

**Ninth Annual International Workshop on Advanced Materials  
(IWAM 2017)**

*Sunday, February 19 – Tuesday, February 21, 2017*

*Al Hamra Convention Center  
Ras Al Khaimah, United Arab Emirates*

**His Highness Sheikh Saud bin Saqr Al Qasimi  
Member of the Supreme Council of UAE  
and Ruler of Ras Al Khaimah**

**Welcoming Message**

February 2017

Dear Participants,

It gives me great pleasure to welcome you to Ras al Khaimah to attend the 9<sup>th</sup> RAK-CAM International Workshop on Advanced Materials (IWAM-2017). The Ras al Khaimah Centre for Advanced Materials (RAK-CAM) was officially launched in October 2007 under the Chairmanship of Professor Tony Cheetham of the Department of Materials Science at the University of Cambridge. A world class Scientific Advisory Board was established and its members will be attending this workshop. The scope of RAK-CAM embraces materials science in its broadest sense, from well-known construction materials such as concrete and glass, to the sophisticated materials that underpin the function of solar cells, catalytic converters, computers and cell phones. Our program reflects that diversity of purpose.

The previous IWAM meetings, held in February 2009-2016, were each attended by over 100 scientists from across the world and proved to be great successes. On the occasion of this 9<sup>th</sup> RAK-CAM workshop, we have once again attracted an outstanding group of speakers and participants who will present their work in both oral and poster sessions. I hope that you will enjoy this special occasion and that you will continue to support our long-term goal of establishing a leading centre for materials research here in the Middle East.

**His Highness Sheikh Saud bin Saqr Al Qasimi  
Ruler of Ras Al Khaimah and Member of the Supreme Council of the UAE**

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## Welcome to IWAM 2017

IWAM-2017 marks the ninth International Workshop on Advanced Materials organized and sponsored by the Ras Al Khaimah Centre for Advanced Materials (RAK CAM). The objectives of the workshop are to have in-depth discussions on the fundamental science and applications of Advanced Materials, including nanostructured materials and nanotechnology, and to stimulate international research collaboration with RAK CAM in diverse areas ranging from chemical, electronic and magnetic materials to environmental, renewable energy and biomedical applications. The general theme of IWAM-2017 is “*Innovation in Energy Materials*”.

The program includes 24 invited talks by a group of world leaders in Advanced Materials addressing topics dealing with research that has the potential for the greatest impact on developing clean and renewable forms of energy, nano medicine for improved diagnostics and therapy, and a clean healthy environment. In addition, a tutorial on solar energy, 9 student talks and two poster sessions with 79 poster presentations are planned as an integral part of the workshop program. We are again very grateful to colleagues at the American University at Ras Al Khaimah for reviewing and selecting all poster abstracts. The synergism produced by bringing together more than 100 researchers and students from 18 countries with research interests in diverse areas of the field of advanced materials is expected to enhance scientific collaboration which will take this field a step closer to realizing its enormous potential for the betterment of mankind.

I hope that you will find the program intellectually stimulating and rewarding and that you will enjoy your stay at Ras Al Khaimah.

*Professor Tony Cheetham*  
Chairman, RAK CAM

# **Workshop Program**

## **Ninth Annual International Workshop on Advanced Materials (IWAM 2017)**

**Al Hamra Convention Center, Ras Al Khaimah, UAE**

*Sunday, February 19 – Tuesday, February 21*

### **Saturday 18<sup>th</sup> February**

<b>14:00 onwards</b>	<b>Check-in at Hilton Al Hamra Beach &amp; Golf Resort</b>
<b>18:00-22:00</b>	<b>IWAM Registration &amp; Reception</b> <i>Hilton Al Hamra</i> <i>La chalet garden (weather permitting)</i>

## Day 1: Sunday 19<sup>th</sup> February 2017

<b>Session I</b>	<b>Opening Session</b>	<b>Start time: 08:30</b> <b>End time: 10:00</b>
<b>08:30</b>	<b>Welcome &amp; Overview of RAK CAM</b>  <b>Professor Tony Cheetham</b> Chairman, Ras Al Khaimah Centre for Advanced Materials	
<b>09:00</b>	<b>Keynote Address</b>  <b>His Highness Sheikh Saud bin Saqr Al Qasimi</b> Member of the Supreme Council of UAE and Ruler of Ras Al Khaimah	
<b>09:30</b>	<b>Regional Topic</b>  Ras Al Khaimah, United Arab Emirates	
<b>10:00</b>	<b>Coffee Break</b>	

<b>Session II</b>	<b>Electronic Materials</b>	<b>Start time: 11:00</b> <b>End time: 12:20</b>
	<b>Chair: Wang</b>	
<b>11:00</b>	<b>Advanced Materials for Future Computing Technologies using Spins and Ions</b>  <b>Stuart Parkin</b> Max Planck Institute for Microstructure Physics Halle, Germany	
<b>11:40</b>	<b>GaN Nanostructures for Phosphor Free White Light Emission by Molecular Beam Epitaxy</b>  <b>S. B. Krupanidhi</b> Materials Research Centre Indian Institute of Science Bangalore, India	
<b>12:20</b>	<b>Lunch &amp; Learn (lunch provided)</b>	

