of the Swelling Behavior of Alginate and Alginate/Clay Beads Cross-Linked with Ca^{2+}

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Studies on the swelling behavior of polymer-based and polymer/clay beads are limited despite the large field of applications such as drug delivery due to their high biocompatibility and the simple gelatinization process. In this work, the swelling behavior of polymer (sodium alginate) and polymer/clay beads prepared by ionotropic gelation in the presence of calcium chloride has been investigated.

Three different types of clay have been used: sodium (Na) clay, cetylpyridinium (CPC) clay and pillared (Al) clay type. The beads were characterized in terms of physical aspect by calculating the hydration rate, the yield and the sphericity. To evaluate the swelling behavior, the beads were exposed to different conditions including pH, temperature variation and salts (monovalent, divalent, trivalent) at various concentrations. The water-uptake was quantified by comparing initial and final weights.

The results showed different capsules swelling behavior depend on the incubation medium. The experimental monitoring showed an increase in water-uptake capacity at high temperature for alginate beads (275%) while a syneresis occurred in saturated salt solutions. The same phenomenon was observed at low and high pH.

The results of our experiment indicate that hybrid beads have a higher water-uptake than alginate beads due to the presence of clays, except the CPC beads because they are hydrophobic, which make them suitable for the encapsulation and release of various hydrophilic and hydrophobic substances.

Poster I.6

Fabrication of Metalosomes (Metal Containing Cationic Liposomes) using Single Chain Surfactant as Precursor via Formation of Inorganic Organic Hybrids

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Herein, we demonstrate the formation of liposomes from single-chain cationic surfactants with the help of metal as a part of the counter ion and these metal embedded liposomes are termed as metalosomes. It is a noteworthy advancement in the area of self-assembled molecular structures since we are preparing metal embedded liposomes (metalosomes) from a water soluble single chain cationic surfactant, which is otherwise a property or the arrangement made by double tailed surfactants or more precisely lipids which are poorly water soluble. The metallosurfactants depict the successful formation of cationic metalosomes (with/without cholesterol) and the formation, structure and size has been verified using TEM, FE-SEM, DLS XRD and SAXS. The comparison of metalosomes in different solvents provides further insight of microstructure and solvent environment effects on the self-assembly of metallosurfactants. In addition, we have evaluated the encapsulation ability of metalosomes for fluorescein dye. High encapsulation efficiency of Metallosomes makes them promising candidates for many applications in future, especially because of water solubility.

Poster I.7

Modification of Gold Nanoplates into Gold Nanosquares to Increase Sensitivity of Plasmonic Sensors

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Gold nanoparticles have received tremendous attention in recent years for various applications such as biological imaging, chemical sensing, drug delivery and phototherapeutics due to its unique surface plasmon resonance (SPR) properties. Localized surface plasmon resonance (LSPR) properties of metallic nanostructures, such as gold, are very sensitive to the dielectric environment of the material, which can simply be adjusted by changing its shape and size through modification of the synthesis procedure.

In this study, gold nanostructures focusing on gold nanosquares (AuNSs) have been fabricated by modifying the recipe of gold nanoplates (AuNPs) on indium-tin oxide (ITO) substrate using seed mediated growth method (SMGM). From previous studies, there are many possible AuNP shapes such as hexagon, semi-hexagon, triangular and spherical resulting in broad optical spectra, which are not optimum for plasmonic sensors. Therefore, having a homogeneous shape might increase the sensitivity of the LSPR sensor.

AuNSs were synthesized through two main processes namely seeding process and growth process. Seeding process was used deposit a seed layer onto the substrate. Then, the growth of AuNSs were carried out at 28-30 °C in the presence of polyvinylpyrrolidone (PVP) as a stabilizing and shape-directing agent in the polyol synthesis of metallic nanoparticles. In this process, the molarity of PVP and the growth time were investigated to study the density and homogeneity of AuNSs. As a result, the AuNSs were been successfully synthesized using SMGM. However, the formation of byproduct such as rod, triangular, spherical shape were also present. Hence, the growth time was varied from 2-8 hours and labelled as GT2, GT5 and GT8 to obtain the optimum density, size and shape of AuNSs. After 2 hours, small spherical to square particles were observed. Bigger particles formed after 5 hours growth time with a small amount of byproduct such as nanorods. 8 hours resulted in the largest particle size compared to other samples. Further, the amount of byproduct formed also increases. The average size of AuNSs for GT2, GT5, and GT8 are 1058.28 nm^2, 1195.19 nm^2 and 4309.01 nm^2. Despite the smallest aspect ratio, highest intensity, and biggest particles, GT8 is not the most optimum growth time as more byproduct produced. Thus, 5 hours is the optimum growth time with aspect ratio 1.10 and surface density of 63%. The XRD results show all samples have the presence of two peaks at 38.195° and 44.393° indicating gold nanosquares, with their crystal orientation of (111) and (200).

Poster I.8

Evaluating the Potential Use of Waste Eggshells in Lead Adsorption Using Response Surface Methodology

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Lead is a highly toxic pollutant to human health and the environment. It is regularly identified in domestic as well as industrial wastewater. To mitigate its negative effects, environmentalists and materials scientists have been working on developing efficient and cost-effective lead removal techniques. This research falls in the same category as such ongoing efforts, whereby waste eggshells were examined for their efficiency in removing lead from polluted synthetic wastewater. The eggshells were locally sourced from restaurants and bakeries in the city of Al Ain. The eggshell membranes were removed and the eggshells were then washed, dried, and crushed to the appropriate particle size. Preliminary test results show that eggshells have a high potential as an adsorbent, with lead removal of up to 98%. Further testing will include batch adsorption experiments using a factorial experimental design to assess statistically significant adsorption-related parameters, including particle size, contact time, pH, adsorbent dose, and initial lead concentration. The statistically significant parameters will then be utilized in Response Surface Methodology for the modeling and optimization of the adsorption process. Future work will also include the development of continuous flow adsorption columns. The lab-scale setup will provide a stepping stone towards determining the potential industrialization of the process. This research will provide evidence to the feasibility of recycling an abundant food waste to achieve environmental sustainability and reduce pollution.

Poster I.9

Synthesis of Curcumin Based Novel Nano Hybrid Composite with ZnO and its Application for Biological Activity

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Curcumin is a natural component present in turmeric and its synthetic derivatives are a versatile biomaterial which has a wide range of biological importance, unfortunately it lacks bioavailability predominantly due to its poor aqueous solubility. The intention of the present investigation was to develop a novel nanocomposite of curcumin derivative named 3,5-bis((E)-3-methoxy-4-(prop-2-yn-1-yloxy)styryl)isoxazole with ZnO nanoparticles in order to improve its aqueous-phase solubility and develop its efficiency. Therefore, we have constructed an aqueous soluble curcumin derivative/ZnO nanocomposite from the insoluble synthesized curcumin derivative and poorly soluble ZnO nanoparticles. We used two step concerted top down methods for curcumin derivative preparation utilizing a mixed type of mechanical using zirconia beads and ultrasonic milling.

The synthesized ZnO nanoparticles, nanocurcumin derivative and the nanocomposite were analyzed with dynamic light scattering (DLS), and powder X-ray diffraction (XRD) along with spectroscopy techniques. The calculated average particle size of ZnO nanoparticles is ~40 nm, curcumin derivative is ~ 28 nm and nano-composite from XRD was found to be ~50 nm.

The observed results demonstrated that the title nanomaterials showed excellent antibacterial activity against, *Escherichia coli*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*. The nanocomposite showed negligible hemolytic activity (less than 5%) proving that the material expresses negligible cellular toxicity. All the observed results show that it has great potential for antibacterial applications.

Poster I.10

Characterization of Bioactive 3D-printed Biodegradable Bone and Dental Fixation Prosthetics

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Fixation of bone fractures take place using metallic plates and screws that are usually considered bioinert. These prosthetics were not found absolutely bioinert as they undergo corrosion over time after implantation. In addition, these prosthetics are normally removed through an additional surgery after bone fixation. The current work deals with the use of single-use biodegradable bone and dental prosthetic devices that are bioactive and will maintain fixation duties until it eventually degrades. Moreover, the enhanced bioactivity of the prosthetics provides a better augmentation with the fractures body and does not contain parts that need an additional surgery for removal. In the current study, a biodegradable polymer based on poly(□-hydroxy esters) was 3D printed into highly porous device. After chemical treatment in a highly basic medium, the porous prosthetics were evaluated in a simulated body fluid to assess their bioactivity as compared with the as-prepared porous prosthetics. Moreover, the mechanical properties of the highly porous 3D parts were evaluated before and after being impregnated with bone-like calcium phosphate cement.

Poster I.11

Characterization of Hydroxyapatite-Containing Zinc Polycarboxylate Cement for the Treatment of Bone Fracture

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Bone fractures are usually treated with bone cements and or mechanical fixation depending on the extent of fracture. Zinc polycarboxylate bone cements have been studied as stand-alone cements or as composites with inorganic and organic components, which are usually added to improve the strength and bioactivity of the cement. In the current study, bone-like hydroxyapatite (HAp) nanoparticles have been added to ZnO nanopowder prior to its hydration with acrylic-based polymeric solution to form the final set modified cements. The effect of adding up to 20 wt% of HAp NPs to ZnO powder on the setting reactions of the modified composite cements made thereafter has been investigated. Moreover, the variation of compressive and tensile strengths of the HAp-Zn polycarboxylate composites and the morphological changes observed as a result of the addition of HAp NPs has been studied. Due to the high surface area of the HAp NPs by virtue of theirs size (< 20 nm), improved mechanical properties of zinc polycarboxylate cement was observed where it is estimated that NPs act as true fillers within the porous polymeric matrix. These cement composites are highly believed to be superior to pure cements due to the improved mechanical properties and presence of HAp as an additional source of bioactivity for enhanced treatment of bone fractures.

Poster I.12

Comparative Study of CTS-nHA and CTS-nBG Composite based Scaffolds for Hard Tissue Engineering Applications

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The idea of composite synthesis using natural polymer (chitosan) and ceramic nanoparticles (hydroxyapatite and bioglass) may be considered as a solution for hard tissue engineering. In this paper, we describe a comparative assessment of biocompatible and biodegradable composite based scaffolds with enhanced biological characteristics. Chitosan (CTS) has the ability to bind with growth factors, glycosaminoglycans and DNA (anionic molecules). The biocompatibility and the cationic nature of chitosan makes it effective as bone grafting material. The hydroxyapatite nanoparticles (nHA) were synthesized by hydrothermal method and 50% SiO_2-42.5% CaO-7.5% P_2O_5 bioglass nanoparticles (nBG) were synthesized by sol-gel method. The nHA and nBG have a greater surface area and inert properties, which mean they can used for tissue engineering applications. The porous composite based scaffolds have been fabricated by freeze drying method. Scanning electron microscopy (SEM), transmission electron microscopy (TEM), and fluorescence microscopy were used to study various properties such as microstructure, size and surface topography of composites or scaffolds. Fourier transform infrared spectroscopy (FTIR), x-rays diffraction (XRD) and Brunauer, Emmett, and Teller analysis (BET) were used to analyze the physicochemical characteristics of synthesized nanoparticles and composites. Simulated body fluid was used to check the mineralization behavior of composite. These composite based scaffolds can prompt to the advancement of artificial creation of hard tissue alternates.

Poster I.13

Green Silver Nanoparticles by and Against the Two-Spotted Spider Mite, *Tetranychus urticae*

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Biosynthesis of nanocides is being pro rata increased with the amount and concentration of raw material that are provided to agricultural pests. The formation of biological silver nanoparticles (AgNPs) has presented an evolutionary paradigm specifically by *Tetranychus urticae*. Furthermore, the production of silk webs is expanding the effect of AgNPs effectively. Bionanoparticles of silver produced from the green form of *T. urticae* which caused certain mortality percentages over 97% against the same species, while they were more than 92% and 90% against *Spodoptera littoralis* and the red form of *T. urticae*. In the same trend, bioproduct from the red form of *T. urticae*, caused mortality over 88%, 94% and 90% in case of treatments against *T. urticae* green form, *T. urticae* red form, and *S. littoralis*, respectively. Subsequently, AgNPs as bio-ovicides resulted from the green form of *T. urticae*, caused sterility over 90%, 85% and 87% in case of treatments against *T. urticae* green form, *T. urticae* red form, and *S. littoralis*, respectively. Also, AgNPs from the red form of *T. urticae*, caused sterility over 88%, 94% and 90% in case of treatments against the same arrangement of mentioned pests. Moreover, data revealed that individuals of the green form populace invested more energy moving and less time resting than populace of the red form of *T. urticae* which means increased production of AgNPs.

Poster I.14

Development of Metal-Organic Frameworks based Nanocomposites for Impedimetric Sensing of *Staphylococcus arlettae*

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Metal-organic frameworks (MOFs) have emerged as materials with great potential for their extended applications. Owing to their ease of synthesis, large surface to volume ratio and flexible framework functionality, MOFs can also be explored in the development of efficient biosensors. However, the poor electrical conductivity is a bottleneck to exploit them in the development of electrochemical sensing devices. Recent investigations indicate that MOFs can be assembled on conducting surfaces and such assemblies can be explored for impedimetric responses. Among the various categories of biosensors, the electrochemical devices offer some definite advantages such as fast response time, convenient handling, and high sensitivity.

The present work reports the assembly of Cu MOF composite on a conducting polymer substrate. The conducting thin film functionalized platform was then comprehensively characterized with various analytical techniques, such as FT-IR and UV-visible spectroscopy, X-ray diffraction analysis, electron microscopy, and surface area. The charge conduction properties of the doped MOF have been confirmed with I-V and cyclic voltammetry experiments. The sensing platform was then applied for the electrochemical detection of *Staphylococcus arlettae*. The fabricated biosensor displayed quantitative response for the target bacteria with short response time and low limit of detection.

Poster I.15

Green Silylation of Cellulose Fibers for Oil Spill Remediation

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Cellulose-rich cotton fibers were chemically modified to enhance their hydrophobicity. In conventional methods, chemical modification is performed in the solution phase which entails significant amount of chemical waste. In the present study, a gas–solid silylation reaction was used to graft alkyl groups on cotton fibers and the method does not require the use of a solvent. The modified cotton fibers were characterized by IR-spectroscopy, TGA analysis and SEM–EDS. The degree of substitution varied between 0.1 ~ 0.3 per glucose residue. The ability of the fibers to remove oil from the surface of simulated sea-water was investigated and all the modified fibers have adsorption capacity at least five times that of unmodified cotton. The oil adsorption capacity was optimized by varying factors such as fiber–oil contact time, temperature, and length of the grafted alkyl chains. Cotton fibers modified with dialkylsilyl ethers were found to have the best adsorption capacity of 18 g oil/g of modified cotton and a fiber–oil contact time of 10 min at 25 °C.

Poster I.16

Enhanced Structural Stability and Catalytic Activity of Sol-gel Prepared Ti(IV)-doped-Fe_2O_3 Nanoparticles and Ti(IV)-Fe(III) Mixed Oxides

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Doping γ-Fe_2O_3 with Ti(IV) ions and modifying TiO_2 with different concentrations of Fe(III) ions was found to lead to significant enhancement in structural stability as well as to modification of the composites textural properties and catalytic activity. The observed modification resulted in enhanced stability of the structure of the Fe(III) oxide magnetic polymorph, γ-Fe_2O_3, which is of great importance in various magnetic applications [1,2].

A sol-gel method was used to prepare composites with Fe(III) nitrate and Ti(IV) butoxide in 2-propanol in the presence of propylene oxide as a gelation agent. In the absence of Ti(IV) dopant ions, a mixture of γ-Fe_2O_3 and α-Fe_2O_3 was obtained after calcination at temperatures in the range of 300-400 °C. However, the presence of Ti ions in concentrations as high as 10% suppressed the conversion to α-Fe_2O_3 resulting in a pure γ-Fe_2O_3 phase after calcination at 500 ºC, and no binary oxide phases were observed after calcination at temperatures as high at 650 °C.

The presence of Ti(IV) ions resulted in significantly larger surface areas and higher porosities. While the undoped γ-Fe_2O_3 possessed a surface area around 75 m^2/g, its doped counterpart containing 10% Ti exhibited a surface area of 151 m^2/g and significant mesoporosity. Doping also enhanced reducibility of γ-Fe_2O_3 which was reflected in its enhanced catalytic activity in the catalytic oxidation of toluene. Similarly, the presence of Fe(III) ions in TiO_2 matrix resulted in structural, textural, and chemical modifications including enhanced oxidation catalytic activity.

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Poster I.17

Tuning of the Dopant Size and Valance State in TiO_2 Thin Films for Efficient Photocatalysis

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TiO_2 has been widely studied for its optoelectronic and catalytic applications since the discovery of the photocatalytic activity of TiO_2 in 1972. However, due to large band gap of TiO_2 (3.0 - 3.2 eV), most of the absorption occurs in the UV range, where the visible spectrum contributed only 5 - 8%. To enhance its photocatalytic activity under the visible light, TiO_2 requires band gap tailoring, which can be achieved by doping. On the other hand, almost 90% of the terminating surfaces (101) of TiO_2 are non-reactive and a small portion of remaining 10% is (100) which are most reactive ones. Thus, structural and morphological modifications are desirable for enhanced efficiency towards the catalytic reaction.