	<p><b>Solar Cell Tutorial - from Silicon to Carbon-based Materials</b></p> <p><b>Andrew Holmes</b>  School of Chemistry, Bio21 Institute  University of Melbourne  Victoria, Australia</p>
<b>12:20</b>	<p><b>Lunch</b>  <i>Al-Jazeera Restaurant</i></p>

<b>Session III</b>	<b>Energy Storage and Conversion</b>	<p><b>Start time: 14:20</b>  <b>End time: 16:50</b></p>
	<b>Chair: Dinca</b>	
<b>14:20</b>	<p><b>“Beyond Li-NMR”: Studies of Na and Mg Batteries and Li Dendrites</b></p> <p><b>Clare Grey</b>  Department of Chemistry  University of Cambridge  Cambridge, United Kingdom</p>	
<b>15:00</b>	<p><b>A Facile Method to Synthesize TiO<sub>2</sub>/Graphene-Metal Nanocomposites via Sol-Gel Technique for Solar Energy</b></p> <p><b>Edreese Alsharaeh</b>  Department of Chemistry  Alfaisal University  Riyadh, Kingdom of Saudi Arabia</p>	
<b>15:30</b>	<p><b>Perylene Diimide as Electron Transporters in Organic Solar Cells</b></p> <p><b>Sridhar Rajaram</b>  Jawaharlal Nehru Centre for Advanced Scientific Research  Bangalore, India</p>	

<b>16:10</b>	<p><b>Towards Rational Catalyst Design? Molecularly Engineered Frameworks for Hydrogen Evolution Photocatalysis</b></p> <p><b>Bettina Lotsch</b> Max Planck Institute for Solid State Research Stuttgart, Germany</p>
<b>16:50</b>	<p><b>Coffee Break</b> <b>Free time for informal discussions</b></p>

<b>Session IV</b>	<b>Graduate Student and Post-Doctoral Researcher Talks</b>	<b>Start time: 17:30 End time: 18:30</b>
	<b>Chair: Seshadri</b>	
<b>17:30</b>	<p><b>Shape-Memory and Self-Healing Effects in Mechanosalient Molecular Crystals</b></p> <p><b><u>Durga Prasad Karothu</u>, James Weston, Israel Desta, and Panče Naumov</b> Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, UAE</p>	
<b>17:40</b>	<p><b>A Universal Method of Producing Three-Dimensional Architectures of Two-Dimensional Materials</b></p> <p><b><u>Yarjan Abdul Samad</u> and Kin Liao</b> Cambridge Graphene Center (CGC), Electrical Engineering Division, The University of Cambridge, Cambridge, United Kingdom</p>	
<b>17:50</b>	<p><b>Mapping Molecular Changes Associated with Avascular Necrosis using Raman Spectrometry</b></p> <p><b><u>Ahmed Al Ghaithi</u>, Sultan Al Maskari, and John Husband</b> Oman Medical Specialty Board, Muscat, Oman College of Medicine, Sultan Qaboos University, Muscat, Oman College of Science, Sultan Qaboos University, Muscat, Oman</p>	
<b>18:00</b>	<p><b>Light Trapping in Perovskite Solar Cell with Metallic Nano-Structures</b></p> <p><b><u>Arul Varman Kesavan</u>, Arun D Rao and Praveen C Ramamurthy</b> Department of Materials</p>	



	Engineering Indian Institute of Science Bangalore, India
<b>18:10</b>	<p><b>Structure and Dynamics of Perovskite Formamidinium Lead Iodide: Phase Transitions, Reentrant Properties, Persistent Molecular Motion, and Large Positive Thermal Expansion</b></p> <p><b><u>Douglas Fabini</u>, Geneva Laurita, Constantinos Stoumpos, Ting-Ann Siaw, Song-I Han, Mercuri Kanatzidis, and Ram Seshadri</b>  Department of Materials University of California Santa Barbara  Santa Barbara, California, USA</p>

<b>Session V</b>	<b>Poster Session</b>	<b>Start time: 18:30</b> <b>End time: 20:30</b>
<b>18:30</b>	<b>Poster Session I</b> <i>Al Hamra Convention Center</i>	

*End of Day 1*

## **Day 2: Monday 20<sup>th</sup> February 2017**

<b>Session VI</b>	<b>Computational Materials Science</b>	<b>Start time: 09:00 End time: 11:00</b>
	<b>Chair: Seshadri</b>	
<b>09:00</b>	<b>Liquids, Crystals, Liquid Crystals, Plastic Crystals, &amp; More...</b>  <b>Michael Klein</b> College of Science and Technology Temple University Philadelphia, Pennsylvania, USA	
<b>09:40</b>	<b>Probing Nano-particle Properties using Computation and Synchrotron Radiation</b>  <b>Richard Catlow</b> Department of Chemistry, University College London UK Catalysis Hub, Harwell School of Chemistry, Cardiff University	
<b>10:20</b>	<b>The Yielding Transition in Amorphous Solids</b>  <b>Srikanth Sastry</b> Jawaharlal Nehru Centre for Advanced Scientific Research Bengaluru, India	
<b>11:00</b>	<b>Coffee Break</b>	

<b>Session VII</b>	<b>Nanomaterials</b>	<b>Start time: 11:30</b> <b>End time: 12:50</b>
	<b>Chair: Klein</b>	
<b>11:30</b>	<p><b>Photochemical and Thermochemical Generation of Hydrogen by Water Splitting</b></p> <p><b>C. N. R. Rao</b> Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore, India</p>	
<b>12:10</b>	<p><b>Recent Developments of Graphene-based Materials and Metal-Organic Frameworks for Clean Energy and Environmental Applications</b></p> <p><b>Samy El-Shall</b> Departments of Chemistry &amp; Chemical and Life Science Engineering Virginia Commonwealth University Richmond, Virginia, USA</p>	
<b>12:50</b>	<p><b>Lunch</b> <i>Al-Jazeera Restaurant</i></p>	

<b>Session VIII</b>	<b>Inorganic Materials - I</b>	<b>Start time: 14:30</b> <b>End time: 16:30</b>
	<b>Chair: Parkin</b>	
<b>14:30</b>	<p><b>Engineering Next Generation Hybrid Nanocapsules for Bioimaging and Biosensors</b></p> <p><b>John Wang</b> Department of Materials Science and Engineering National University of Singapore</p>	

<b>15:10</b>	<p><b>3D Printing of Metals: Challenges and Opportunities for Materials Science and Engineering</b></p> <p><b>Upadastra Ramamurty</b> Department of Materials Engineering Indian Institute of Science Bangalore, India</p>
<b>15:50</b>	<p><b>Magnetocaloric Materials: Function, Rapid Preparation, and Rational Screening</b></p> <p><b>Ram Seshadri</b> Materials Department and Department of Chemistry and Biochemistry Materials Research Laboratory, University of California Santa Barbara, California, USA</p>
<b>16:30</b>	<p><b>Coffee Break</b> <b>Free time for informal discussions</b></p>

<b>Session IX</b>	<b>Graduate Student and Post-Doctoral Researcher Talks</b>	<b>Start time: 17:30</b> <b>End time: 18:30</b>
	<b>Chair: Grey</b>	
<b>17:30</b>	<p><b>PEI Functionalized Multiwall Carbon Nanotubes for Uranium Adsorption</b></p> <p><b><u>Muna Alrebaki</u>, Mohammad Al-Harashseh and Mohannad Al-Jarrah</b> Department of Chemical Engineering Jordan University of Science and Technology, Irbid, Jordan</p>	
<b>17:40</b>	<p><b>Evaluating Performance of Newly Synthesized ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S Nano Photocatalyst for Degradation of Organic Pollutants and Enhanced Biogas Production from Sludge</b></p> <p><b><u>Muzammil Anjum</u>, Rajeev Kumar, and M. A. Barakat</b> Department of Environmental Sciences King Abdulaziz University, Jeddah, Saudi Arabia</p>	
<b>17:50</b>	<p><b>Amorphous Mixed Metal Hydroxide of Co and La as an Excellent Co- Catalyst for Photoelectrochemical Oxygen</b></p>	

	<p><b>Evolution Reaction</b></p> <p><b><u>Manjeet Chhetri</u>, Sunita Dey, and C. N. R. Rao</b>          New Chemistry Unit, Chemistry and Physics of Materials Unit          Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India</p>
<b>18:00</b>	<p><b>Defect Order and Disorder in Group 4 MOFs</b></p> <p><b><u>Matthew Cliffe</u> and Clare Grey</b>          Department of Chemistry, University of Cambridge, Cambridge, UK</p>

<b>Session X</b>	<b>Poster Session</b>	<b>Start time: 18:30</b> <b>End time: 20:30</b>
<b>18:30</b>	<p><b>Poster Session II</b>  <i>Al Hamra Convention Center</i></p>	

*End of Day 2*

## Day 3: Tuesday 21<sup>st</sup> February 2017

<b>Session XI</b>	<b>Inorganic Materials and Nanoscience</b>	<b>Start time: 09:00</b> <b>End time: 10:20</b>
	<b>Chair: Ramamurty</b>	
<b>09:00</b>	<b>Topology – From the Materials Perspective</b>  <b>Claudia Felser</b> Max Planck Institute Chemical Physics of Solids Dresden, Germany	
<b>09:40</b>	<b>Carbon Nanotubes Dispersed Coating System and its Applications</b>  <b>Takashi Yanagisawa</b> Nanotechnology Development GSI Creos Corporation Tokyo, Japan	
<b>10:20</b>	<b>Coffee Break</b>	