In this work, two dopants neodymium (Nd) and vanadium (V) were used to dope TiO_2 thin films. The experimental and simulation work show that the dopant ion size and valence state along with the growth conditions play an important role. The preferred (004) and (211) textured surfaces were successfully obtained when TiO_2 was doped with Nd and V, respectively. The doping of V and Nd also contributed to the visible and IR spectrum. Thus photocatalytic efficiency can further be enhanced by using these modified TiO_2 chips.

Poster I.18

Magnetic Framework Composites as New Catalysts for Biodiesel Production through Esterification Reaction

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Metal-organic frameworks (MOFs) consisting of metal linked to organic linkers have grabbed the attention in major fields ranging from catalysis, separation, adsorption, to sensing due to their large surface area and high porosity. To enhance their applications, additional functionality can be added to the MOF; one example are magnetic framework composites (MFCs) that are synthesized by the adherence of previously prepared magnetic nanoparticles to the surface of the MOF.

In our experiment, five MFCs were synthesized based on MOF-74 by solvo-thermal synthesis with different metals (Mg, Zn, Mn, Co, and Ni) and each was fully characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), infrared spectroscopy (IR) and Brunauer-Emmett-Teller (BET) measurements.

In general, MFCs have great potential in many applications such as catalysis and drug delivery. In particular, we recently proved their great catalytic activity in the esterification reaction of levulinic acid into butyl levulinate (a biodiesel of high potentials). Their catalytic activity was compared by detecting the produced ester on GC (gas chromatography) in which Mn-MFC gave the best results.

Poster I.19

Carbon-doped TiO_2 Photocatalysts for Visible Light Photodegradation of Methylene Blue

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Methylene blue (MB), a dye widely used in the textile industries, contributes with other dyes to harm the environment, especially water. In order to provide new tools for the removal of these organic pollutants present in wastewater, many efforts have been devoted to develop photocatalytic applications under visible light irradiation. In this context, carbon-doped titanium dioxide was used to investigate the photocatalytic degradation of MB.

These photocatalysts were prepared through different methods including sol-gel process, hydrothermal and solvothermal methods. Different sources of carbon were used including glucose, graphite, fullerene and acetic acid. The obtained materials were characterized by means of X-ray diffraction (XRD). Their morphological and textural properties were studied using N_2 adsorption-desorption at 77 K. While, their optical properties were studied by UV-Visible diffuse reflectance spectroscopy and photoluminescence.

In this work, the effects on the photocatalytic activity of carbon ratio as well as the effect of each preparation method were studied. Indeed, carbon-doped TiO_2 has been found to be viable in degrading our pollutant model under visible light. This may be due to the extension of the absorption of the light to the visible region by the narrowing of the band gap. The results also revealed that these photocatalysts may reduce the charge recombination and enhance photo-induced charge separation, which improved the photocatalytic activity. It was also proven that hydrothermal method was the most efficient preparation method of carbon doped TiO_2 photocatalysts dedicated to the degradation of MB.

Poster I.20

Hydrothermal Synthesis of $BiVO_4/TiO_2$ Hetero-Nanojunction for Methylene Blue Degradation under Solar Light Irradiation

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Chemical dyes have dangerous impacts on the environment and health of mankind. Methylene blue (MB) is one of the organic dyes which is present in textile industry effluents, and heterogeneous photocatalysis is a promising alternative for the degradation of these pollutants. Titanium dioxide (TiO_2) is one of the most common metal oxide photocatalyst for degradation of organic pollutants, because of its chemical stability and relatively high photocatalytic activity. Nevertheless, TiO_2 has a wide band gap energy (3.2 eV), which limits its absorption to UV light range. In this field, a challenge for semiconductor photocatalysts is to insure a low cost, narrow band gap, stable electron-hole pair, visible light active and heterojunctional photocatalysts. In recent years, and due to its narrow band gap energy, nanostructured bismuth vanadate ($BiVO_4$) has attracted substantial attention of several researchers.

Herein, we report a facile two-step hydrothermal method for the synthesis of $BiVO_4/TiO_2$ with heterojunction structure. This work aims to study the effects of $BiVO_4$ content on the catalytic photodegradation reaction of methylene blue (MB) under solar radiation using $BiVO_4/TiO_2$. The structural and textural characteristics of the synthesized materials were studied by means of different physico-chemical techniques such as N_2-sorption isotherms at 77 K, X-ray diffraction (XRD), Raman spectroscopy, diffuse reflectance spectroscopy (DRS), photoluminescence spectroscopy (PL) and ICP analysis. The incorporation of $BiVO_4$ extends the absorption edges to the visible light range which enhances the photosensitized degradation of MB.

Results revealed that appropriate $BiVO_4$ loading can inhibit TiO_2 crystallite growth and favors stabilization of the TiO_2 anatase phase. Photocatalytic test revealed that the as-obtained products possessed high photocatalytic activity, especially for low $BiVO_4$ amounts. This could be due to the formation of a heterojunction between $BiVO_4$ and TiO_2 which induces more efficient separation of excess charge carriers and reduces the electron-hole recombination rate.

Poster I.21

Synthesis and Characterization of TiO_2 Photocatalysts Doped with Transition Metals: Application in Wastewater Treatment

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Water pollution is attracting increased attention of specialists around the world. To eliminate or reduce the harmful effects of water pollutants, several processes are implemented such as heterogeneous photocatalysis which is revealed as a promising tool for photocatalytic removal of toxic water pollutants. Due to its non-toxicity, chemical stability and relatively low cost, titanium dioxide was considered as one of the most performant photocatalysts. However, the limit of its activity to the UV region and the rapid electron-hole recombination limit its efficiency. To overcome this problem, doping TiO_2 was a promising option showing an improvement of the photocatalytic activity by extending its absorption to the visible region and reducing the recombination of photogenerated charges.

The present study consists of doping TiO_2 nanoparticles with a series of transition metals (Co, Cr, Fe and Zr) using a sol-gel process and the prepared samples were evaluated in the photodegradation reaction of methylene blue, which is a synthetic dye posing a real problem of water contamination.

The as-prepared photocatalysts have been characterized by means of X-ray diffraction, Raman spectroscopy, N_2 adsorption–desorption measurements at 77 K, UV–vis diffuse reflectance spectroscopy and photoluminescence spectroscopy (PL). In the first part of this study, the effect of calcination temperature was investigated. Pure TiO_2 nanoparticles calcined at 400 °C possess the highest photocatalytic activity thanks to its highest specific surface area and its low gap band energy, in addition to a low recombination rate of the photogenerated electron-hole. The second part of the work was dedicated for TiO_2 doping. Doped TiO_2 nanoparticles have revealed the presence of anatase structure, a reduction of the band gap energy and a shift of the absorption band of TiO_2 to the visible region.

The photocatalytic activity showed an apparent improvement for TiO_2 when doped with zirconium compared to other doped and pure TiO_2 photocatalysts, which was related to the increase of the surface defects. Thus, the photocatalytic activity for the photodegradation of methylene blue was enhanced. Further, this study reveals that the photocatalytic performance of TiO_2 may be improved optimization of preparation parameters, such as calcination temperature or by doping. Certain elemental ions could not be used to dope TiO_2 due to their negative impacts on the photocatalytic activity, while other ones result in enhanced TiO_2 photocatalytic efficiency.

Poster I.22

Synthesis of CuO-GO/TiO_2 Visible Light Photocatalyst for 2-Chlorophenol Degradation, Pretreatment of Dairy Wastewater and Aerobic Digestion

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In the present study, photocatalysts such as copper oxide (CuO) and titanium dioxide (TiO_2) were coupled with graphene oxide (GO) for the synthesis of visible light active CuO-GO/TiO_2 composite photocatalyst for the decomposition of 2-chlorophenol (2-CP) and complex aromatics in real dairy wastewater. Photocatalytically treated dairy wastewater was further purified by aerobic digestion. The results revealed that the composite material improved 2-CP degradation. 86% removal was achieved with $k = 0.0101\ min^{-1}$ at pH 5.0. The effect of pollutant concentration showed that the decomposition of 2-CP increases with increased irradiation time and decreases with increased 2-CP concentration. Further testing showed high stability of CuO-GO/TiO_2 composite where 85.8% degradation of 2-CP was achieved after three cycles. For treatment of real dairy wastewater, photocatalysts increase the solubilization of organic matter and a 24% higher sCOD (from 5764 mg/L to 7536 mg/L after 6 hours) was observed compared to photolysis (without catalyst) pretreatment. This improves the aerobic digestibility of dairy wastewater where tCOD was significantly lowered from 12747 mg/L to 134.8 mg/L within 27 days of the process. Overall, the present study revealed that the CuO-GO/TiO_2 composite material could be an efficient catalyst for removal of toxic organic pollutants and treatment of dairy effluent, thus can be applied in wastewater treatment plants with a dependency of extensively available visible light.

Poster I.23

Organic Waste as a Feedstock to Sustainable Hydrogen Fuel: A Solar Driven Quantum Leaf

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Lately the conversion of waste to wealth has attracted great attention of researchers worldwide. The global usage of fruits and vegetables necessitates research efforts for recycling or reusing non-edible waste (peels, pulp, etc.) for innovative application development. Motivated by the need, we herein present the facile process for recycling organic waste into eco-friendly carbon quantum dots (CQDs) followed by their usage as efficient photoelectrode for solar driven hydrogen production via PEC water splitting. An architectural design is implemented on the conversion of *Citrus limetta* waste pulp into highly fluorescent, eco-friendly and low cost CQDs by one-step pyrolysis-assisted green route. These CQDs exhibit highest quantum yield of 63.3% compared to similar green synthesized CQDs, which is advantageous for many applications. Further, the surface of TiO_2 nanofibres (TNF) photoanode as a modelled photocatalyst, was modified by these CQDs, which enhance the overall light absorption by tailing into visible light spectrum and, thus, substantially expedites water splitting reactions in 0.1 M NaOH alkaline aqueous solution. The fabricated CQDs/TNF demonstrate a high current density of ~5.6 mA/cm^2 over TNF (~1 mA/cm^2), at applied vs. RHE under simulated AM 1.5 G solar illumination. Further, the Rct value measured in the similar conditions for TNF and CQDs/TNF electrodes to be ~111 Ω from ~140 Ω, respectively, which confirms the higher diffusion of channelized electrons under light illumination for CQDs/TNF photoanode over TNF. The CQDs/TNF photoanode show extended range of light response, which can be attributed to the existence of the electronic coupling between π states of CQDs and conduction band of TNF and enhances the water reduction for H_2 generation. The hydrogen evolution for CQDs/TNF electrodes was measured to be 260 μmolh^{-1}. This study serves as a proof-of-concept for the ability of solar-driven quantum leaf i.e. CQDs/TNF to address the global challenges: organic waste alleviation and hydrogen fuel production.

Poster I.24

Enhancement of Visible Light Photocatalysis and Anaerobic Digestion of Wastewater Sludge

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Visible light photocatalysts of Cr_2O_3/C_3N_4 composites with varying melamine concentrations were prepared by a high temperature calcination method. The composite samples were characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), UV-visible spectroscopy and particle size analysis. These analyses demonstrate coexistence of both Cr_2O_3 and C_3N_4 in the composites. The Cr_2O_3/C_3N_4 catalysts were tested for photocatalytic degradation of 2-chlorophenol in wastewater and solubilization of sludge in anaerobic digestion process to enhance biomethane production. The catalytic performance of Cr_2O_3, with 6% melamine (precursor of C_3N_4), improved the photocatalytic degradation of 2-chlorophenol under visible light. Further, application of Cr_2O_3/C_3N_4 for photocatalytic pretreatment of sludge released the soluble substances in solution in which sCOD was increased from 431 mg L^{-1} to 3666 mg L^{-1} after 6 hours and VS content decreased by 9.1%, which indicates that the short pretreatment time could avoid further mineralization of organic matter to complete degradation. These results can provide a useful basis and reference for the multi applications of visible light Cr_2O_3/C_3N_4 photocatalyst for enhancement of degradation of toxic pollutant in wastewater and sludge stabilization with bioenergy production.

Poster I.25

Synthesis and Catalytic Properties of Metal Nanoparticles in Biodegradable Polymers Coated Polyurethane Sponge Substrate

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During the last decade, magnetic nanoparticles (MNPs) gain a great interest because of their prospective applications in the biomedical field. However, several drawbacks involve the synthesis of magnetic nanoparticle include, the need for templates or surfactants, prolonged reaction times and multiple process steps. In this study, we have reported a rapid and straightforward method through a one-step hydrothermal synthesis by a quick microwave assisted synthetic route of Co_3O_4 nanoparticles with tailored structural and magnetic properties, furthermore characterized by FT-IR, TEM, DLS, UV-Vis, XRD techniques. The XRD and TEM studies show that the as-synthesized nanoparticles possess cubic morphology with a high degree of crystallinity, additionally, Co_3O_4 MNPs exhibit magnetic properties at room temperature. On the other hand, understand the properties of the nanoparticles and their effect on the body is crucial before any clinical uses, thus in vitro cytotoxicity evaluation will be studied. Moreover, MNPs surface modification and coating need to consider in order to improve the biocompatibility. As a result, the synthesized MNPs will enable them to be used in further development of MRI diagnostic systems, induced magnetic hyperthermia as well as a targeted drug delivery system.

Poster I.26

Synthesis of a Novel Mixed-Shape ZnO with Metal Nanoparticles Embedded in Graphene Oxide with a Powerful Photoactivity for Degradation of Methylene Blue

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Nanocomposite materials based on metal nanoparticles and graphene oxide (GO) have attracted considerable research interest due to their potential applications, including surface-enhanced Raman scattering, catalysis, sensors, biomedicine and antimicrobials. In this study, several GO/ZnO nanocomposites were synthesized via changing the GO to ZnO nanoparticle ratio (6.25, 3.125, 1.25, 0.625 and 0.125%). As synthesized nanocomposites were evaluated as photocatalysts for degradation of organic pollutants present in water. The degradation of methylene blue (MB) was investigated as a model pollutant. An optimum catalytic activity of 84% was achieved using a nanocomposite with 3.125% GO, exposed to irradiation of sunlight for 90 min. Furthermore, copper, palladium and silver nanoparticles were used as dopants to study their effects on photocatalytic activity. GO/ZnO/Cu and GO/ZnO/Pd nanocomposites showed that the activity toward MB degradation was decreased to ~ 50% and ~70%, respectively. However, a significant increase in the activity of MB degradation was achieved using GO/ZnO/Ag nanocomposite.

Poster I.27

Nanocomposite Fibers of Chitosan-Graphene Oxide Supported Copper Nanoparticles Based Perceptive Sensor and Active Catalyst for Nitrophenol in Real Water

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Copper nanoparticles templated at chitosan-coated graphene oxide (GO) nanocomposite fibers (Cu@CH+GO) were prepared via solution-based fiber formation and followed by treatment with a metal salt solution and $NaBH_4$. The prepared nanocomposites were utilized for the detection and catalytic reduction of 4-nitrophenol (4-NP). Cu@CH+GO exhibited a high sensitivity of 1.729 micro-$AmM^{-1}cm^{-2}$ and a detection limit of 3.5 mM toward 4-NP. In addition, high catalytic activity was observed for the reduction of 4-NP with an apparent rate constant of 1.3096 min^{-1} using 7 mg of Cu@CH+GO catalyst. In addition to the catalytic activity of Cu@CH+GO, it could be easily recovered by simply pulling the fiber from the reaction medium. Moreover, Cu@CH+GO catalyst was also examined in real samples and found to be efficient in the detection and reduction of 4-NP. This novel approach provides a new route for simultaneous detection and reduction of 4-NP and can be a time and cost-effective tool for environmental safety.

Poster I.28

Effect of Light Irradiance on Electrical Performance of GaInNAs Multiple Quantum Well (MQW) p-i-n Diode

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The properties of dilute nitride such as miscibility gap and large conduction band offset make this semiconductor very promising for photonic applications. This paper presents an investigation of light irradiance on electrical performance of dilute nitride GaInNAs with multiple quantum well (MQW) p-i-n diode on Hellish structure. The performance in this work refers to the magnitude and quality of generated dark current, the spectral response in dilute nitride absorption regions and responsivity.

The GaInNAs MQW p-i-n diode was grown on n-type GaAs (100) substrate using molecular beam epitaxy (MBE) system equipped with a radio frequency plasma source for nitrogen incorporation. Two 10 nm undoped GaAs graded layers were initially grown at the top and bottom of intrinsic region with 10 sandwiched GaAs and AlGaAs layers. It consists of a 600 nm emitter p-doped GaAs barrier with Be = 2 x 1018 cm^{-3} followed by 40 nm a p-doped AlGaAs with Be = 2 x 1018 cm^{-3}, a GaAs top layer with Be = 4 x 1018 cm^{-3}, a base contact consisting of 1900 nm n-doped GaAs with Si = 2 x 1017 cm^{-3}, 20 nm n+-doped GaAs with Si = 2 x 1018 cm^{-3} and n+-GaAs as a substrate. Electrical characterization, i.e. current-voltage (I-V) measurements, were performed using a Keithley source measurement unit (SMU) at room temperature. The light irradiance was illuminated using portable solar simulator (PECCELL technology) and light irradiance on 0.258 kW/m^2, 0.467 kW/m^2, 0.670 kW/m^2, 0.967 kW/m^2 and 1.077 kW/m^2 using reference cell meter (Newport) through ORIEL cell position.