<b>Session XII</b>	<b>Sensors and Catalysis</b>	<b>Start time: 11:00</b> <b>End time: 12:00</b>
	<b>Chair: Holmes</b>	
<b>11:00</b>	<b>Production of H<sub>2</sub>S Sensors Based on CuO Nanoprticles and Semiconducting Organic Membranes</b>  <b>Ahmad Ayesb</b> Department of Mathematics, Statistics and Physics Qatar University Doha, Qatar	
<b>11:30</b>	<b>Additive Technologies for Fluid Catalytic Cracking</b>  <b>Natalie Herring</b> Johnson Matthey Process Technologies	

	Savannah, Georgia, USA
<b>12:10</b>	<b>Group Photo</b>
<b>12:30</b>	<b>Lunch</b> <i>Al-Jazeera Restaurant</i>

<b>Session XIII</b>	<b>Metal-Organic Frameworks</b>	<b>Start time: 14:30</b> <b>End time: 17:00</b>
	<b>Chair: Felser</b>	
<b>14:30</b>	<b>Designer Porous Materials for Clean Energy and Water</b>	
	<b>Mircea Dinca</b> Department of Chemistry Massachusetts Institute of Technology Cambridge, Massachusetts, USA	
<b>15:10</b>	<b>Tuning Structure and Connectivity of Zinc Phosphate MOFs through SBU Engineering</b>	
	<b>Ramaswamy Muragavel</b> Department of Chemistry Indian Institute of Technology Bombay Powai, Mumbai 400076, India	
<b>15:40</b>	<b>Hybrid Organic-Inorganic Perovskite Halides</b>	
	<b>Tony Cheetham</b> Department of Materials Science and Metallurgy University of Cambridge Cambridge, UK	
<b>16:20</b>	<b>Closing Remarks</b>	
	<b>Tony Cheetham</b>	
<b>17:00</b>	<b>Coffee Break</b>	
<b>19:00</b>	<b>Dinner Banquet at the Palace hosted by</b>	

	<p><b>His Highness Sheikh Saud bin Saqr Al Qasimi</b></p>
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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 19, 2017; 11:00

## **Advanced Materials for Future Computing Technologies Using Spins and Ions**

**Stuart S. P. Parkin**

Max Planck Institute for Microstructure Physics  
Halle, Germany  
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The era of computing technologies based on charge currents is coming to an end after more than 40 years of exponential increases in computing power that have been largely based on shrinking devices in two dimensions. A new era of “Beyond charge!” will evolve over the next decade that will likely be based on novel materials and phenomena whose innate properties are derived not from the electron’s charge but from spin currents and from ion currents. In some cases new functionalities will arise that can extend charge based devices but in other cases fundamentally new computing paradigms will evolve. An important new paradigm will be devices that are innately three-dimensional, such as Racetrack Memory,<sup>1,2</sup> a novel memory storage device that relies on the current induced motion of domain walls along nanoscopic racetracks. Recent discoveries show that charge currents can be converted to pure spin currents via the spin Hall effect in conventional<sup>3</sup> and unconventional metals,<sup>4</sup> with high efficiency. This enables the current driven motion of magnetic domain walls at great speeds,<sup>5</sup> the fundamental underlying principle of Racetrack Memory. Ionitronic,<sup>6,7</sup> bio-inspired devices that may mimic the extremely energy efficient computation systems in the biological world are also compelling. In this talk I will discuss spintronic and ionitronic materials and devices and how they may lead to novel computing technologies.

### References:

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Sunday, February 19, 2017; 11:40

## **GaN Nanostructures for Phosphor Free White Light Emission by Molecular Beam Epitaxy**

**S. B. Krupanidhi, B. Roul, Greeshma Chandan and Rohit Pant**

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Indian Institute of Science  
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Conventionally, Indium gallium nitride (InGaN) based white LEDs are popularly used for lighting in displays. These LEDs are generally fabricated by adding yttrium aluminum garnet (YAG) yellow phosphor on top of high-power blue LED chips to enable white light emission. However, wavelength-conversion loss and degradation of the phosphors tend to shorten the lifetime of these LEDs.

Due to these short-comings, realization of phosphor-free white-light emitters is becoming an important goal to achieve highly reliable high-power white-light-emitting diodes (LEDs). However, most of the earlier reported methods have not been applied to practical use due to their complexity. We demonstrated a novel growth method for phosphor-free white-light emitters with in-situ processing. In addition, adding graphene layer for p-type contact further improved the device performance.

Present talk describes the growth processes of nanostructured GaN, and other intermittent layers including the monolithic InGaN/GaN heterostructure, along with graphene layer, in correlation to the final device characteristics.

Sunday, February 19, 2017; 12:20

## **Solar Cell Tutorial - from Silicon to Carbon-based Materials**

**Andrew B. Holmes**

School of Chemistry, Bio21 Institute  
University of Melbourne  
Vic. 3010 Australia  
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Solar cells harness the excitation energy from photons emitted by the sun and convert this into electrical energy, resulting in the flow of an electric current through an appropriate circuit.

This tutorial will outline the basic principles of a silicon-on-glass solar cell module and the results will be compared with those obtained from a thin film of a blend of a donor and acceptor mixture of conjugated light harvesting organic materials.