Electrical characteristics of the dilute nitride p-i-n diode with MQW can be generally modelled using Shockley equation, the reverse current was increased with changes of light irradiance of -32.2 mA, -45.4 mA, -59.8 mA, -74.9 mA and -90.1 mA with 0.258 kW/m^2, 0.467 kW/m^2, 0.670 kW/m^2, 0.967 kW/m^2 and 1.077 kW/m^2, respectively. The highest short-current density 0.08 (± 1.33 x 10^{-3}) mA/cm^2, fill-factor 53.62 (±0.268) and lowest efficiency 0.02% on 1.077 kW/ m^2 light irradiance were obtained from the electrical characteristics.

In this work, it has been demonstrated that dilute nitride p-i-n diode with multiple quantum well generates dark current in the GaInNAs intrinsic layer. The MQW also results in an increase of the dark current. Further studies are ongoing to fully understand this behavior in the p-i-n diode.

Poster I.29

Transparent Conducting p-Type Nickel Oxide Fabricated by Annealing of Phosphorous Doped Electroless Nickel

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Transparent conducting oxides have wide spread applications for a variety of optoelectronic devices. Typically, n-type oxides used are zinc oxide, indium oxide, tin oxide, and their doped variants, with indium tin oxide being the most commonly used n-type conductor. Similarly, there is intensive research on developing p-type oxides, especially for sensors, memory devices, transparent electronics, and photovoltaics. Nickel and copper oxides, along with their doped variants, are the most commonly used p-type oxides. Nickel (II) oxide (NiO) is normally prepared either by vapor deposition or by a wet chemical route. The key to developing these oxide layers is to balance the optical transparency with the electrical conductivity.

We have used a two-step process for the synthesis of NiO thin films. The first step involves electroless deposition of Ni on quartz substrates activated through Au-Pd alloy sputtering. This mode of activation also allows for patterned deposition, which is crucial for device fabrication. We found that the mode of activation and bath conditions affect the kinetics and were able to extract the activation energies for the process. By varying both bath conditions and substrate activation, we were able to identify the rate controlling step in the electroless process.

Subsequently, air annealing was carried out to oxidize the Ni to form NiO. Along with oxidation, this step lead to the formation of defect states, which have an impact on the optical gap and the carrier mobility. The effect of annealing conditions on the optoelectronic properties of the film was investigated in detail. The oxide films were characterized by 3D non-contact optical profilometer for thickness measurement, scanning electron microscopy with energy dispersive spectroscopy for morphology and composition, UV-Visible spectroscopy to calculate the absorbance, and I-V measurements for electrical conductivity.

Electroless deposition of Ni leads to co-deposition of phosphorous, which acts as a dopant in the NiO. The amount of P can be varied by the chemical bath pH and our results show that this affects the deposition rate, optical transparency, and electrical conductivity. In addition, Hall-effect measurements and x-ray photoelectron spectroscopy (XPS) analysis can help us gain more insight regarding carrier type, mobility, and concentration. XPS data also tells us about the P content of the films as a function of bath pH and annealing temperature, which will be used to understand the stoichiometry of the NiO thin films. Thus, the two-step process developed in this work represents a simple and low-cost route to form p-type NiO transparent conductive films. The concept can be extended to other electroless deposition systems and can be used to form a variety of pure and doped metal oxide films.

Poster I.30

Observation of Large Topological Hall Effect in Antiskyrmion Hosting Compound $Mn_{1.4}PtSn$

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Skyrmions are topologically stable vortex-like spin structure which are considered to be a potential candidate for future high density memory devices. They have been detected in many chiral and polar compounds such as MnSi, FeGe, Co-Mn-Zn, GaV_4S_8, and $VOSe_2O_5$. Three types of vortex spin structure have been predicted and observed so far namely, Bloch, Néel and antiskyrmions. Existence of these exotic spin structures depends upon the crystal symmetry. Recently, by means of Lorentz transmission electron microscopy, antiskyrmions have been discovered in Mn-based tetragonal Heusler compound $Mn_{1.4}PtSn$ and $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$. Antiskyrmion is considered to be anti-particle of Néel or Bloch type skyrmion because it consists of opposite topological winding number. Due to this topologically stable spin nature, it can give rise to non-vanishing Berry phase in real space. This could result in nonzero topological Hall Effect (THE). Here, we report large THE and its origin in single crystals of antiskyrmion hosting compound $Mn_{1.4}PtSn$. We show for the first time that THE has contributions both from real and momentum-space Berry phase.

Poster I.31

The Effect of h-BN/Graphene on the Efficiency of DSSCs

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Due to their low cost, simple fabrication procedure, and strong adjustable features such as transparency and power of conversion efficiency, dye sensitized solar cells (DSSCs) are a promising alternative for silicon-based solar cells. One of the main concerns of DSSCs is the weak amount of absorption level; therefore, there is a need to find a better surface passivation technique that will help in absorbing more light intensity.

Nanomaterials have different properties than bulk materials. Materials with nanometer dimensions, typically less than 100 nm, contain superior properties that have a remarkable importance to nanotechnology.

In this work, TiO_2/h-BN/graphene nanocomposites were synthesized via microwave method. As synthesized nanocomposed were used as the working electrode, in addition to N-719 dye, which was coated onto the TiO_2 and carbonated glass or Pt as the counter electrode to fabricate quick, cost effective and eco-friendly DSSCs.

These nanocomposites were then fully characterized to confirm the formation of TiO_2/h-BN/graphene nanocomposites with pure anatase phase of TiO_2. Structural properties and morphology were characterized using X-Ray diffraction (XRD) and transmission electron microscopy (TEM). Thermal properties were studied using thermogravimetric (TGA). Chemical and optical properties were studied using infrared radiation (IR) and UV-visible spectroscopy. The synergistic effect of h-BN/graphene will improve the efficiency of DSSCs vastly regarding surface passivation and the components that the nanocomposites provide.

Poster I.32

Multifunctional Hybrid Diode: Study of Photoresponse, High Responsivity, and Charge Injection Mechanisms

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A multifunctional hybrid heterojunction diode is developed on porous silicon and its current density-voltage characteristics reveal a good rectification ratio along with other superior parameters such as ideality factor, barrier height and series resistance. The diode also functions as an efficient photodiode to manifest high photosensitivity with high responsivity under illumination with broadband solar light, UV light, and green light. The diode is also carefully scrutinized for its sensitivity and repeatability over many cycles under UV and green light and is found to have a quick response and extremely fast recovery times. The notable responsivity is attributed to the generation of high density of excitons in the depletion region by the absorption of incident photons and their separation by an internal electric field besides an additional photocurrent due to the charging of polymer chains. The mechanisms of generation, injection and transport of charge carriers are explained by developing a schematic energy band diagram. The transport phenomenon of carriers is further investigated from room temperature down to a very low temperature of 10 K. An Arrhenius plot is made to determine the Richardson constant. Various diode parameters as mentioned above are also determined and the dominance of the transport mechanism of charge carriers in different temperature regimes such as diffusion across the junction and/or quantum tunneling through the barriers are explained. The developed multifunction heterojunction hybrid diodes have implications for highly sensitive photodiodes in the UV and visible range of electromagnetic spectrum that can be very promising for efficient optoelectronic devices.

Poster I.33

Effect of Deposition Angle on Morphological and Optical Properties of Sputtered Tin Nitride Thin Films

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With potential commercial applications in optoelectronic devices, growth and characterization of nitride thin films is an area of considerable research interest. Tin-nitride is a IV-group nitride, which has not received much attention earlier due to difficulties associated with growth of pure tin nitride phase. Since trajectory of target particles is normally rectilinear in magnetron sputtering, placing the substrate at an oblique angle with respect to the direction normal to the target may result in changed crystallographic orientation of deposited thin-films.

In our previous study, we optimized the process parameters for the growth of pure tin-nitride thin-films, while keeping magnetron flux normal to the substrate surfaces. In this work, we studied the effect of deposition angle on the growth of polycrystalline tin nitride thin films. Tin nitride films were deposited with 3“ target on glass and Si substrate at a substrate temperature of 600 °C and target to substrate distance of 10 cm at two different angular positions, 45 and 90, of target flux onto the substrate surface. To improve confidence in obtained results, we deposited tin nitride thin-films at two RF powers, 15 and 20 W, for both angle of depositions.

Structural properties of deposited polycrystalline thin-films were studied using X-ray diffraction (XRD) Scanning electron microscopy (SEM) and UV-Vis spectroscopy were used to study morphological and optical changes in deposited tin-nitride thin-films with varying deposition angle.

XRD analysis reveals that the same crystal planes are present at both deposition angles but their intensity varies with varying angle of deposition, which is consistent for films deposited at both RF powers. In contrast to the minor changes observed in structural properties, surface morphology was found to vary significantly. Morphological study of tin-nitride films reveals that although films deposited at both deposition angles were uniform, samples with the 90 angle of deposition have particle size ~10 times higher than film deposited at 45 angle of deposition for both RF powers. Tin-nitride thin films deposited at 90 degrees and 20 W RF power demonstrated porous, uniform surface morphology, whereas, film deposited at 45 degree angle of deposition had a very dense surface structure along with the presence of few lumps in the deposited film surface. The drastic change in maximum transmitted light intensity from 29% to 80% is also observed between films deposited at 90 and 45 angle of deposition, respectively for the tin-nitride thin films deposited at 15 W RF power.

Based on these results, we conclude that, although the angle of deposition does not affect the crystallographic orientation, it has a significant effect on optical properties and surface morphology of tin-nitride thin-films in terms of film's microstructure, porosity and compactness.

Poster I.34

Emergence of Two Dimensional Spin Polarized Electron Gas at the Surface of Polar Insulators

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We report 2-dimensional electron gas at the basal surface terminated at shuffle planes containing oxygen atoms of polar insulators, wurtzite BeO and ZnO, based on first-principles density functional theoretical (DFT) analysis. We analyze this bulk insulator to surface metal transition as a function of distance of separation at the plane that cleaves the bulk crystal into surfaces, and find a critical distance dc at which the oxide shuffle surface becomes metallic. In typical DFT calculations, this distance corresponds to the thickness d of vacuum separating the periodic images of slabs of a crystal. This happens when the energy shifts in the conduction bands with d lead to pinning of the Fermi level in the conduction band.

From the density of states projected onto atomic orbitals, we demonstrate that the electron charge density is accumulated at the metal-terminated surface. While both BeO and ZnO are non-magnetic in their bulk form, their oxygen-shuffle surfaces constitute a spin-polarized 2-dimensional electron gas with a nonzero magnetization, which also depends on the distance d.

In their bulk from, both polar insulators possess a macroscopic electric polarization along c-axis of the wurtzite structure. In a non-magnetic state, the projected density of states exhibit a peak at the Fermi level, comprising of oxygen orbitals, causing the Stoner instability. Secondly, macroscopic electrostatic potentials in the slab of these oxides show a polar field, which leads to polar catastrophe. Together, these two mechanisms results in a two dimensional spin polarized electron gas in the shuffle surface of insulating polar oxides.

We expect these surfaces or nanothin slabs of BeO and ZnO to exhibit interesting magneto-electric coupling, and it should be rich and useful in various applications including electronic and magnetic devices.

Poster I.35

Insights into the Characteristic Gap Level and n-Type Conductivity of Rutile TiO_2

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It is well known that intrinsic rutile TiO_2 has two characteristic properties: gap level and n-type conductivity, but their origins remain controversial. In the present work, insights into these two characteristic properties have been probed using the Heyd-Scyseria-Ernzerhof (HSE) hybrid functional method in the framework of the density functional theory (DFT). Detailed thermodynamic and kinetic investigations have been conducted to elaborate the favorability for the formation of the possible n-type defects and unintentional impurities in rutile TiO_2. Results show that oxygen vacancy is clearly identified to induce a deep localized state inside the forbidden energy region through localizing two excess electrons at two Ti^{4+} ions along the [001] direction and reducing them into Ti^{3+} ions, accounting for the characteristic gap level observed experimentally. The eg orbital (x2-y2 type) composition of this gap level offers an accountable explanation of the experimentally measured ferromagnetism in TiO_{2-x}, while the electron transition from this characteristic level is contributable to the photocatalytic behaviors and visible photoluminescence of slightly reduced TiO_2. Also, unintentional incorporation of hydrogen substitution for oxygen acts as a shallow donor, providing a consistent explanation of the n-type conductivity in TiO_2. The fundamental understanding of these characteristic properties and the associated functionalities would be essential to improving and expanding the practical applications of TiO_2-based materials and devices.

Poster I.36

Efficiency Improvement of Organic Solar Cells by Using solvent Vapor Annealing and Thermal Vapor Annealing

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Fullerene solar cells are becoming a feasible choice due to advanced developments in donor materials and improved fabrication techniques of devices. Recently, sufficient optimization and improvements in processing techniques like incorporation of solvent vapor annealing (SVA) with additives in solvents has become a major reason for prominent improvements in the performance of organic solar cell-based devices . On the other hand, the challenge of reduced open circuit voltage (Voc) remains. This study presents an approach for significant performance improvement of overall device based on organic small molecular solar cells (SMSCs) by following a two step technique that comprises thermal annealing (TA) and SVA (abbreviated as SVA+TA). In case of exclusive use of SVA, reduction in Voc can be eliminated in an effective way. The characteristics of charge carriers can be determined by the measurement of transient photo-voltage (TPV) and transient photo-current (TPC) that determines the scope for improvement in the performance of device by two step annealing. The recovery of reduced Voc is linked with the necessary change in the dynamics of charge that lead to increased overall performance of device. Moreover, SVA and TA complement each other; therefore, two step annealing technique is an appropriate way to simultaneously improve the parameters such as Voc, fill factor (FF), short circuit current density (Jsc) and PCE of small molecular solar cells.

Poster I.37

Performance Improvement of Supercapacitors by using h-BN/RGO as Material Electrodes

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Owing to the high specific surface area of 2D nanomaterials, graphene and boron nitride have been widely investigated as effective materials in energy storage applications. This attention is attributed to the excellent electrical, optical and mechanical properties for these materials. Recently, supercapacitors have been shown to exhibit great potential as high performance energy sources for advanced technologies due to their high energy density and power density.

This work demonstrates a simple synthesis of hybrid h-BN/RGO as electrode material of supercapacitors and assembly in coin type with different electrolyte and different percentages of carbon black. The results show that the hybrid h-BN/RGO electrode could be used in large-scale production using existing economical, and highly effective supercapacitors fabrication technique.

Poster I.38

Vertically Aligned Tree-like Carbon Nanostructures as Electrode for Electrochemical Capacitors

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Vertically aligned tree-like carbon nanostructures are grown using plasma enhanced chemical vapor deposition (PECVD) method using electron cyclotron resonance (ECR) plasma system. The nanostructures are multiwalled carbon nanotubes, aligned perpendicular to the surface of the substrate with carbon films attached like "branches" of a tree[1]. The material with its vertical alignment and tree-like morphology has a very high exposed surface area, and this material is speculated to act as a high-performance electrode of electrochemical capacitors (EC) or supercapacitors[2-4].The electrochemical performance of the material as electrode has been studied in symmetric two-electrode configuration. The material is deposited on stainless-steel substrates of 12 mm diameter (area 1.13 cm^2). The material has shown a specific areal capacitance of 0.55 mF cm^{-2} (4.6 F cm^{-3}) at a current density of 0.88 mF cm^{-2} as compared to the value of 0.08 mF cm^{-2} (0.66 F cm^{-3}) for vertically aligned carbon nanotube films of same thickness, for the same current density. These results indicate that this material is a promising candidate for electrode material of supercapacitor.

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Poster I.39

TiO_2/g-C_3N_4 based Biodegradable Nanolubricant towards Improving Tribological Properties

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In recent years, the use of bio-lubricants, for instance, vegetable oil has gained popularity owing to the renewability, inherent biodegradability, and low eco-toxicity. This is indeed advantageous because mineral oil is non-renewable and toxic. However, vegetable oil may undergo changes in chemical and physical composition at elevated temperature and pressure which restrict them from being widely used for tribological applications. To improve these properties, the molecular structure may be modified or additives can be introduced into the vegetable oil.

Additives help to improve the wear performance of the vegetable oil at high speed, high temperature and high load. There are several additives such as graphite, MoS_2, hexagonal boron nitride and zinc dialkydithiophosphates (ZDDP), which are commonly used for anti-wear, extreme pressure and corrosion resistance applications. However, these additives often decrease machine life. In this regard, 0D and 2D nanomaterials have been explored extensively for tribological applications owing to their special properties, making them suitable for rolling, polishing, mending effect and uniform tribofilm formation. In order to harvest the synergistic effect of rolling and enhanced sliding motion with mending effect, a nanoadditive was designed which combines the best of 0D and 2D nanomaterials.

Tribological modification of vegetable oil by the addition of TiO_2/g-C_3N_4 nanocomposite has been studied. The nanoadditive was prepared by a two-step synthesis route. The combined effect of the nanocomposite dispersion in a vegetable oil has led to the formation of a thermally stable nanolubricant that shows excellent oil dispersion stability in the absence of surfactant. Tribological characterization was completed using a four-ball tester following ASTM standard D5183. The performance improvement on the nanoadditive dispersion in vegetable oil has been quantified by coefficient of friction, wear scar diameter, wear rate and surface roughness analysis. Data show that the use of biodegradable TiO_2/g-C_3N_4 nanocomposite dispersed vegetable oil can exhibit very good lubrication behavior for tribological applications. The effective decoration of the TiO_2 on the g-C_3N_4 sheets unlocks the synergistic effects of the anti-wear behavior of TiO_2 coupled with the inter-layer sliding behavior of g-C_3N_4 sheets. These results serve to prove the potential viability of TiO_2/g-C_3N_4 based biodegradable nanolubricant towards improving friction and wear resistance in the area of tribology.