Advances in the development of organic bulk heterojunction solar cells will be summarized, culminating in the production of printed solar cells on a strip of polyethylene terephthalate.

Finally, the use of perovskite materials will be introduced as a possible solution to the production of efficient thin film flexible solar cells.

Sunday, February 19, 2017; 14:20

## **“Beyond Li-NMR”: Studies of Na and Mg Batteries and Li Dendrites**

**Raphael Clement,<sup>†</sup> Phoebe Allan,<sup>†</sup> Josh Stratford,<sup>†</sup> Paul Bayley,<sup>†</sup>  
Nicole Trease,<sup>†</sup> Clare P. Grey,<sup>†</sup> Hee Jung,<sup>‡</sup> Andrew J. Ilott,<sup>§</sup> Alexej Jerschow<sup>§</sup>**

<sup>†</sup>Chemistry Department, University of Cambridge, Cambridge, UK

<sup>‡</sup>Chemistry Department, Stony Brook University, New York, USA

<sup>§</sup>Department of Chemistry, New York University, New York, USA

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This talk will describe the use of NMR and MRI spectroscopy to characterize a series of “beyond-Li” electrode materials. The NMR results are combined with complementary techniques such as pair distribution function analysis of (X-ray) scattering data. In the sodium-ion battery case, <sup>23</sup>Na NMR spectroscopy can be used to follow changes in local structure in a manner very similar to that performed on lithium-ion battery materials and the application of the method to study anode materials such as Sb and hard carbon Sn will be described. The use of NMR and MRI (magnetic resonance imaging) to link structural changes with electrolyte concentrations will be demonstrated for lithium metal anodes.

Sunday, February 19, 2017; 15:00

# **A Facile Method to Synthesize TiO<sub>2</sub>/Graphene-Metal Nanocomposites via Sol-Gel Technique for Solar Energy Harvesting**

**Edreese Alsharaeh and Abelrahman Soliman**

Department of Chemistry  
Alfaisal University  
Riyadh, Saudia Arabia  
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Solar energy harvesting is considered one of the most promising clean alternative energy resources. Dye Sensitized solar cells based on TiO<sub>2</sub> has been extensively studied in the last two decades. With the excellent thermal and electrical properties of graphene and plasmonic properties of metal nanoparticles, nanocomposites based on the aforementioned materials will be excellent candidates for solar energy harvesting. In this work, we are reporting a facile method of preparing photoactive materials based on TiO<sub>2</sub>/Graphene/AgI nanocomposites. The nanocomposites were characterized via XRD, TEM, XPS, UV-visible spectroscopy, FT-IR, and Raman spectroscopy. The thermal stability of the prepared nanocomposites were tested by the thermal gravimetric analysis technique (TGA). The materials also were tested for photo-degradation of MB dye, and phenols in both the UV and Visible spectra respectively and shows excellent photo-degradation (100% in 4 hours for the MB and 70% in 3 hours for the phenol). The prepared nanocomposites were tested as active materials in Dye-Sensitized Solar Cells DSSCs.

Sunday, February 19, 2017; 15:30

## **Perylene Diimide as Electron Transporters in Organic Solar Cells**

**Sridhar Rajaram**

Jawaharlal Nehru Centre for Advanced Scientific Research  
Bangalore, India

Solar cells play a pivotal role in our search for renewable sources of energy. Organic solar cells are one class of cells amongst various options. The low processing costs associated with their manufacture is one of the attractive advantages. Correlation of molecular architecture to device performance is extremely important for optimizing the performance of organic solar cells. In this context we have been involved in developing a novel electron transporter for organic solar cells using perylene diimides. We hypothesized that inducing a twist in the structure of perylene diimides might increase the short circuit current density. In this talk, I will detail our studies on developing a twisted perylene as an electron transporter for organic solar cells.

# **Towards Rational Catalyst Design? Molecularly Engineered Frameworks for Hydrogen Evolution Photocatalysis**

**Bettina V. Lotsch**

Max Planck Institute for Solid State Research  
Heisenbergstraße 1, Stuttgart, Germany

The conversion of sunlight into storable chemical fuels through photocatalysis has been identified as a viable strategy to alleviate future energy shortage. Although a number of potent semiconductors for solar water splitting are at hand, key features such as earth-abundance, stability and low toxicity still need to be addressed, thus calling for new material solutions for sustainable photocatalysis. While heterogeneous systems excel through their stability, homogeneous catalysts offer the potential to tune every step in the photocatalytic mechanism through molecular engineering. Combining the best of both worlds opens up new possibilities for the design of tailor-made photocatalysts.