Poster I.40

Synthesis of Nano-Sized High-Entropy Carbide Powder by Electrochemical Deoxidation for Possible Application in Supercapacitors

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In recent years, entropy-stabilized materials have been receiving attention as alloys, oxides, borides, carbides, nitrides and carbo-nitrides due to their large compositional design space [1]. The concept of high-entropy materials, initially starting from alloys, has gained importance because the combination of simple crystallography and complex chemistry enables the synthesis of new structural and functional materials with unique properties. By applying conventional methods such as arc melting and spark plasma sintering, it is difficult to bring these materials from bulk to nanoscale. Therefore, alternative processing routes are required to prepare nanoscale materials with controlled chemical composition, phase composition and particle size. Significant research efforts are currently being undertaken in the world over towards the preparation of high-entropy materials by economically-favorable and environmentally-friendly processes.

In the present study, the FFC-Cambridge process, originally developed for the single-step electro-deoxidation of oxides into metals, was used for the first time to synthesize high-entropy carbides. To that end, sintered discs of mixtures of TiO_2, Nb_2O_5, Ta_2O_5, ZrO_2, HfO_2 and C were employed as the cathode, versus a graphite anode in a bath of molten $CaCl_2$ at 1173 K, in order to convert them into (TiNbTaZrHf)C high-entropy carbide (HEC). XRD analysis of the HEC powders prepared demonstrated that single-phase face-centered cubic material can be prepared by optimizing the composition of the oxide/carbon precursor. SEM analysis revealed that the as-reduced materials were nano-grained with particle size in the range of 75-100 nm, and STEM-EDX elemental mapping confirmed their compositional homogeneity down to nano-scale level.

The synthesized HEC powder, with the unique features of single-phase crystallography and nano-sized morphology, is considered to be a promising candidate material for supercapacitor applications. The supercapacitive behavior was evaluated in a conventional three-electrode cell with 1 M KOH as the electrolyte, a platinum foil as the counter electrode, and Ag/AgCl as the reference electrode. The experimental results obtained in these investigations will be highlighted in the presentation.

Another key conclusion of this study is that the new electrochemical approach should be scalable towards the production of larger quantities of material, thereby offering a straightforward, low-energy and cost-affordable process for the preparation of high-entropy carbides, and related materials, with attractive properties.

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Poster I.41

Feasibility of Quantum Dot Based Lasers in Blue and Green Region

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Inorganic lead halide perovskite ($CsPbX_3$: X: Cl, Br, I) nanocrystals (NCs) are well-known for their high photoluminescence (PL) efficiency and stability as compared to organic lead halide perovskite. The high PL yield of these NCs makes them an ideal candidate for light emitting applications with broader tunability (400 to 700 nm). Replacing anions in $CsPbX_3$ from Cl to Br to I, or changing the size yields PL emission in blue, green and red region. In the present work, we demonstrate facile lasing tunability at low threshold in $CsPbBr_3$ and $CsPbCl_3$ quantum dots.

$CsPbBr_3$ quantum dots were synthesized by the reported hot injection wet chemical method. The size of quantum dots is 5.5 ± 0.98 nm as calculated from the transmission electron microscopy image analysis. The measured PL yield of these quantum dots is about 95 % having full width at half maximum 132 meV without any passivating layer of other semiconductor material (like core shell CdSe/CdS quantum dots). Temperature dependent PL study in the range 10-300 K gives the small value of exciton-longitudinal phonon coupling (49.4 meV) with high exciton binding energy (50 meV). The PL spectrum recorded at 10 K under xenon lamp excitation shows the excitonic luminescence feature at 2.42 eV (512 nm) and a hump type feature at 2.38 eV (521 nm). If the same sample is excited using a pico-second laser, it is observed that the low energy feature evolves into a sharp peak having very high intensity as compared to the excitonic peak intensity. The low energy peak is attributed to the stimulated emission peak as a result of biexcitonic recombination.

As we change the composition of halide, i.e. Br to Cl, the emission changes from green to blue. $CsPbCl_3$ quantum dots were synthesized using the same method. Size of quantum dots is about 5.3 ± 1.1 nm and shows emission at 3.04 eV (408 nm) with full width at half maximum of 97 meV. The PL yield of these quantum dots is very low~7 % at room temperature but at low temperature (10 K) PL intensity shows 90 times enhancement as compared to room temperature. At low temperature excitonic peak is observed at 3.022 eV and biexcitonic peak is at 2.97 eV (418 nm). The biexcitonic binding energy of about 50 meV is observed in these quantum dots.

By changing the halide composition in $CsPb(Br/Cl)_3$ quantum dots one can tune the emission and lasing action from blue to green region of visible region. The notable result is in $CsPbBr_3$ and $CsPbCl_3$ NCs reveal the stimulated emission. At low temperature, biexcitonic feature appears well resolved (which yield stimulated emission) while at room temperature, fitting of the data is required to distinctly observe the biexcitonic feature. The high PL emission yield, large excitonic ad biexcitonic binding energy and defect tolerant nature of these quantum dots makes them an ideal candidate for low threshold based quantum dot lasers.

Poster I.42

Microwave-Assisted Synthesis of Some Potential Bioactive Imidazolium-Based Room-Temperature Ionic Liquids

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Chemical industries are being directed toward finding alternatives to toxic or hazardous volatile organic compounds (VOCs). For these problems ionic liquids (ILs) appear to be suitable solutions due to several outstanding properties, such as zero-vapor pressure, good chemical and thermal stability, low flammability, excellent solubility for many organic and inorganic compounds and high ionic conductivity.

The general definition of ILs are organic salts with a melting-point below 100 °C which contain organic cation, and various organic and inorganic anions. The numerous combinations made between the cation and the anion permits the design of appropriate ILs for a particular application. ILs have been dramatically expanding in popularity as a new generation of chemicals with potential uses in various areas in industry. Additionally, several studies have shown the very interesting biological activity of ILs against both environmental and clinically important microorganisms.

Following on from our work on the synthesis of ILs, recent results concerning an efficient green method for the preparation of novel functionalized imidazolium ionic liquids using microwave containing combined antibacterial, antifungal and antitumor Pharmacophore sites will be presented.

Poster I.43

Design, Microwave Synthesis and Characterization of Some New Bioactive Functionalized Imidazolium-based Ionic Liquids

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Ionic liquids (ILs) have recently emerged as an alternative to volatile organic compounds (VOCs) as solvents in synthetic organic chemistry. They are synthesized from an anion and an organic cation, such as imidazolium, pyrolidinium or pyridinium and are good solvents that readily dissolve many organic, inorganic and organometallic compounds. They also have many advantageous physicochemical properties, such as zero vapor pressure, high thermal and chemical stability, a low melting point and high ionic conductivity.

Following on from our work on the synthesis of ILs, we report an efficient green method for the preparation of novel functionalized imidazolium-based ionic liquids using microwave irradiation containing combined antibacterial, antifungal and antitumor pharmacophore sites. The newly prepared ILs demonstrate promising antimicrobial and antitumor activity.

Poster I.44

Microwave-Assisted Synthesis of Novel Imidazolium, Pyridinium and Pyridazinium-based Ionic Liquids and/or Salts and Prediction of Physico-Chemical Properties for their Toxicity and Antibacterial Activity

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A few decades ago, room-temperature ionic liquids (RTILs) and salts usually composed of large organic cations and inorganic or organic anions appeared as an emerging class of ecofriendly compounds alternative to volatile organic compounds (VOCs) due to their outstanding physical and chemical properties such as negligible vapor pressure, excellent thermal and chemical stability, outstanding dissolving capacity, excellent ionic conductivity, non-flammability, and recyclability [1–3]. These characteristics make them very attractive for applications in a myriad of different fields and have, therefore, been investigated for a broad range of applications. However, possession of these properties does not necessarily make them a greener alternative.

Thus, the purpose of this work was the synthesis of new class of imidazolium, pyridinium and pyridazinium-based ionic liquids. Furthermore, the antimicrobial activity of the new synthesized ILs were investigated against six types of human pathogen was in order to assess to their potential toxicities. Results showed that some compounds demonstrated promising antimicrobial activity. Based on the theoretical study, it has been concluded that physicochemical analyses might prove to be a suitable method to correlate the structural features of newly synthesized ILs derivatives with their promising antimicrobial activity and may contribute to the development of novel antimicrobial agents against drug resistant [4].

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Poster I.45

Preparation of $CaCO_3$-HDPE Composite Sheets and their Physiochemical Characterization

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Traditionally, paper is derived from wood by pressing together moist fibers of cellulose pulp followed by drying into sheets. The quality of paper is determined from properties such as its thickness, texture, and strength. A stunning global demand of paper is marked by greater than 350 million tons of paper produced annually, leading to a rise in deforestation and consequently global warming. In addition, a large amount of water is used during traditional paper production process, which consequently produces significant amounts of wastewater and residual sludge waste, complicating wastewater treatment and sludge disposal. Therefore, alternatives to the wood-based paper sheet for a variety of paper-based applications are of significant interest. Also, replacing traditional paper with a wood-free material will substantially improve forestation, and hence reduced global warming. This research focuses on development of a polymer composite sheet using a low-cost naturally abundant filler; calcium carbonate ($CaCO_3$) and high-density polyethylene (HDPE) polymer as a replacement of the traditional wood fiber-based sheets. The composite sheets are expected to have a higher mechanochemical durability. Composite sheets are prepared by melt blending technique followed by compression with varying compositions. The effect of changing filler and polymer concentrations and use of additive will be discussed. Structural, thermal characterization and wettability of prepared composite sheets will be presented.
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Poster I.46

Thermally Reduced Graphene/Polyethylene Nanocomposites: Study of Melt Crystallization

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A unique combination of excellent electrical, thermal, and mechanical properties makes graphene a multi-functional reinforcement for polymer nanocomposites. However, incorporating graphene in polymers induces micro-structural changes leading subsequently to alterations in the functional properties of the resultant nanocomposites. One of the fundamental properties that effects the functional properties of nanocomposites is the crystallinity of nanocomposites. In this research, crystallization kinetics of graphene/polyethylene nanocomposites are investigated in the melt. X-ray diffraction, Raman spectroscopy and scanning electron spectroscopy were used to characterize the nanocomposites. The crystallization and melting behavior of nanocomposites was studied using differential scanning calorimeter, whereas degradation temperature was studied via thermogravimetric analyzer. These results are considered as the first step in understanding how the microstructure of polyethylene changes with the addition of graphene.

Poster I.47

Synthesis of Multivariate Metal-Organic Frameworks

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Metal-organic frameworks (MOFs) are robust extended structures built from an organic link and inorganic joint components. MOFs are used as rigid platforms for physical interactions such as gas storage and purification, as well as chemical reactions such as catalysis and post-synthetic modification of MOF links. Metal-organic frameworks are commonly synthesized by different routes including solvothermal, mechanochemical, sonochemical, microwave assisted or electrochemical methods. Most MOFs have been synthesized using a single type of link and inorganic joint unit. In order to enhance the performance and to develop novel applications using MOFs, we have outlined a strategy for synthesizing a new kind of MOF from multiple organic linkers known as multivariate metal-organic frameworks (MTV-MOFs). Such a construct is successfully achieved by using a reaction-diffusion framework (RDF) at room temperature. Our synthesis system is based on the separation of the reactants into two parts, inner and outer. Initially, 1,3,5-benzene tricarboxylic acid (BTC) is dissolved in the gel matrix and then the outer containing the copper salt is added on the top of the gel matrix and allowed to diffuse through the inner electrolyte forming thereby the MOF-199 crystals. Based on this initial success, other organic linkers incorporating different functional groups (e.g. Isophthalic acid, 5-hydroxyisophthalic acid, 5-aminoisophthalic acid, and 5-cyanoisophthalic acid) have been mixed in different ratios within the gel matrix leading to the formation of multivariate MOF-199 (MTV-MOF-199). The resulting MTV-MOFs are fully characterized using PXRD, BET, TGA, SEM, and NMR. Furthermore, the new MTV-MOFs are used to remove the organic methylene blue dye from water and demonstrated higher removal compared to the original MOF-199. More importantly, a magic ratio of BTC: OH-BDC (1:1) in MTV-MOF-199 crystals is found to be crucial to efficiently remove MB from the water.

Poster I.48

Fabrication of Multiferroics and High Refractive Index Glasses by Containerless Process

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Recently, bulk glass, glass-ceramics and multiferroic materials have attracted attention due as low cost optical, multiferroics, magnetic and electronic materials. Among these, nickel ferrite is one of the most versatile and technologically important ferrite materials which has great potential applications due to typical ferromagnetic properties, low conductivity, high electrochemical stability and catalytic behavior. On the other hand, alumina based ceramics have significant applications due to their refractory nature, hardness, strength, transparency in the infrared region, and chemical resistance. In the present study, containerless solidification of alumina-based glass-ceramics and $NiFe_2O_4$ melt, where the undercooling level can be treated as one of the experimental parameters, was carried out to study the glass, glass-ceramics and multiferroic phases using an aerodynamic levitator (ADL). The containerless levitation under deep undercooling conditions can achieve novel microstructures such as refined grain size, stable/metastable phases and glassy phases.

A spherical sample was levitated by an ADL and completely melted by a CO_2 laser. Then, the droplet was cooled by turning off the CO_2 laser. The surface temperature and solidification behavior of the levitated droplet was monitored by pyrometer and a high-speed video. Among the rare earth aluminum perovskites, La, Nd and Sm aluminum perovskites solidified as glass and Eu-Lu aluminum perovskites solidified as crystalline phases. The $NdAlO_3$ glass phase showed a high refractive index of ~1.89, suggesting that containerless levitation is an elegant technique for fabrication of new glass and crystalline ceramics from an undercooled melt. The x-ray diffraction (XRD) and the cross sectioned scanning electron microscopy (SEM) images confirm the existence of glass, glass-ceramics and multiferroic $NiFe_2O_4$ phases. In order to confirm the thermal stability, samples were annealed at various temperatures using thermogravimetric and deferential thermal analysis (TG/DTA). These results confirm formed phases are stable after annealing at 1473 K. The magnetic properties of the as-solidified samples were studied using vibrating sample magnetometer (VSM). These results indicate that stable multiferroic $NiFe_2O_4$ phases solidify directly from the undercooled melt.

Poster I.49

Giant Room Temperature Ferroelectricity in Ferromagnetic $SmMnO_3$

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Type-II multiferroic materials can lead to new magneto-electric device applications due to the exquisitely coupled magnetic and ferroelectric orders. However, for device applications such as new non-volatile memory and sensors, there are no simple systems which have spontaneous room-temperature ferroic properties. By breaking the inversion symmetry of these materials the ferroic properties can be tuned and room temperature multiferroicity can be achieved. Here, we demonstrate giant room temperature ferroelectricity in vertically aligned nanocomposite (VAN) films of $(SmMnO_3)_{0.5}(Bi,Sm)_2O_3)_{0.5}$ grown by pulsed laser deposition on single crystal (001) $SrTiO_3$, whereas bulk SMO is paraelectric and A-type antiferromegnet (AFM) with $T_{N,FM}$ of ~ 60 K. The VAN structure makes the SMO component of the films a type II ferroelectric, with $T_{C,FE}$ = >300K. At the same time, it is a ferromagnet with $T_{C,FM}$ = 90K. The measured room temperature electric polarization P (≈3.9 $\mu C/cm^2$) is the highest among all reported spin-driven ferroelectric *o*-*R*MnO_3 films (*o*: orthorhombic, *R*: rare earth materials). Also, the ferromagnetic moment (M_S) *i.e.* ~1.02 μ_B/Mn @ 10 K of the ferroelectric SMO VAN is comparable to the ferromagnetism (~1.0 μ_B/Mn @ 10K) measured in *o*-$LuMnO_3$ thin films which is not ferroelectric at room temperature.

The ferroelectricity arises from a large *in-plane* compression of -3.6% (vector sum of in-plane orthogonal compressive strain) as well as an *out-of-plane* tension of +4.9% induced in the composite. This compares to much lower in-plane values, i.e. -1.1% for plain SMO film. The large *in-plane* strain produces an E-type AFM from a bulk A-type AFM phase, which then induces ferroelectricity in the SMO. DFT calculations show that the Mn-O bond length and out-of-plane Mn-O-Mn bond angle decreases and increases, respectively. This enhances the ferromagnetic in-plane nearest (J_1) and antiferromagnetic in-plane next-nearest neighbour (J_2) interactions of Mn moments which produces the E-type AFM coupling. The 3D strain engineering VAN approach gives a completely new way to design multiferroics, and gives promise for obtaining near room temperature multiferroicity in *R*MnO_3 films.

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Poster I.50

Photocatalytic Degradation of Nizatidine in Aqueous Solution by $BiVO_4$ Catalyst Under Ultraviolet Radiation

Naji Ahmed Aldubaili, **Mohammed Misbah Uddin, Ahmed Alzamly, Soleiman Hisaindee, Muhammad A. Rauf, Ahmad Alzamly, Rengaraj Selvaraj, and Mohammed Meetani**

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Nizatidine is a histamine H_2 receptor antagonist that inhibits stomach acid production, and is commonly used in the treatment of peptic ulcer and gastroesophageal reflux diseases. The presence of this compound and other drugs in surface water and wastewater is a serious issue and has been acquiring increasing interest because of unidentified environmental effects and probable damage to aquatic life. Nizitidine could escape intact from conventional treatment plants, and consequently be released into the environment. In this study, $BiVO_4$ photocatalysts were prepared and characterized, then photocatalytic activity for degradation of Nizatidine drug in aqueous solution using UV irradiation was evaluated. Approximately 75% degradation of the dye solution was achieved in 180 min. The kinetic studies showed that photodegradation of Nizatidine follows first order reaction kinetic model. Effective parameters such as pH, photocatalyst dose and contact time were investigated and optimized. Furthermore, Nizatidine degradation products were analyzed using LC-MS/MS. Finally, a reaction pathway is proposed based on the intermediates detected.

Poster Session II

Al Hamra Convention Center

Monday, February 25, 2019 18:30-20:30

II.1 Anionic MOF as a Template for Solvent-free Synthesis of Perovskite Quantum Dots

Sohini Bhattacharyya and Tapas K. Maji
Chemistry and Physics of Materials Unit
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II.2 Synthesis and Characterization of Inorganic Bi-Layer Bi_2S_3-Cu_xS by Sequential Chemical Bath Deposition

Shital M. Sonar, P. K. Baviskar, Habib M. Pathan, and Prakash B. Ahirrao
School of Physical Science
Kavayitri Bahinabai Chaudhari North Maharashtra University, Jalgaon, India

II.3 Reducing the Harmful Impact of the Prepreg Scrap from Domestic Aerospace Industries Using Compression Molding to Preserve UAE Environment

Mariam Alhammadi, Haliemah Alabdouli, Aya Mansour, Hend Alqaydi, Alya Almuhairi, Waleed Khalil, and Ali Alnaqbi
Department of Mechanical Engineering
United Arab Emirates University, Al Ain, United Arab Emirates

II.4 Effects of Voids Growth on the Damage of Polypropylene

Belabbas Bachir Bouiadjra, Abdulmohsen Albedah, Faycal Benyahia, and Sohail M. A Khan Mohammed
Department of Mechanical Engineering
Djillali Liabes University, Sidi Bel Abbes, Algeria

II.5 Comparative Study of Thermomechanical Behavior of Plates in Insulating Materials

Fatima Zohra Kettaf and Amine Bouziane Hammou
Department of Mechanical
University of Sciences and Technology of Oran, Oran, Algeria

II.6 Effects of Mineral Additions on the Mechanical Strength of Cement Mortar

Miloud Driss, Mohamed Amine Hamadouche, Noureddine Della, and Nadia Driss
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Mascara University, Mascara, Algeria

II.7 Determination of Dapsone Drug in Treated Wastewater with β-cyclodextrine Sensitized Flourescence Spectrometry

Ahmad M. Alhalabi, Noor I. Badawi, Nada Elmari, Ameena Ahmed, Hind Hasan, Naji A. Aldubaili, Munjed Maraqa, and Mohammed Meetani
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II.8 Effect of Catalysis-Clustering on Gas-sensing Performance

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Poster II.1

Anionic MOF as a Template for Solvent-free Synthesis of Perovskite Quantum Dots

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Nanocrystal quantum dots (QDs) are one of the emerging materials for optoelectronic applications and devices, although they often suffer from poor stability and activity owing to aggregation. Thus, confining them in nanospaces to isolate them will enhance their stability and activity, thereby increasing their processability in advanced optoelectronic devices. Metal-organic frameworks (MOFs) are ideal candidates for this purpose owing to their high surface area, porosity, flexibility and tunability. AMOF-1 $\{[Zn_3(L)_2][(NH_2Me_2)_2].9H_2O$;
(L = 5,5-(1,4-phenylenebis(methylene))bis(oxy)diisophthalic acid)$\}$ is a 3D flexible anionic MOF where the charge neutrality is maintained by guest dimethylamine (DMA) anion. By the virtue of this, AMOF-1 is capable of efficiently capturing heavy metal cations like Cd(II), Hg(II) and Pb(II) from aqueous medium. We seek to convert the Pb(II) encapsulated MOF into a value-added QD@MOF composite for optoelectronic devices. With this in mind, in a novel post-synthetic approach, we have incorporated $CsPbX_3$ (X= Cl, Br, I) QDs into the pores of AMOF-1. $CsPbX_3$@1 composites not only exhibit enhanced fluorescence lifetime and quantum yields than their bulk counterparts, they also show unprecedented stability in a wide range of solvents. The incorporation of these quantum dots also causes a 104 fold increase in the inherent electrical conductivity of the MOF. Thus this unique one-step synthetic technique can facilitate the formation of a new nanocomposite involving QDs and MOF for advanced optoelectronic applications.

Poster II.2

Synthesis and Characterization of Inorganic Bi-Layer Bi_2S_3-Cu_xS by Sequential Chemical Bath Deposition

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Heterojunctions have interesting optical properties, which make them attractive for solar cell and other optoelectronic device applications. A semiconductor heterojunction is a junction between two chemically different semiconductors having different band gaps. Good performance of a heterojunction in any device depends on the selection of semiconductors with useful energy gaps.

In the present investigation, a simple and inexpensive chemical deposition route was used to deposit bismuth trisulphide (Bi_2S_3) and copper sulphide (Cu_xS) thin films on fluorine doped tin oxide (FTO) coated glass substrates. Deposition of n-Bi_2S_3 was carried out by sequential chemical bath deposition (S-CBD) using bismuth nitrate and sodium sulphide as cationic and anionic precursors, respectively. UV-visible spectroscopy shows the band gap is 1.38 eV for n-Bi_2S_3 and after post annealing treatment of Bi_2S_3 thin film, X-ray diffraction confirms orthorhombic crystal structure of n-Bi_2S_3. Copper sulphide (Cu_xS) shows poor adhesion on glass substrate as well as FTO. Therefore, a buffer layer of Bi_2S_3 was grown on FTO by S-CBD and then p-Cu_xS deposited on n-Bi_2S_3 by S-CBD to enhance the adhesion of copper sulphide film to the substrate. Copper sulphate and sodium sulphide were used as cationic and anionic precursors, respectively, in the deposition of p-Cu_xS. Optimization of preparation parameters led to the formation of a good heterojunction between the n-Bi_2S_3 and p-CuxS films. The structural, surface morphological, optical, and electrical properties of n-Bi_2S_3, p-CuxS and its heterojunction were investigated via different characterization techniques.

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Poster II.3

Reducing the Harmful Impact of the Prepreg Scrap from Domestic Aerospace Industries Using Compression Molding to Preserve UAE Environment

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The need for high performance and capability to design material characteristics to meet specific requirements has made composite materials the first choice for many aerospace applications. Due to their various design engineering advantages, the need for composite materials has sprung up in the past few years. Carbon fiber reinforced polymers (CFRP), in specific, have superior strength to weight ratios, offering enormous potentials in the industry. On the other hand, massive quantities of pre-preg CFRP waste from production might become a real concern in the future for the following reasons:

- Environmental impact: the increasing amount of CFRP produced raises concerns on waste disposal and consumption of non-renewable resources.
- Legislation: recent European legislation is enforcing strict control of composite disposal; it is required that automotive vehicles that had been disposed after 2015 are 85% recyclable.

A solution has been developed by turning CFRP waste using compression molding into a valuable resource and closing the loop in the CFRP life-cycle. This project aims to investigate the properties of prepreg CFRP waste and identifying how this waste can be one of the good choices toward more sustainable aerospace subsidiaries industrial products.

The process starts by using a shredding machine to shred prepreg CFRP remnants, while measuring the level of pollution using an air quality meter device, a dangerous level of pollution was determined. Assembling the mold, cleaning, waxing and compacting the shreds were the essential steps for the compression process. Maintained pressure and heat were applied to the compacted mold design for a specific period of time. Cooling, removing the sample and re-cleaning to repeat the process for 10 different samples. Testing goals were to define different mechanical properties such as the modulus of elasticity and compression strength.

Overall, comparing our results with properties of steel, it was found that they were close, which means that the material is strong and ductile enough to be used in different useful applications such as non-structural elements under compression and in civil applications too.

Poster II.4

Effects of Voids Growth on the Damage of Polypropylene

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The damage of semi crystalline polymers is very complex because of their heterogeneity. In general under mechanical loading, the damage of these polymers occurs by micro voids coalescence. In this study, the effect of the voids growth on the damage of polypropylene (PP) was analyzed using experimental and numerical approaches. The Gurson-Tvergaard-Needleman (GTN) model was implemented in FE model to predict the damage of the polymer. The predicted results were compared to the experimental ones. There is good agreement between the numerical and the experimental results. The relative difference does not exceed 11%. The GTN model predicts that the voids growth follows an exponential function as the strain of the polymer increases.

Poster II.5

Comparative Study of Thermomechanical Behavior of Plates in Insulating Materials

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This paper presents a comparative investigation on the thermomechanical behavior of several insulating materials having different elastic, plastic or inelastic properties. The bending analysis of the square plates under a sinusoidal distribution of thermomechanical loads is carried out using a refined four-variable plate theory. Flexural analysis of square plates under mechanical, thermal and thermomechanical loads are also presented. Five materials are studied: ceramics, wood, glass wool, cork and polystyrene. The influence of the thickness and the thermal load on the thermomechanical bending behavior of the plates is studied. The main conclusions found are :

a) When the Young's modulus increases the deflexion decreases.
b) For purely thermal loading, the influence of plate thickness on the deflexion is negligible.
c) A thermomechanical loading gives an important deflexion than purely thermal or purely mechanical loading.
d) The normal stress is continuous in the direction of the thickness. It is in tension below the median plane and in compression above the median plane.
e) The normal stress is maximum on the faces, and null on the average plane.
f) The variation of the tangential stress is parabolic across the thickness, it takes a maximum value at the median plane of the plate, while on the surfaces, it is zero.
g) The effect of the thermal load is important on the normal and tangential stresses.

Poster II.6

Effects of Mineral Additions on the Mechanical Strength of Cement Mortar

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In the cement industry, the search for a cheaper binder using industrial wastes and natural resources has become a major concern to overcome the deficit in Portland cement manufacturing. However, despite the technical, economic and ecological advantages reported by the use of composite cements, the latter remain associated with disadvantages. It is, therefore, necessary to know whether multi-component (ternary) cements have synergistic effects so that their ingredients can compensate for their mutual weaknesses. The purpose of our work is to study the effects of the incorporation of mineral additions such as natural pozzolana (active addition), limestone fillers (inert addition) and silica fume (very active addition) on the mechanical properties of mortars made according to different combinations based on these additions. This will determine optimal dosages for binary cements and optimum couples for the best performers ternary cements. The results from this research work confirm that 10% limestone fillers (LF) improves the resistance of binary mortars at young age (2 days), while 30% of natural pozzolan (NPZ) and 10 % silica fume (SF) contribute positively in the long term (90 days). For ternary mortars, the couples (10-30% NPZ/10% CF) and (10-30% NPZ/10% SF) seem the most effective because they develop resistances comparable to that of the long-term control mortar (90 days).

Poster II.7

Determination of Dapsone Drug in Treated Wastewater with β-cyclodextrine Sensitized Flourescence Spectrometry

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Dapsone is an antibiotic which is used to treat skin disorders. The presence of this compound and other drugs in surface water and wastewater is a serious issue and has attracted increasing interest because of their unidentified environmental effects and probable damage to aquatic life. Dapsone could escape intact from conventional wastewater treatment plants, and consequently is released into the environment. In this project, we utilize a host-guest supramolecular approach where we confine dapsone (as a guest) inside the cavity of a macromolecule, cyclodextrin (as a host) and determine its amount using high performance liquid chromatography with fluorescence detection (HPLC-FLD). Earlier experiments revealed that the addition of β-cyclodextrine (β-CD) to aqueous solution of dapsone enhanced its fluorescence signal. The average enhancement caused after the addition of the host (β-CD) to the guest solutions in basic media was up to 23 times . Therefore, an HPLC-FLD method has been developed to detect dapsone in raw and treated domestic wastewater samples. Preliminary results showed that there was a very significant increase in fluorescence emission intensity after the addition of β-CD to dapsone solutions, even at very low concentrations. The formation of host-guest interactions was explored using 1H NMR and it was confirmed by the shifted signals.

Calibration curves were constructed for dapsone without β-CD and after addition of β-CD to the mobile phase. It was found that the calibration curve slope, which is a measure of the method sensitivity, was substantially improved, but varied based on the concentration of β-CD and the pH of the mobile phase solution.

Poster II.8

Effect of Catalysis-Clustering on Gas-sensing Performance

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We present a theoretical investigation, based on a combined of density-functional theory (DFT) and non-equilibrium Green's-functional (NEGF) formalism, to study the effect of catalysis-clustering on the sensor response. Specifically, the scope is to compare the adsorption and transport properties after chemisorption of CO_2 molecules on iron (Fe) ad-atoms deposited on graphene nano-ribbons (GNR) in two different ways: (i) Five Fe ad-atoms deposited on GNR in scattered fashion; and (ii) A cluster of five Fe atoms deposited on GNR. Results of atomic relaxations yield binding energies of $E_{bind}(Fe\text{-}GNR)$ and $E_{bind}(CO_2\text{-}Fe)$ to be stronger in the case of scattered Fe ad-atoms than in the case of Fe cluster. Consistent with this trend, density of states at Fermi level as well as Bader charge analysis corroborate larger effects in the case of scattered Fe ad-atoms. Furthermore, the results of IV-curves calculations confirm stronger deviations in the case of scattered Fe ad-atoms and, consequently, stronger sensor response. This work suggests stronger sensitivity and selectivity to be reached by scattering ad-atoms of the transition-metal catalysis and with an optimization of their density. As the sensor response is based on the deviation of conductance from before to after the exposure to the gas, our results have indeed a direct application to fabricate solid-state based gas sensors working with high sensitivity at room temperature, to detect toxic and hazardous gases such as CO_2.

Poster II.9

Nonlinear Postbuckling Analysis of Carbon Nanotubes with a Nonlocal Zero-Order Shear Deformation Theory

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A simple nonlocal zeroth-order shear deformation theory is proposed for the nonlinear postbuckling behavior of nanoscale beams of carbon. The novelty in this formulation is that, in addition to including the nonlocal effect according to the nonlocal elasticity theory of Eringen, the shear deformation effect is considered in the axial displacement within the use of shear forces instead of rotational displacement like in existing shear deformation theories. Governing equations are obtained from the principle of virtual works together of the nonlocal differential constitutive relations of Eringen. Closed-form solutions for the critical buckling load and the amplitude of the static nonlinear response in the postbuckling state for simply supported and clamped nanoscale beams are examined and discussed. Comparison studies are carried out to check the validity of obtained results.

Poster II.10

Anticancer Activity of Zinc Peroxide Nanocomplex using Magnetic Hyperthermia

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Recently, nanoparticles (NPs) have received much attention due to their use in cancer therapy. This work demonstrates the utilization of zinc peroxide (ZnO_2), a magneto sensitive NP complex and its heating efficiency under alternating magnetic field. The ZnO_2 nanocomplexes (NCs) were synthesized using a chemical method in an inert atmosphere at room temperature using ferric salt solutions and zinc peroxide nanoparticles. X-ray diffraction was used to study crystalline structure and both scanning and transmission electron microscopy were used to study morphology. The prepared ZnO2 NCs were of spherical morphology and approximately 20 nm in size. The cytotoxicity evaluation of the ZnO_2 NCs performed *in-vitro* on fibrobalast cancer cells using 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay shows low toxicity. The specific absorption rate (SAR) value of 910 W/g (at $H=10\ KAm^{-1}$) was estimated from the rate of temperature rise curve upon exposure to magnetic field of frequency 470 kHz. This heat-generating capability is tested by interacting the ZnO_2 NCs with the extracellular matrix of fibroblast tumor cells, which shows potential damage to the matrix under magnetic stimuli. This interaction is attributed to the unique ability of the ZnO_2 NCs reactive oxygen species generation, leading to oxidative stress and eventually cell death when the anti-oxidative capacity of the cancer cell exceeds and considered as the lead mechanisms for observing its cytotoxicity towards cancer cells. The newly prepared ZnO_2 NCs with heat generation upon exposure to magnetic field and with cytotoxicity against cancerous cells demonstrates its use in magnetic hyperthermia applications.

Poster II.11

Enhanced Electrochemical Performance of Lithium Sulphur Battery using h-BN/RGO Nanocomposite Based Cathode

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Composite 2D materials and graphene oxide (GO) in energy storage devices form a major new branch of material science research. The 2D materials are in nanometer scale, which have properties that are significantly different from the same materials in bulk form. These properties are important in this dimension and exhibit changes in storage electric charges. For example, GO is able to store charges more than graphite which is in the bulk size.

In this work, a simple, cost effective, methodology is reported to design h-BN/RGO nanocomposites used as cathodic materials for the lithium sulphur battery (LiS). TEM images showed the hBN nanosheets are uniform and densely covered on the surface of GO. The results showed that the hBN/RGO nanocomposites electrode prepared by this technique could be used for large scale production using existing economical, and highly effective LiS battery fabrication technique. The interpretation of these results in view of the proposed structures and the electrochemical performance of the nanocomposites will be presented.