We have recently developed a class of “soft” photocatalysts based on carbon nitrides and covalent organic frameworks (COFs),<sup>1</sup> which are abundant and molecularly tunable organic semiconductors. I will review our recent progress in the rational design of triazine- and heptazine-based systems for hydrogen evolution and highlight possible catalyst optimization strategies – through doping,<sup>2</sup> exfoliation,<sup>3</sup> functionalization,<sup>4</sup> as well as active site engineering.<sup>5,6,7</sup>

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Sunday, February 19, 2017; 17:30

## **Shape-Memory and Self-Healing Effects in Mechanosalient Molecular Crystals**

**Durga Prasad Karothu, James Weston, Israel Desta, and Panče Naumov**

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There has been a growing interest in polymorphic transitions involving substantial and sudden structural changes affecting physical and thermodynamic property of a material without altering its chemical composition. This property is essential for revealing the mechanism of the molecular packing of organic crystals, which might provide key technical information for molecular mechanical actuators and artificial muscles. Single crystals of terephthalic acid are mechanically compliant and reversibly shape-shift between forms I and II. While the transition of form II to form I on heating is spontaneous, in absence of significant defects, the reverse transition (form II to I) upon cooling to room temperature is latent, and can be stimulated by applying local pressure, whereby crystals leap to several centimeters. This mechanosalient (mechanically induced leaping) effect is due to sudden release of strain which has been accrued in form I that becomes metastable at room temperature. High-speed optical scanning and electron microscopy recording of the transformation reveal that large crystal domains are very rapidly transformed, and these transitions are separated by periods of latency required for stress accrual. *In situ* X-ray diffraction confirmed that the mechanosalient effect is related to the strong anisotropy of the intermolecular interactions, where layers of strongly hydrogen-bonded acid molecules are weakly bonded by  $\pi$ - $\pi$  interactions and can slide atop each other during the transition. This behavior resembles closely that of superelastic terephthalamide crystals, in line with the close similarity of their supramolecular structures.



Sunday, February 19, 2017; 17:40

# **A Universal Method of Producing Three-dimensional Architectures of Two-dimensional Materials**

**Yarjan Abdul Samad and Kin Liao**

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More than two thousand two-dimensional (2D) materials exist which have been identified after the successful isolation of graphene 2D materials. The properties of these 2D materials are different from their bulk counterparts, which make them potentially useful for several applications. One of the most important properties of 2D materials is their high surface area. In order to exploit these high surface areas, three-dimensional (3D) porous, connected and free-standing architectures of such 2D materials were proposed and in some cases proven to be possible by simulation based studies. Nonetheless, to date the only experimentally realized 3d architectures of 2d materials are those of graphene and graphene based 2D materials. Here, we report a universal method of creating 3D architectures of any 2D material. The technique is simple and facile including coating of moderately hydrophilic colloidal suspension of any 2D material on a thermally consumable polymeric template typically Polyurethane (PU) based. Three prominent 2D materials, molybdenum disulphide ( $\text{MoS}_2$ ), tungsten disulphide ( $\text{WS}_2$ ) and reduced graphene oxide (RGO), were used to demonstrate the method. Monolithic 3D architectures of density as low as  $1 \text{ mg}\cdot\text{cm}^{-3}$  were successfully formed. Flexible and stretchable conductors based on 3d structures of RGO were developed by infusing polydimethylsiloxane (PDMS) elastomeric polymer. These conductors show piezoresistive behavior as they change their resistance on the application of an external pressure/strain. With a strain gauge of more than 30 the RGO based 3D flexible and stretchable conductor is the most sensitive RGO/graphene based 3d conductor reported to date. When connected to human body as a wristband, the RGO 3D flexible and stretchable conductor is able to accurately sense the heartbeat rate as well as the magnitude of blood pressure.

Sunday, February 19, 2017; 17:50

## **Mapping Molecular Changes Associated with Avascular Necrosis using Raman Spectrometry**

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Bone avascular necrosis is pathological condition which results from interruption of blood supply to the bone. Though it is poorly understood condition, it is a common end process of traumatic or non-traumatic factors that compromise the precarious blood flow to the bone. The result of bone ischemia is the death of marrow and osteocytes and classically results in the failure of the necrotic part. Due to the lack of resolution and sensitivity of the existing diagnostic modalities, the aim of this study was to apply Raman spectrometry to avascular necrotic bones and map their molecular changes associated with avascular necrosis

Avascular necroted femoral heads were obtained under Institutional permission from sickle cell disease patients who underwent total hip replacement due to avascular necrosis (n= 7) and stored at -20 °C until further processing. Samples were cut into half and scanned with Raman spectrometer (I- Raman Ex Bwtek system). Scanned areas correlated with preoperative magnetic resonance scans.

All Raman spectra were baseline corrected and normalised to the phosphate peak ( $960\text{ cm}^{-1}$ ). Ratios of phosphate: Amide I, phosphate: proline, and phosphate: carbonate were calculated. Results suggest that there is a significant difference ( $p=0.001$ ) in density between diseased bone area and normal one. The exploration of this disease using Raman spectroscopy can facilitate the analysis of the overall biochemical signature of avascular necrosis on the femoral heads.