Poster II.12

Experimental Characterization of Polymer Filter Bags for Phosphate Dust Collector

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Polymer fiber bags used for baghouse phosphate dust collectors were characterized using X-ray diffraction (XRD), X-ray fluorescence (XRF) and Raman spectroscopy. The aim of this work is a comparative study in the chemical composition of filter material adopted for the phosphate collection system installed in the drying unit of Beni-Idir, Khouribga, Morocco. Four filter samples were examined. The first sample, filter F1, is made with polyacrylonitrile (PAN) and coated with polytetrafluoroethylene (PTFE). The second sample, filter F2, is the same as the first but in degraded state, and is used for twelve months of filtration and cleaning stages. The third sample, filter F3, is an intensive filter jet with coanda injector and combi-jet (IFJCC). The fourth sample, F4, is a treated polymer filter. A comparison of the three filter types will be presented. The results reveal that both the PAN filter and the phosphate dust deposit has an orthorhombic crystalline structure, while the IFJCC and polymer treated filters have a monoclinic crystalline structure. XRD suggests that the PAN filter, IFJCC filter, and polymer treated filter have crystallites size of 91, 72, and 66 nm respectively. XRF and Raman spectroscopy demonstrate that the F3 and F4 have similar chemical compositions.

Poster II.13

Synthesis of Carbon-Metal Double Layered Oxides for the Removal of Congo Red from Aqueous Solution

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A low-cost, novel carbon-metal double layered oxide (C/MnCuAl-LDOs) nanoadsorbent was synthesized by co-precipitation, for the adsorption of Congo red (CR), using modified carbon derived from pyrolysis of polystyrene (PS) plastic waste. The synthesized C/MnCuAl-LDOs has a crystalline structure with a high surface area of 60.43 m^2/g and pore size of 99.85 Å. Adsorption of CR using prepared adsorbents from aqueous solution under equilibrium and kinetic conditions were evaluated against different pH values (4–10), CR concentrations (25–250 mg/g), contact time (0–310 min) and temperature (30–50 °C). The obtained results revealed that C/MnCuAl-LDOs showed maximum adsorption capacity for CR among all the used adsorbents. The optimum equilibrium time was 180 min, whereas acidic medium (pH 4.5) favored the maximum adsorption of CR up to 317.2 mg/g on C/MnCuAl-LDOs. The adsorption kinetics followed the pseudo-second-order model, whereas Freundlich adsorption isotherm fitted best to obtained data in comparison to Langmuir adsorption isotherm. The results suggested that C/MnCuAl-LDOs is an efficient material for the removal of organic pollutants from the wastewater.

Poster II.14

Defect Mediated Broadband Emission in $ZnAl_2O_4$ Investigated through Photoluminescence Spectroscopy and Rietveld Refinement

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$ZnAl_2O_4$ has been an attractive material due to its robust luminescence properties and promise for applications such as in solid state lighting, optoelectronic devices, catalysis, ceramics, etc. Significant efforts have been made by researchers to explore the luminescence in doped $ZnAl_2O_4$ system. However, luminescence in its undoped state can be tuned by varying the synthesis method, temperature conditions, creation of defects and cationic vacancies. The formation of defects enhances its properties to a significant level. We have observed a brilliant white and intense near infrared (NIR) emission, simultaneously, in undoped $ZnAl_2O_4$/ZnO nanocomposite system prepared through combustion route using urea as a fuel. White luminescence has been observed in the sample processed at a much lower temperature than reported by other researchers i.e. at 550 ºC. The emission has been ascribed to various types of shallow and deep donor/acceptor defects such as oxygen vacancies, zinc interstitials, cation antisite defects, cationic vacancies, etc., existing in the crystal lattice. White emission switches to blue on annealing owing to rearrangement of various defects accompanied by conversion of $ZnAl_2O_4$/ZnO to $ZnAl_2O_4/\alpha\text{-}Al_2O_3$ which predicts its applicability as a sensor. NIR emission enhances to almost double in intensity on annealing. Suitable values of illuminating engineering society colorimetric parameters such as fidelity index, luminous efficiency of radiation, color gamut, etc. infers the good quality emission. Broad photoluminescence spectra of both the samples have been deconvoluted in order to obtain the information about each individual component contributing towards emission. Various transitions generating emission in the visible and NIR region are ascribed to different defect levels present in forbidden band gap region and are depicted through band model diagrams. Rietveld refinement of the X-ray diffraction (XRD) patterns of both as-prepared and annealed samples has been carried out to evaluate crystalline structure. Presence of a secondary phase, percentage of each phase, vacancies of zinc and oxygen has been determined from the Rietveld refinement. Transmission electron microscopic analysis has revealed the change in morphology from spherical to polyhedron and increase in crystallite size on annealing. Electron diffraction studies also complemented the results of XRD. High quality emission in visible and NIR region predicts their potential applications such as solid state lighting and *in-vivo* bioimaging, respectively.

Poster II.15

Enantioseparation of Ibuprofen Drug in Treated Wastewater using HPLC with β-cyclodextrine Sensitized Fluorescence Detection

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Ibuprofen is a synthetic compound used widely as an anti-inflammatory drug. Nowadays, the presence of Ibuprofen in wastewater is becoming a serious issue and is considered as a threat to the environment. Ibuprofen can easily reach plants as a result of not being treated and removed efficiently in the conventional wastewater treatment facility. In this work, we utilize a host-guest supramolecular approach to confine Ibuprofen (as a guest) inside the cavity of a macromolecule, β-cyclodextrin (β-CD) (as a host). We aim to separate Ibuprofen enantiomers and determine their levels using high performance liquid chromatography with fluorescence detection (HPLC- FLD). Earlier spectrofluoroscopic experiments show that the addition of β-CD to aqueous solution of Ibuprofen enhanced its fluorescence signal. Moreover, β-CD is chiral selector since it is made of sugar molecules bound together in a ring (cyclic oligosaccharides) that has chiral carbons within. Therefore, separation of Ibuprofen enantiomers is possible, after the addition of β-CD to mobile phase solution composed of 5.0 mM β-CD in 25 mM phosphate buffer, pH 6: ethanol (85:15). Method development and validation will be reported and discussed. Moreover, the new method will be used to detect and quantitate the Ibuprofen enantiomers in ground and treated domestic wastewater samples.

Poster II.16

Low-temperature Synthesis of Hard Metal Nanoparticles from Liquid Ammonia

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Nanoparticles are an interesting field of research, because they show size dependent properties. The optical properties of nanoscale materials can show quantum effects like plasmon resonance. Another effect is, as described by Dresselhaus, the effect of reduced thermal conductivity in nanocomposite materials.[1] Additionally, the physical properties can undergo massive changes, like the melting-point depression or the increased hardness of materials.[2]

For nanoparticle synthesis, a well-defined system to generate monodisperse particles is needed. A controlled reaction environment is very important to synthesize transition metal nitride nanoparticles. Reactions in liquid ammonia are used to avoid oxygen and carbon during the reaction. Another advantage is the low temperature utilized for the condensation of ammonia (b.p. -33 °C), which inhibits the particle growth. Earlier, reactions in liquid ammonia have been used for synthesis of (reactive) base metal nanoparticles by Feldmann *et al.*[3] We used the low reduction potential of sodium in liquid ammonia and generated solvated electrons to synthesize transition metal nitride nanoparticles from different metal salt precursors.[4, 5] Here, we present an interesting synthesis route for surfactant-free group IV nitrides, which are already known in bulk as hard materials, like TiN or ZrN. Future work will focus on densifying the nanomaterial via spark plasma sintering to generate materials with nanoscale grain boundaries, to further investigate phenomena like the Hall-Petch or thermoelectric properties.

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Poster II.17

Highly Efficient Hydrothermal Green Synthesis of Reduced Graphene Oxide for Wastewater Purification Applications

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Exponential rise of the global population coupled with industrialization causes severe environment pollution, especially of water resources. Due to the limited useful water sources present on earth, it is necessary to protect them from various types of pollutants. Developing carbon-based adsorbent materials for wastewater purification have received much attention in recent times, owing to their low cost, high surface area, natural abundance and eco-friendly nature. Here, we have prepared highly efficient hydrothermal green synthesis of reduced graphene oxide (rGO) with tulasi (Holy Basil) green tea extract. As prepared rGO shows efficient adsorption of toxic organic dyes from aqueous solutions. The adsorption kinetics was evaluated using pseudo-first and pseudo-second order kinetic models. The maximum adsorption capacity values are analyzed using linear Langmuir and Freundlich adsorption isotherm models. The maximum adsorption capacity of rGO reaches 416.7 mg/g for methylene blue dye at equilibrium under aqueous solutions based on the Langmuir adsorption isotherm model. The highly efficient adsorption capacity of rGO could be attributed to the formation of high surface area with mesoporous surface at the adsorbed sites of the adsorbent which efficiently increases the adsorption rate. It is believed that the developed green synthesis will offer a facile route for gram scale production of highly efficient rGO for treating various types of toxic dyes in industrial wastewater.

Poster II.18

Studies on Low-Dimensional Misfit Layered Calcium Cobalt Oxide

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Misfit layered compounds (MLCs) possess unique structure and properties. MLCs can be considered as stacking of two components alternatively in layer by layer fashion.[1-3] MLCs are thermodynamically stable compared to their individual components. Lattice parameters of one of the components of MLCs doesn't match the other and that leads to mutual structural modulation. $Ca_3Co_4O_9$ (Ca_2CoO_3-CoO_2) is a misfit compound, which is shown to be a good thermoelectric and cathode material for solid oxide fuel cells. We have investigated these materials and formed one-dimensional nanotubes and two-dimensional nanosheets.[4, 5] In this presentation, I will focus on synthesis routes to make them into one- and two-dimensional nanotubes and nanosheets, respectively. The growth mechanism of formation and structural characterization will be presented. How the structure influences the electrical properties on individual nanotubes will also be presented.

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Poster II.19

Diameter Dependent Transport Properties of Core/Shell Nanowires for Nano-Electronic Device Applications

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One dimensional core/shell nanowires (NWs) have attracted attention due to the possibility of easily tuning their energy gap, a useful property for applications in next-generation electronic devices. In this work we are focused on Si or Ge based metallic core/shell nanowires, their morphology and transport properties, which would make them applicable in different sorts of electronic industries. Our work starts from the analogy with already synthesized Si and Ge-NWs, where the NW core is replaced by arsenic (As) and antimony (Sb). These NWs are optimized with two different diameters of 1.1 Å and 2 Å. We have observed the transition from semiconducting to metallic behavior for As/Si and As/Ge with the increase in diameter. The quantum conductance study from electronic band structure properties shows the increase in conductivity with the diameter of the nanowire. Further, we have investigated current-voltage (IV) characteristics for the NWs. The NWs with 1.1 Å diameter show nonlinear IV with negative differential conductance (NDC) effect that could be useful for a potential application in atomic scale device for fast switching. However, with increasing diameters, we have observed Ohmic nature in the NWs. It has been found that current values in accordance with applied voltage show a strong dependence on the diameter of the NWs. The tunable transport properties of core/shell nanowires with Ohmic character show a comprehensive picture as possible electron connector on the nanoelectronic device and technological applications.

Poster II.20

Functionalized Graphene Oxide-Epoxy Nanocomposite: A Hybrid Nanocoating for Corrosion Prevention of Mild Steel in Saline Medium

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The aim of the present research is to study the effect of graphene oxide (GO) and functionalized graphene oxide (FGO) as a nanofiller on the corrosion protection ability of epoxy coatings on mild steel in saline media. GO was modified with 2-amino-4-methylthiazole and characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), thermogravimetric analysis (TGA), and surface of the coated sample was analyzed using contact angle technique. 0.2 wt.% of GO and FGO were incorporated into epoxy resin by mechanical agitation and sonication. GO and FGO epoxy nanocomposites were coated on mild steel substrate by spin coating method. The formation of a protective film on the mild steel was confirmed using SEM. The anti-corrosive properties of nanocomposite coatings were investigated by electrochemical impedence spectroscopy and potentiodynamic polarization methods in 3.5% NaCl medium. The results indicated that FGO based polymer coatings exhibited superior barrier and corrosion protection properties due to their two dimensional sheet structures, uniform dispersion and exfoliation in epoxy matrix, hydrophobic nature and stopping up tiny pores properties.

Poster II.21

Synthesis and Characterization of GO-QDs@Ag-MOF Nanocomposite for Synergistic Antibacterial Activity

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Resistant microscopic organisms are an undeniably genuine risk for the wellbeing of the world. Multifunctional hybrid nanocomposites of graphene oxide quantum dots (GO-QDs) with silver metal-organic framework (Ag-MOF) were synthesized to study its antibacterial efficacy. These nanocomposites were characterized by field emission scanning electron microscopy (FESEM) and powder X-ray diffraction (PXRD). Antibacterial activity of GO-QDs@Ag-MOF have been evaluated against representative bacterial strains including gram-positive (*B. subtilis*) and gram-negative (*E. coli*), using CLSI recommended qualitative disk diffusion approach. The synergistic nanocomposite of GO-QD and tunable Ag-MOF fostered an enhanced antibacterial activity compared to either of its individual components. We determined that charge transport between components, GO-QDs and Ag-MOF, is key to the electrostatic interactions of the composites with the bacterial cell membranes. The functionalized nanocomposite allows the release of silver in the extracellular environment. The released silver ions further interact with high affinity to thiol-ligands of the biological entities. The reaction result in the formation of metallic silver (AgO) and silver sulfides (Ag_2S), suggested as critically important for the composites to inhibit bacterial growth. An enhanced bactericidal activity of nanocomposite could also be linked to morphological features like increased surface area and specific surface chemistry. This study introduces that GO-QDs@Ag-MOF nanohybrids have significant bactericidal effect.

Poster II.22

Anion Substituted Solution-Processed Cu_2ZnSnS_4 Nanocrystals and Thin Film for Photovoltaic Applications

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Nanocrystals of multi-element chalcogenides, such as Cu_2ZnSnS_4 (CZTS) and $Cu_2ZnSnSe_4$ (CZTSe), are considered as potential building blocks for low-cost thin-film photovoltaics. In the present investigation, we have synthesized CZTS and CZTSe nanocrystals by hot injection method. Physicochemical properties of synthesized nanocrystals studied by using various characterization technique. X-ray diffraction (XRD) and Raman spectroscopy reveal that the nanocrystals showing pure phase kesterite CZTS and CZTSe. The optical properties demonstrated that the prepared nanocrystals have good absorption in 300-1100 nm range with band gap energy of 1.56 and 1.03 eV for CZTS and CZTSe, respectively. Transmission electron microscopy (TEM) results revealed that the monodisperse spherical nanocrystals observed with average particle size 23 and 28 nm for CZTS and CZTSe nanocrystals, respectively. Exact positions of energy levels of CZTS and CZTSe were calculated using ultraviolet photoelectron spectroscopy (UPS), which help to understand the electronic band structure and charge transfer mechanism. Furthermore, we have prepared thin films of CZTS and CZTSe nanocrystals on molybdenum (Mo) coated glass substrates to measure the photocurrent response. CZTSe nanocrystals show significantly enhanced photocurrent response compared to CZTS.

Poster II.23

Development of a Protocol to Reduce Nanoparticle Toxicity in Plants

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Nanomaterials have presented as a new technology for the current era with the entry and use of nanomaterials in industry, agriculture and day to day life. Thereby, it is possible for nanomaterials to be present in the food chain of our ecological system. It is therefore necessary to find a remedy to reduce toxicity introduced by nanomaterials. Thus, a protocol was developed to reduce the effect of metal nanoparticles. Two species of millet, i.e. *Eleusine corcana* Gaertn. (finger millet) and *Paspalum scrobiculatum* L. (Kodo millet), were selected as model plants. Copper nanoparticles (CuNPs) were synthesized by the chemical reduction method. EDTA was used as a capping agent to stabilize the nanoparticles during synthesis. Uncoated nanoparticles were taken as reference to compare the effect of EDTA capping agent on the toxicity of CuNPs on plant growth. Synthesized nanoparticles were characterized using XRD and TEM to determine crystallite size and particle size, respectively. Original Cu from MS media was replaced with CuNPs, both in coated and uncoated forms and *in vitro* studies were conducted to study their effects on morphological and biochemical parameters after 15 days of seedling germination. Both coated and uncoated CuNPs treated plants displayed reduced growth compared with untreated plants, however significantly less reduction in biomass, root and shoot lengths, chlorophyll content and peroxidase enzyme activity was noted in coated CuNPs treated plants in comparison to uncoated CuNPs treated plants. The results obtained suggested that the extreme toxicological effect of nanoparticles on plant growth can be reduced by coating of nanoparticles. This study thus highlights the use of coating agents as an aid for reducing NP toxicity.

Poster II.24

Lipid Bilayer-SPION-Based Nanosystem as a Vaccine Delivery System in the Treatment of Leishmaniasis

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Over the course of history, vaccinations have proved to be one of the most effective prevention methods for infectious diseases. The main purpose of vaccines is to trigger an immune response. Vaccines are mainly divided into three subgroups: attenuated, inactivated, and subunit vaccines. This work focuses on subunit vaccines, which use fragments of the microorganism to trigger the immune system response. Leishmaniasis is a disease caused by a protozoan parasite of the genus *Leishmania*. To date, there is no effective vaccine for prevention of *Leishmania* due to the lack of appropriate adjuvant that would trigger the immune system to produce the desired response. In this work, the use of coated superparamagnetic iron oxide nanoparticles (SPIONs) for the treatment of Leishmaniasis will be discussed. In the initial stage of the work, SPIONs are encapsulated inside a bilayer lipid system, thus acting as an adjuvant. Then, the bilayer system will be conjugated with the transmembrane protein, the antigen, to create vaccine for the Leishmaniasis.