Sunday, February 19, 2017; 18:00

## **Light Trapping in Perovskite Solar Cell with Metallic Nano-Structures**

**Arul Varman Kesavan, Arun D Rao and Praveen C Ramamurthy**

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In thin film solar cells, light absorption is critical factor and further enhancement for a given system is one of the significant ways to improve efficiency. Various active layer growth methodologies adopted in the perovskite solar cells to achieve high performance devices. One of the ways to improve the optical absorption is by introducing metallic nanostructure in the perovskite solar cell. The presence of metallic nanostructures can contribute to the light absorption by scattering which will increase light path length in the cell, by creating electromagnetic field in the semiconducting layer, or by repeated absorptions/reflections of light toward the active layer and hence improved conversion efficiency. In this work, three different (Al, Ag and Cu nanoparticle) polydispersed metallic nanostructures was investigated as a light tapping agents in p-i-n structured perovskite solar cell. The metallic nanostructure incorporated at the interface in the perovskite solar cell showed wide optical absorption improvement. This absorption enhancement and hence the conversion efficiency was observed for all the three metallic structures. The obtained results showed metallic nano-structure introduced on the electron collecting interface layer offers light trapping enhances the photoelectron collection, reduces the charge recombination loss and also electrical transport properties in the device. The coupled effect offers improved short circuit current density (JSC) and fill factor (FF) and hence the higher power conversion efficiency.

Sunday, February 19, 2017; 18:10

# **Structure and Dynamics of Perovskite Formamidinium Lead Iodide: Phase Transitions, Reentrant Properties, Persistent Molecular Motion, and Large Positive Thermal Expansion**

**Douglas Fabini, Geneva Laurita, Constantinos Stoumpos, Ting-Ann Siaw, Song-I Han, Mercuri Kanatzidis, and Ram Seshadri**

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The hybrid organic–inorganic perovskite  $\text{HC}(\text{NH}_2)_2\text{PbI}_3$  (formamidinium lead iodide) and its alloys constitute the absorbers in today’s highest performing perovskite photovoltaics, but the structure and dynamics of this nascent material are poorly understood compared to the well-studied  $\text{CH}_3\text{NH}_3\text{PbI}_3$  (methylammonium lead iodide). Competing interactions associated with molecular motion, hydrogen-bonding tendencies, thermally activated soft octahedral rotations, and the propensity for  $\text{Pb}^{2+}$  lone pair stereochemical activity give rise to rich temperature-dependent polymorphism. We describe the evolution of the structure and dynamics of  $\text{HC}(\text{NH}_2)_2\text{PbI}_3$  between 2 K and 490 K, which is marked by multiple structural phase transitions and a glassy freezing of molecular motion. Synchrotron X-ray powder diffraction reveals an unusual reentrant pseudosymmetry in the  $\beta$ – $\gamma$  transition, which is reflected in the optical properties. The coefficient of volumetric thermal expansion near ambient temperature is perhaps the largest for any extended crystalline solid, posing great challenges for application. The dynamics of molecular motion are investigated via solid state nuclear magnetic resonance, dielectric spectroscopy, calorimetry, and ab initio calculations, and are shown to be markedly different from those of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , with implications for carrier transport and recombination in optoelectronic devices. This high-performance photovoltaic absorber displays incredible structural complexity and illustrates the delicate balance between energetic and entropic factors in dense, 3D connected hybrid materials.

Monday, February 20, 2017; 09:00

## **Liquids, Crystals, Liquid Crystals, Plastic Crystals, & More...**

**Michael Klein**

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My talk will first 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, CH<sub>4</sub>, CCl<sub>4</sub>, O<sub>2</sub>, and CH<sub>3</sub>OH.

Molecules with internal degrees of freedom and/or flexibility, such as, surfactants, lipids, dendrimers, peptides, or even proteins, self-assemble into an array of distinct condensed phases. Using selective examples, the talk will survey some of the intriguing phases exhibited by Nature. (e.g., *ACS Nano*, Article ASAP, DOI: 10.1021/acsnano.6b06419 Publication Date (Web): November 9, 2016)

Monday, February 20, 2017; 09:40

# **Probing Nano-particle Properties using Computation and Synchrotron Radiation**

**Richard Catlow**

Department of Chemistry, University College London  
UK Catalysis Hub, Harwell  
School of Chemistry, Cardiff University

Optimising the performance of nano-particulate based materials requires a detailed understanding of their structures, dynamics and reactivities at the atomic and molecular level. Computational chemistry and physics provide uniquely powerful tools in developing atomic level models for nano-structures. Their power is even greater when they are used in conjunction with advanced experimental techniques, especially those employing synchrotron radiation (SR). This lecture will illustrate the scope of joint computational/experimental investigations of nano-particulate based catalysts by reference to the following three recent studies:

- Structure - reactivity relationships in titania supported gold catalysts;
- Optimising photocatalytic properties of nano-alloy based catalysts;
- Restructuring of alloy nano-particles during catalytic operation. We will discuss how the detailed information gained from this concerted computational/experimental approach can assist the optimisation of catalytic performance