Poster II.25

Gene Silencing in Huntington's Disease: shRNA Delivery using Magnetic Iron Oxide Nanoworms

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Huntington's Disease (HD) is a dominant genetic disorder resulting from a trinucleotide repeat, CAG repeats, in the Huntington gene (HTT). Symptoms of the disease include cognitive decline, chorea, and dystonia. These symptoms manifest between the ages of 30 and 50. Disease-modifying therapies are currently not available for HD patients. Silencing of the HTT gene is a potential curative therapy for HD. Gene silencing can be achieved through RNA interference (RNAi) mechanisms. RNAi includes the delivery of small interfering RNA (siRNA) or short hairpin RNA (shRNA). Although siRNA suppression of a gene is very popular, it unfortunately requires repeated dosing and can exhibit off target effects. On the other hand, shRNA dose can last years and exhibits less off target effects. In this work, we will conjugate a DNA plasmid that encodes for shRNA to magnetic iron oxide nanoworms. This will allow for specific and efficient targeting. The DNA plasmid will be designed and synthesized along with the magnetic iron oxide nanoworms, which will then be followed by their conjugation. Cytotoxicity studies will be conducted, as well as *in vitro* and *in vivo* assessment of the effectiveness of the therapy. This method can serve as a potential disease-modifying therapy for HD.

Poster II.26

Synthesis of $Al(OH)_3$/CuMnAl-LDH Nanocomposites as Novel Adsorbents for Congo Red Dye Removal

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A novel lamellar $Al(OH)_3$/CuMnAl-layered double hydroxide (LDH) nanocomposite was successfully synthesized via hydrothermal method and tested as a superior adsorbent for the removal of Congo red (CR) dye from aqueous solution in comparison to its precursors; $Al(OH)_3$ and CuMnAl-LDH. The spectroscopic and chemical structure were analyzed by X-ray diffraction (XRD), transmission electron microscope (TEM), scanning electron microscopy (SEM), photoluminescence (PL) and UV-visible analysis. Several parameters such as temperature (30-50 °C), contact time (15–300 mins), pH (4-10), and dye concentration (100-500 mg/L) were used to investigate the removal efficiency. $Al(OH)_3$/CuMnAl-LDH nanocomposite displayed excellent properties for removal of CR dye, for instance the highest value of adsorption capacity was 172 mg/g; 210 min, followed by CuMnAl-LDH (102 mg/g; 210 min) then $Al(OH)_3$ (32 mg/g; 90 min). The results revealed that anion exchange and hydrogen bonding are mainly responsible for the adsorption of CR dye onto $Al(OH)_3$/CuMnAl-LDH nanocomposite. The presence of Cu (II) ions (synergistic effect) and NaCl salt (antagonism effect) interfered with the adsorption of CR dye onto $Al(OH)_3$/CuMnAl-LDH nanocomposite. However, the presence of Cr (VI) ions had no significant effect. Furthermore, the heavy metal removal efficiency by $Al(OH)_3$/CuMnAl-LDH nanocomposite in a single batch experiment showed a high adsorption capacity of 18.85 mg/g for Cu (II) ions and no adsorption for Cr (VI) ions. The adsorption kinetic and isotherm models of CR dye on $Al(OH)_3$/CuMnAl-LDH nanocomposite revealed that the experimental model fits the pseudo second order and Langmuir model. The developed nanocomposite showed excellent potential and could be useful in treating industrial wastewater.

Poster II.27

Covalent Calix[4]arene Nanocapsules for Efficient Camptothecin Delivery

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Covalent self-assembly has enabled the synthesis of morphologically diverse materials for a range of applications.[1] Different molecules, including macrocycles such as porphyrins[2] and cucurbiturils[3], have been used as building blocks of such materials, but covalent self-assembly of conformationally-flexible monomers, such as calixarenes, has proven more challenging. Herein, we assembled functionalized calix[4]arene and simple aromatic amines through dynamic imine bond formation under microwave irradiation. The obtained structures exhibited the morphology of uniform nanocapsules ~200 nm in diameter with a shell thickness of ~20 nm. The nanocapsules were synthesized in absence of any template and represent the first example of any covalently self-assembled structure based on calixarene.

The capsules, which were found to be stable under physiological conditions and non-cytotoxic, were loaded with a hydrophobic drug camptothecin, whose delivery is challenging because of its hydrophobic nature. We presumed that the drug would favorably interact with the hydrophobic cavity of calix[4]arene as well as capsule interior. A high drug loading of almost 21 % was attained and its release was enhanced in acidic conditions and in presence of a competitive binder, glutathione, which suggests that camptothecin can be preferentially released in tumor conditions. Studies on breast cancer cells demonstrated a 33-fold higher cytotoxicity for breast cancer cells ($IC_{50} = 1.7\ \mu g\ mL^{-1}$) than noncancerous cells ($IC_{50} = 57.6\ \mu g\ mL^{-1}$). Confocal microscopy revealed that camptothecin-loaded capsules started to interact with cell membranes of breast cancer cells after 3 hours of incubation. The drug molecules were internalized after 24 hours and cells started to exhibits signs of fragmentation and cell death after 48 hours of incubation. These results demonstrate the potential of calixarene-based systems for effective drug delivery.

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Poster II.28

Chemical Sensor Development with Ag@Nd_2O_3 Nanoparticles for Environmental Remediation

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In this approach, a selective and sensitive chemical sensor (4-Nitrophenol; 4-NP) based on silver doped neodymium oxide aggregated nanoparticles (Ag@Nd_2O_3 NPs) has been developed by electrochemical method. Initially, Ag@Nd_2O_3 NP was prepared by facile wet chemical method and fully characterized by UV–vis, FT-IR, XRD, FE-SEM, XPS, and XEDS techniques. The NPs were applied to the glassy carbon electrode (GCE) with the help of conducting binders called nafion. The fabricated Ag@Nd_2O_3/nafion/GCE has good selectivity and sensitivity and is linear over concentration ranging from 1.0 pM–0.1 mM. The sensitivity value of the fabricated GCE was 0.2215 $\mu A \mu M^{-1} cm^{-2}$. The above mentioned electrode has a low limit of detection, which was 0.43 pM. The prepared electrode was simple and easy to handle with an electrometer. In short, the prepared chemical sensor was environmentally and eco-friendly for the detection of various toxic and hazardous chemical pollutants.

Poster II.29

Synthesis and Characterization of SPIONs linked with polyethylene glycol (PEG) -Thiols coated with Gold Nanoparticles for Hyperthermia Applications

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Potent cancer therapeutics have been required to properly treat various types of cancers which cause more than nine million deaths annually worldwide. Current cancer therapies are insufficient and remain a big challenge. This project aims to outsmart cancer and avoid drug resistance. Recently, core/shell nanocomposites have proved to be effective in treating a broad range of cancers by utilizing the photothermal ablation concept. The synergetic effect of optical shell and magnetic core of the nanocomposites play a major role in selectively damaging the cancerous cells through heating when applying near infra-red (NIR) laser. In the current study new hybrid gold (Au) encapsulating magnetic nanoparticles (Fe_3O_4NPs) were utilized for the hyperthermia treatment. The specific objectives were to: (1) synthesis of core-shell nanostructures, (2) developing optical hyperthermia. The physicochemical properties of as-prepared core-shell nanostructures were studied through X-ray diffraction analysis (XRD), Ultraviolet–visible spectroscopy (UV-Vis), thermal gravimetric analysis (TGA), Scanning electron microscopy (SEM), High-resolution transmission electron microscopy (HRTEM) and Dynamic light scattering (DLS). In this study, we explored several key aspects of the NIR light-triggered photothermal hyperthermia modal approach. The 2nm gold shell showed a plasmonic absorption in the NIR region, thus, causing heating of the cells upon irradiation with the NIR laser. In addition, the magnetic core amplifies the heating effect, yielding unprecedented heating efficiency in the hyperthermia model. Development doses (400 mg/mL and 500 mg/mL) of the prepared core-shell nanocomposites showed significant results upon irradiation with NIR laser reaching heating therapeutic window of 45-50 ˚C leading to apoptotic cell death. The prepared core/shell nanocomposites with the significant heating effect could be used in hyperthermia treatments.

Poster II.30

Effect of Ageing on the Optical Properties and Morphology of Gold Nanorods

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This report explores the effect of ageing time of growth solutions toward physical, structural, morphological and optical properties of gold nanorods (GNRs). By varying the ageing time of growth solutions, the formation of rods can be controlled, which has a significant impact on GNR morphology. Modification of two-step synthesis namely seed-mediated growth method (SMGM) had been used to synthesize GNRs due to its simplicity, stability and high reliability. GNR thin films were deposited on glass substrates using a simple drop-drying technique. X-ray diffraction (XRD), UV-vis spectroscopy and field emission scanning electron microscopy (FE-SEM) were used to characterize the as synthesized GNRs and GNR thin films. Different ageing times resulted in solutions of different colors, and therefore, different optical spectra for the transverse surface resonance peaks (t-SPR) around 450 and 630 nm and longitudinal surface resonance (l-SPR) peaks (630 to 850 nm). 20 hours of ageing time resulted in optimized peak intensity at 0.55 a.u. with t-SPR at 630 nm and l-SPR at 850 nm. Increased ageing time resulted in increased GNR aspect ratios, which are in the range of 2.64 ± 0.02 to 4.23 ± 0.05. XRD results show that the crystal orientation of the GNRs is in the (111) direction.

Poster II.31

Effect of Synthesis Condition on Local Electronic Structure and Luminescence Properties of $SrZnO_2$ and Nanoparticles

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$SrZnO_2$ nanoparticles have been widely used for applications as a luminescent material. Nanoparticles synthesized by combustion synthesis using different fuels, glycine and mono ethanolamine, showed a remarkable change in structural and optical properties. The photoluminescence (PL) study was carried out at different excitation wavelengths. At 325 nm excitation, both samples showed broad emission in visible region, which gave overall white emission. At 270 nm excitation, nanoparticles prepared using ethanolamine fuel emitted in the blue region, whereas, those from glycine fuel showed emission in white region accompanied with sharp emission in near infrared region. These results show that prepared $SrZnO_2$ nanoparticles exhibit multiple emission centers, which are sensitive to excitation wavelength. Moreover, using different fuels for the synthesis of $SrZnO_2$ nanoparticles resulted in creation of different lattice defects. The local electronic structure was studied using X-ray absorption spectroscopy (XAS) technique at both Zn K edge and Sr K edge. The experimental spectra at both Zn K edge and Sr K edge showed different features in both samples. Theoretical absorption spectra were simulated using FEFF9 software for better understanding of local electronic structure of $SrZnO_2$ nanoparticles. From theoretical simulation, we found that near edge region displays features due to the presence of oxygen vacancies in the lattice. The investigation of extended X-ray absorption fine structure (EXAFS) region at Zn K edge and Sr K edge provides information about interatomic distances, coordination number, disorder term in both the samples. From both PL and XAS study, it is inferred that local electronic structure and luminescence response of $SrZnO_2$ nanoparticles can be tailored by varying synthesis conditions.

Poster II.32

Phase Miscibility and Dynamic Heterogeneity in PMMA/SAN Blends through Grafting of Polymer Chains on Graphene Oxide

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Agglomeration of nanoparticles due to van der Waals forces of attraction in a host polymer matrix can be improved by using polymer grafted nanoparticles. In this work we have functionalized SAN polymer chains onto the surface of graphene oxide (GO) and investigated how the phase separation temperature, morphology and volume cooperativity of PMMA/SAN blends are influenced. Functionalization of SAN polymer chains on the surface of nanoparticles usually involves the use of large amounts of solvents, many which are detrimental to the environment besides involving cumbersome processes. The polymer functionalized nanoparticles were prepared by a solvent free method where the cyano group in SAN was replaced by oxazoline groups during melt mixing in the presence of zinc acetate and ethanol amine. These newly created oxazoline groups reacted with the COOH group of GO under melt extrusion resulting in grafting of SAN on the surface of GO sheets. The effect of the functionalized nanoparticles on the demixing, local segmental motions and morphology evolution for different annealing times was carefully investigated in a classical LCST system, PMMA/SAN blend, using melt rheology, modulated DSC and AFM, respectively. The changes in viscoelastic behavior in the vicinity of demixing are investigated systematically for the control, and blends with GO and the functionalized nanoparticles. Various models were used to understand spinodal decomposition temperatures of the blends. Interestingly, the phase separation temperature determined rheology and the spinodal decomposition temperature increased significantly in the presence of polymer grafted nanoparticles in comparison to the control and blends with GO. The evolution of the morphology, interfacial driven coarsening as a function of temperature and the localization of nanoparticles were assessed using AFM. The cooperatively re-arranging regions estimated from calorimetric measurements begin to suggest enhanced dynamic heterogeneity in the presence of GO and functionalized nanoparticles in the blends. Our study shows that polymer functionalized nanoparticles delay demixing, suppress coalescence and alter cooperative relaxation in PMMA/SAN blends.

Poster II.33

A Unique Porous Membrane Derived from the Technologically Compatible Poly(ethylene-co-methyl acrylate)/poly(vinylidene fluoride) Biphasic Blend and its Surface Modification for Water Remediation

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A membrane material is developed from poly(ethylene-co-methyl acrylate)/poly(vinylidene fluoride) (EMA/PVDF) blend by chemical etching of the PVDF. EMA/PVDF blends are prepared at various concentrations from 90/10 to 60/40 ratio, and the developed membrane is microporous in nature. Prepared membranes were taken for water permeability measurement, and the 70/30 blend membrane was selected for further filtration studies by considering the blend composition and higher water flux (ca. 500 $Lm^{-2}h^{-1}$). The membrane surface is modified with a nanocomposite prepared using a poly(ethyleneimine) and graphene oxide (PEI/GO) mixture at different concentrations to study the separation efficiency of the 70/30 membrane. Separation of various pollutants such as BSA proteins and antibacterial resistance of the modified membrane with *E. coli* bacteria shows improved results. The modified membrane is also taken for the industrial effluent separation, shows improved water quality at the permeate side.

Poster II.34

Design and Use of Pico-Filter for the Decontamination of Polluted Water

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The pollution of water occurs due to mixing of industrial raw material, garbage and harmful gases with water. Due to its toxicity and high acidity level, polluted water has a capacity to interact with plants and animals, having a specifically harmful effect on human organs. Different industries generate large amounts of contaminated waste water, which is released to rivers and canals creating environmental pollution. Then, contaminated water used for cultivation of vegetables and crops has potential to be very harmful to animal and human health. Therefore, purification of water is necessary. Pico-filter is useful for the purification of water because it removes harmful metals from water. The design of Pico-filter consists of different layers of Pico materials, and results clearly show that it has a high efficiency for the purification of polluted water. Metals such as Fe, Ni, Mn, Mo, Ti, Hg and Ag are removed from the water using Pico-filter. The results show that by using Pico-filter we can achieve the 100 % pure water.

Poster II.35

Solvent Induced 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butanedione Cu(II) Complexes: Synthesis, Structure and Biocidal Activity

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Two novel pseudopolymorphic copper complex crystals, $[Cu(C_{14}H_8O_2F_3)_2\ (C_2H_6OS)_2]$ and $[Cu(C_{14}H_8O_2F_3)_2\ (C_3H_7NO)]$, were grown and characterized by UV-visible, FTIR, and single crystal XRD. With the aid of induced solvents, both complexes form different coordination spheres and exhibit uniqueness in constructing the supramolecular architecture. Interestingly, owing to the intermolecular interaction between fluorine atoms with adjacent molecules, complex 2 constructs a unique 2D single walled open framework filled with coordinated solvent (DMF) molecules through rhomboid channel. Isomorphic differences between the complexes predominantly evince formation of different graph-set descriptors which promote distinct molecular packing. Complexes are biocompatible in nature and potent biocidal (MIC 50 µg/mL) properties against perilous methecilline-resistant *Staphylococcus aureus* (MRSA) through membrane destabilization. Complex 2 could be a potential candidate to combat drug-resistant infectious agents in future, can be warranted.

Poster II.36

Glyco-conjugated Gold Nanorod based Biosensor for Optical Detection and Photothermal Ablation of Food Borne Bacteria

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Food borne bacterial species have been identified as major pathogens in most of the severe pathogen-related diseases among humans. Conventional methods like plating and enzyme-linked immune sorbent assay (ELISA) are time consuming, laborious and require specialized instruments. Nanotechnology has emerged as a great field developing technology for rapid detection of pathogens in recent years. Gold nanorods (AuNRs) have good electro-optical properties due to its broad light absorption band and scattering in surface plasmon resonance wavelength regions. By exploiting the sugar-based adhesion properties of microorganisms, we can use glycoconjugate capped gold nanorods as a potential nanobiosensor to detect food borne pathogens. In the present study, polyethylene glycol (PEG) coated AuNRs were prepared and functionalized with different types of carbohydrates and further characterized by UV-visible spectroscopy, dynamic light scattering (DLS), transmission electron microscopy (TEM). The activity of the as synthesized nanobiosensor was probed by lectin binding assay and also by different strains of food borne bacteria by using spectroscopic and microscopic techniques. Due to the specific interaction between the probe and food borne bacteria (*Escherichia coli, Pseudomonas aeruginosa*), our nanoprobe has shown significant and selective ablation of targeted bacteria. Our findings suggest that our nanoprobe can be an ideal candidate for selective optical detection of food pathogens and reduce loss to food industry.

Poster II.37

Work Function Modulation Studies on Oxide Nanostructure based Chemical and Photosensor Devices

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Oxide nanowires and thin films are prominent materials being researched for applications as sensing materials. The objective of the work is to understand work function changes in the gas sensor and photosensor response of heterostructure metal oxide nanowires and thin films. ZnO nanostructures show appreciable response to various target gases. Here we investigate the enhancement in response of ZnO nanostructures using resistive sensing as well as work function measurements using Kelvin probe system.

The nanostructures are synthesized using hydrothermal methods whereas the thin films are deposited by vapor deposition techniques. The work function studies are conducted under vacuum, in gas ambience and under light illumination (360 nm and 530 nm laser sources). The response of the sensor device fabricated from microrods are studied against gases like CO, H_2 at elevated temperatures. The response of the sensor devices is corroborated with those of the work function measurements which provides insight into the underlying gas-oxide interaction mechanism of oxide sensor devices.

Poster II.38

Y^{3+} Ionic Sensor Development based on (E)-methyl-N´-nitrobenzylidenebenzenesulfonohydrazide Derivatives: Environmental Sample Analysis

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(E)-methyl-N´-nitrobenzylidene-benzenesulfonohydrazide (MNBBSH) molecules were prepared using a simple condensation method from the derivatives of nitrobenzaldehyde and 4-methyl-benzenesulfonylhydrazine and crystallized in EtOH and MeOH. The MNBBSH derivatives were characterized using highly sophisticated spectroscopic instruments for example FTIR, UV-Vis, 1H-NMR, and 13C-NMR. The structure of the MNBBSH compounds were confirmed using a single crystal X-ray diffraction technique and used for the detection of selective trivalent yttrium ion (Y^{3+}) using a reliable I-V practice. A thin layer of MNBBSH was deposited onto a flat GCE with coating binder in order to modify a sensitive and selective Y^{3+} sensor. The modified MNBBSH/GCE sensor exhibited better electrochemical performances such as sensitivity, LOD, LDR, LOQ, short response time, and long-term storage ability towards the metal ion (Y^{3+}). The calibration curve of 2-MNBBSH/GCE sensor was plotted at + 1.1 V over a broad range of Y^{3+} concentration (100.0 pM-100.0 mM), and originated linear. Sensitivity, LOD, LDR and LOQ of the fabricated sensor towards Y^{3+} were calculated from the calibration curve. The prospective 2-MNBBSH/GCE sensor was applied for determination of trivalent Y^{3+} in spiked real samples and satisfactory results were observed.

Poster II.39

Novel Synthesis of Strontium Iron Oxide Nanoparticles and its Application for the Detection of Anti-Inflammatory Drug

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In the present work we have synthesized simple, cost effective, scalable, templet free strontium iron oxide ($SrFeO_2$) nanoparticles using a co-precipitation method. The synthesized $SrFeO_2$ nanoparticles were characterized by X-ray diffraction (XRD), Fourier transformer infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), energy dispersive spectroscopy (EDS) and elemental mapping. $SrFeO_2$ nanoparticles were then used to develop an electrochemical sensor for the detection of anti-inflammatory drug 4-aminoantipyrine (4-AAP). The developed Gr/$SrFeO_2$ sensor was characterized by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) techniques. Under optimized conditions, the developed sensor showed excellent electrocatalytic activity towards the detection of 4-AAP. The sensor exhibited a wide linear range and low detection limit. Moreover, excellent selectivity of the sensor for detection of 4-AAP in real samples was observed.

Poster II.40

Magnetic Graphene Oxide Quantum Dots as Fluorescence Probe for As(III) Sensing

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Due to the excellent photoluminescent properties, graphene oxide quantum dots (GQDs) have attracted great attention over the past few decades for the detection of heavy metal ions in contaminated water. Herein, we have studied the application of magnetic GQDs (Fe-GQDs) for sensing the As^{3+} ions. The prepared magnetic GQDs nanoparticles were characterized using different spectroscopic techniques. Impressively, the prepared Fe-GQDs exhibit good selectivity for As^{3+} ions over a wide range of common coexistent metal ions. This "turn on" sensing of As^{3+} ions can be explained by the fact that the aggregates were formed upon addition of As^{3+} ions, restricted the intra-molecular rotation and thus made the entire system highly emissive relative to the control. The aggregation-induced enhanced emission (AIEE) mechanism was well established from fluorescence anisotropy, DLS, time-resolved photoluminescence, X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy studies. Our study demonstrates that the as-prepared fluorescent Fe-GQDs can be employed as a sensor for ultrasensitive detection of highly toxic arsenic ions in aqueous solution.

Poster II.41

Strain Engineering Enhancement in Thermoelectric Properties of Dynamical Stable 2D Materials: ScP and ScAs

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We investigate the structural, electronic, phonon and thermoelectric properties of newly designed 2D materials, i.e. ScX (X=P, As), using density functional theory and semiclassical Boltzmann transport equations. We find that these nanosheets are chemical, dynamically and thermally stable. These compounds are stabilized in puckered structure and narrow bandgap semiconductors. We notice that electronic band gap can be tuned with the introduction of biaxial strain. Highly dispersed bands of ScP and ScAs, due to strong *p-d* hybridization, give rise to large electrical conductivity (~10^8 S/m). The lattice thermal conductivity (k_l) in the unstrained system is estimated to be 8.3 and 5 W/mK for ScP and ScAs respectively which are less compared to the pristine phospherene (24-110 W/mK) and arsenene (6-30 W/mK). Furthermore, the k_l of these compounds become ultra-low (~ 0.45 W/mK), when they are subjected to optimum tensile strain condition. The strain also brings nearly a two and a three-fold increase in the Seebeck coefficient with respect to the unstrained value in these compounds. Overall, the strain tunable large figure of merit (~0.65-0.9) makes these compounds promising thermoelectric materials.

Poster II.42

Designing Low Strain Graphene/TiO_2 Hybrid Interface for Efficient Separation of Charge Carriers: A First Principles Study

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The hybrid composite of graphene/TiO_2 has been reported as a better photocatalytic candidate with improved electronic properties. The governing mechanism behind the increase in efficiency is attributed to the enhanced interfacial charge transfer and charge separation, which in turn reduces the recombination rate of photogenerated charge carriers. However, the interface suffers from low stability due to the lattice mismatch between TiO_2 and graphene. Conventional approaches report a large lattice mismatch (~8%) between the graphene and TiO_2, which results in low stability. Also, the mechanism of charge transfer at the interface is not clearly understood. Here, we have designed an interface between anatase TiO_2 (001) surface and graphene that reduces the mismatch below 2%. Our proposed model enhances the stability which in turn increases charge transfer between graphene and TiO_2 surface. Using DFT with long range van der Waals dispersive correction, we provide a model to study the charge transfer between graphene and TiO_2.

Poster II.43

Electronic and Optical Properties of Layered 2-D InSe and GaSe Materials: *Ab initio* study

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We present first principles calculations of the electronic and optical properties of InSe and GaSe binary semiconductor compounds. Electronic properties (band structure, density of states, electronic charge density) and optical properties (dielectric function, refractive index, reflectivity, coefficient of extinction) are successfully calculated using self-consistent scalar relativistic full potential linear augmented plane wave method (FP-LAPW) within the generalized gradient approximation (GGA). The Perdew–Burke–Ernzerhof (GGA08) generalized gradient approximation was used for the total energy calculations, while the modified Becke–Johnson (MBJ) was used for the electronic structure calculations. This function was designed to reproduce the exact exchange correlation potential rather than the total energy, and as a result gives significantly improved results such as band gap and electronic structure. This gives us a unique opportunity to test the accuracies of the potentials employed and the calculation schemes in general. We also investigated the electronic properties of the ternary alloy $In_xGa_{1-x}Se$. The virtual crystal approximation (VCA) was adopted to model the alloy. The results are compared with previous calculations and with experimental measurements, we found good agreement with our calculations.

Poster II.44

First Principles Calculations of ^{31}P Solid-State NMR Parameters for Inorganic Phosphate Compounds

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Solid-state NMR can serve as a precision probe of local atomic environments. However, significant difficulty exists in the interpretation of spectra obtained via solid-state NMR due to broad linewidths caused by an array of interactions, including dipole-dipole, quadrupolar, and chemical shielding anisotropy. Additionally, due to the dependence of the chemical shift on the crystal structure of solid materials, making solid-state NMR peak assignments becomes non-trivial. This work utilizes the gauge-including projector augmented wave (GIPAW) method as utilized within the VASP DFT code to compute ^{31}P NMR chemical shift tensors for 22 phosphate compounds. The computed chemical shift tensor parameters are compared to experimentally obtained parameters. A strong correlation is observed between GIPAW calculated isotropic chemical shifts and experimental results. It is demonstrated that the GIPAW method can serve as a valuable tool for making ^{31}P NMR peak assignments for phosphate compounds. Due to the sensitivity of NMR chemical shifts to the local atomic environment, combining solid-state NMR and GIPAW techniques can provide valuable insights into the crystal structure of solids.

Poster II.45

Dirac Crossings in Palladium and Platinum Oxides

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Dirac semimetals are 3D analogs of graphene with unusual electronic transport properties due to symmetry-protected electronic band crossings at the Fermi energy with linear, light-like dispersion. Topological surface states and the enhanced bulk transport due to linear dispersion are both hypothesized to enhance catalytic activity; a growing number of catalysts and noble metals, including pure Pt and Pd, are known to host these features.[1,2] Oxides (Ca,Sr,Na)(Pd,Pt)$_3$O$_4$ have long attracted researchers due to their hole-doping-driven metal-insulator transitions and chemical relationship with historically and commercially important catalysts such as the Adams catalyst and PdO. These oxides are notable for their unusual, nonsymmorphic Pm-3n cubic symmetry and local square-planar coordination. Previous computational work by Li *et al.* identified Fermi level Dirac points in (Ca,Sr)(Pd,Pt)$_3$O$_4$.[3] We present first-principles calculations suggesting that oxide metals Na(Pd,Pt)$_3$O$_4$ host 14 additional Dirac crossings near the Fermi level and that these materials are proximal to an exotic nodal-cube state.

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Poster II.46

Synthesis of New MXenes and Investigation of their Surface Activities

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Since the discovery of MXenes as a new class of two-dimensional materials, more than 20 different MXenes have been synthesized successfully and many more have been predicted theoretically.[1] They are very promising materials for various applications due to their unique physical and chemical properties. Consequentially, they are discussed in the context of a variety of applications, such as battery materials, heterogeneous electrocatalysts, sensors, and many more. Therefore, the synthesis of new members of this class of two-dimensional carbides is of great interest. A variety of precursors is available if the synthesis is based on MAX phases. We have added a new “43”-type carbide MXene to the family.[2] The synthesis of $V_4C_3T_x$ was realized through selective etching of V_4AlC_3 using hydrofluoric acid. The required precursor MAX phase V_4AlC_3 was initially synthesized via a non-conventional solid-state method, microwave heating.[3] Furthermore we target a Cr-based MXene that have not been prepared yet. Based on theoretical investigation however, it is reported to show ferromagnetic properties.[4] Apart from the synthesis of new MXenes our research group also focuses on the surface structure/chemistry of the obtained MXenes and how it influences the materials properties. The products are characterized by means of X-ray powder diffraction, electron microscopy as well as surface sensitive techniques (infrared spectroscopy, nuclear magnetic resonance spectroscopy and X-ray photoelectron spectroscopy).

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Poster II.47

Silver Nanoparticles as a Scavenging Material for New Assay for Polyphenols Metal Scavenging Activity

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Polyphenols are widely used in numerous applications. They are synthesized in plants as secondary major metabolites, their structures are exceedingly varied, they have many roles and functions in plants, and are also very useful in many practical applications [1]. The common structure of polyphenols is aromatic rings with several hydroxyl groups attached. Their role includes participation in self-defense against external pathogens and extreme conditions such as UV light. They can be classified into four categories: (i) phenolic acids, (ii) flavonoids, (iii) stilbenes, and (iv) lignans. The classification is based on the number of phenolic rings they contain as well as the structural elements that binds these phenolic rings [2]. Antioxidant and anti-inflammatory activities are very old identified characteristics of polyphenols, many other biological functions have been identified and they have been attributed to a particular structure of the polyphenols. The wide resonance structure with attached hydroxyl groups makes them very good electron donors or acceptors, scavenging radicals and other reactive oxygen species (ROS) [3]. The antioxidant activity was widely studied using different assays, namely H_2O_2, iron scavenging activity, 2,2-diphenyl-1-picrylhydrazyl (DPPH), ferric reducing antioxidant power (FRAP), oxygen radical absorbance capacity (ORAC) and photochemiluminescence (PCL). However, none of these *in vitro* methods, individually or collectively, are relevant to the actual physiology of the human body [3]. This paper attempts to establish a correlation between the polyphenols content of natural antioxidant and ability to form silver nanoparticles without using reducing agent. Moreover, silver nanoparticle formation was assessed by surface plasmon resonance. Optimization experiments were conducted to understand kinetics, concentration of plant extract and pH. Extracts of turmeric, ginger, garlic, cinnamon and henna were used as natural antioxidants for the preparation of silver nanoparticles.

Poster II.48

Solvent Effects on Electron Transport in Two-Dimensional Materials

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Earth abundant materials for affordable renewable energy storage and conversion promise to address growing world energy demands. In particular, atomically thin, two-dimensional semiconductors are attracting interest as functional components of nanoscale devices for catalysis, solar energy conversion and storage, and flexible electronics. Of central importance to the design and efficiency of such devices is the transport of electrons between and within the semiconducting layers. This behavior can be further complicated by the presence of liquids and other sources of disorder, necessitating a molecular-scale understanding of the principles governing electron transport to inform the knowledge-based design of nanoscale devices. In this work, we use a combination of theory and molecular simulation to elucidate the impact of liquids on electron transport processes in two important areas: (i) water oxidation catalysis by layered manganese oxides and (ii) screening of charge carriers in monolayer MoS_2 by ionic liquids. We first discuss how unique properties of water confined between layered MnO_2 impacts solvent fluctuations that control redox reactions and consequently dictates the rate of electron transfer between the semiconductor and intercalated ions. Strategies that leverage this molecular understanding to inform the design of water oxidation catalysts will then be suggested. We then present a new approach for simulating charge carriers in atomically thin semiconductors. This approach is used to characterize the interactions between an excess electron and a sulfur vacancy in monolayer MoS_2, as well as the screening of these interactions by an ionic liquid. Implications of this work for the development of ionic liquid/MoS_2 devices will also be discussed.

Poster II.49

Thermal Insulation Material Based on PLA and Date-Pit Powder

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Most engineers moving towards improving society by various applications do not affect the environment. The field of this study is to evaluate the possibility of using available wastes, such date pits (DP), as a filler in thermoplastic biopolymer matrices for the preparation of insulating composite material to reduce energy consumption and loss in buildings. Utilization of insulating materials widely in construction will ultimately result in a reduction in energy consumption. Thereby positively impacting the environment through reduction of carbon emissions (e.g. CO_2).

Poly lactic acid (PLA), a biodegradable polymer that can be derived from renewable raw materials such as corn starch and sugarcane, may be used as a thermoplastic matrix in order to develop a biodegradable composite. The PLA-DP composite samples produced were checked for different physical, mechanical and chemical properties to develop a product formulation having best or optimum properties.

Samples were prepared with different percentages, 0-40 wt%, of DP powder using melt extruder and compression machine. Increasing the DP content decreased thermal conductivity of composite samples. Addition of DP to PLA matrices slightly reduced the mechanical strength of composites; however, the measured mechanical strength was greater than that of many commercial heat insulators.

Unquestionably, the research results will have a positive impact on the country’s economy due to the expected decrease in energy loss and contribute effectively in solving environmental problems. The target and creativity of this work is to utilize waste materials for development of waste material-thermoplastic polymeric (biodegradable polymers) composites as heat insulator materials with competitive properties and cost.

Poster II.50

Photoelectrochemical Performance of TiO_2-WO_3 Composite Films for Solar Water Splitting Applications

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Improvement in the photoelectrochemical (PEC) performance of materials for water splitting applications is of interest worldwide. Herein, TiO_2-WO_3 composite films have been successfully deposited on conductive glass substrates by co-sputtering technique with tungsten and titanium metal targets. The as-prepared films were annealed at different temperatures, 200 °C-400 °C . The photoelectrochemical (PEC) performance of the photoelectrode was characterized by the linear sweep voltammetry, and the incident photon-to-current conversion efficiency was measured as a function of wavelength. The films annealed at 300 °C exhibit significantly improved PEC activities compared with other films. The enhanced PEC activity could be attributed to the photogenerated electron transfer from TiO_2 to WO_3 through the interfacial potential gradient in the hybrid conduction bands. Such electron transfer in the hybrid structure facilitated the charge separation and retarded the charge pair recombination. As a result, the films annealed at 300 °C showed the maximum photocurrent density of 400 $\mu A/cm^2$ (at 0 VAg/AgCl) under visible light irradiation, which is about 5 times larger than that of as-prepared films. The enhanced electron transfer within the TiO_2-WO_3 composite films is also confirmed by the electrochemical impedance spectroscopy.

Poster II.51

Atomic Layer Deposition of TiS_2-Nanowall Networks with Superior Performance in Thin Film Rechargeable Batteries

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Employing atomic layered deposition, we have grown TiS_2 thin films using $TiCl_4$ and H_2S as Ti and S precursors respectively. The thin films have been characterized by various techniques microscopic and spectroscopic techniques. Interestingly, the films show nanowall network morphology and exhibit a high surface to volume ratio irrespective of the underlying substrate. The films grown on c-sapphire are crystalline in nature and appears to be amorphous on other substrates. Nanowall networks grown directly on stainless steel substrate show high performance in Na-ion/ Li-ion batteries with TiS_2 as the active electrode without any binder and conductive matrix.

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