Monday, February 20, 2017; 10:20

## **The Yielding Transition in Amorphous Solids**

**Srikanth Sastry, Premkumar Leishangthem, and Anshul D. S. Parmar**

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Bengaluru, India

Amorphous solids are ubiquitous among natural and man-made materials, whose utility as structural materials depends critically on their response to applied stresses. Processes underlying such mechanical response, and in particular their yielding behavior, are not satisfactorily understood. In particular, attempts to understand the yielding of amorphous solids as a sharply defined transition has been the focus of many recent investigations. Although studied extensively, observed yielding behavior can be gradual and dependent on conditions of study, making it difficult to validate theoretical expectations of a sharp yielding transition. Through extensive computer simulations, we demonstrate that oscillatory deformation of model glasses reveal a sharply defined yielding transition, and provide new insights into its character. In contrast to prevailing expectations of diverging scales of avalanche events upon approaching the yielding transition, the statistics of plastic deformation events, or avalanches, reveals no signature of the impending transition, but exhibit dramatic, qualitative, changes across the transition. These results, and their implications for our understanding of the yielding transition, will be discussed.

# **Photochemical and Thermochemical Generation of Hydrogen by Water Splitting**

**C. N. R. Rao**

Jawaharlal Nehru Centre for Advanced Scientific Research  
Bangalore, India

Artificial photosynthesis is a promising method for producing renewable energy by use of sun light. Artificial photosynthesis employing the modified Z-scheme of natural photosynthesis can be exploited both for the oxidation and reduction of water. Oxidation of water is successively achieved by the use of cobalt and manganese oxides with the cations in the 3+ state with one  $e_g$  electron.<sup>1,2</sup> Hydrogen can be produced by the dye-sensitized photochemical process<sup>3</sup> or by the use of semiconductor heterostructures.<sup>4</sup> In this presentation, ways of splitting water will be presented, followed by recent results obtained on the photochemical generation of hydrogen by different strategies specially those involving semiconductor heterostructures of the type ZnO/Pt/CdS<sup>4</sup> or nanosheets of chalcogenides<sup>3,5</sup> such as MoS<sub>2</sub> and MoSe<sub>2</sub>. Recent results on hydrogen generation by the solar-thermal route based on oxides<sup>6</sup> will also be presented. Replacing platinum in electrochemical HER will be examined.

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Monday, February 20, 2017; 12:10

## **Recent Developments of Graphene-based Materials and Metal-Organic Frameworks for Clean Energy and Environmental Applications**

**M. Samy El-Shall**

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This talk will address the development of three classes of heterogeneous catalysts supported on graphene, Metal-Organic Frameworks (MOFs) and hybrid MOFs/RGO (Reduced Graphene Oxide) to efficiently disperse metal nanocatalysts for a variety of chemical transformations for energy and environmental applications. The combined properties of RGO and MOFs can lead to novel hybrid materials characterized by high porosity, large surface area and increased thermal stability which can be used as supporting materials in heterogeneous catalysis. First, we will discuss the superior catalytic activity of Pd nanoparticles supported on graphene 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 MOFs wrapped with thin RGO nanosheets for the biomass-refining of liquids derived from lignocelluloisc sources will be presented. The critical roles of graphene, RGO and MOFs in the dispersion and stability of the supported metal catalysts will be discussed. A general approach for the application of the hybrid support strategy in heterogeneous catalysis will be presented.

Monday, February 20, 2017; 14:30

## **Engineering Next Generation Hybrid Nanocapsules for Bioimaging and Biosensors**

**John Wang**

Department of Materials Science and Engineering  
National University of Singapore

For targeted bioimaging, biosensing and theranostic applications, we have successfully developed a class of PEOlated polymeric micelle/silica as multifunctional nanocapsules. Bioimaging contrast and biosensor agents, such as fluorescent conjugated polymers, CdSe/CdS/ZnS quantum dots (QDs), MnO<sub>2</sub>, Fe<sub>3</sub>O<sub>4</sub> nanocrystals and Au clusters, have been successfully encapsulated into poly(ethylene oxide) (PEO)-based polymeric micelle/silica dual layers via interfacial templating condensation. The encapsulation follows a green and straightforward microemulsion mechanism that directly proceeds in a near neutral pH aqueous environment. No detriment effects to the optical and magnetic properties of fluorescent conjugated polymers, QDs, MnO<sub>2</sub>, Fe<sub>3</sub>O<sub>4</sub> nanocrystals and Au cluster are observed during encapsulation. The core-shell nanocapsules thus generated possess a polymeric micelle framework with a single QD/Fe<sub>3</sub>O<sub>4</sub>/Au clusters encapsulated in the hydrophobic micellar core, an ultrathin (<5 nm in thickness) yet robust silica shell confined to the micellar core/corona interface and free PEO chains dangling on the surface. The free PEO chains effectively prevent nonspecific adsorption of biomolecules to the nanoparticles. Double shielding of polymeric micelle/silica shell remarkably improves the fluorescence resistance of conjugated polymers and QDs to strong acids and highly salted buffers. In vitro testing using MDA-MB-231 breast cancer cells demonstrates that these organic/inorganic dual layer-protected nanocapsules conjugated with folate show noncytotoxicity, bright fluorescence cellular imaging with high target specificity and improved performance in controlled delivery. In this talk, the latest developments in the multifunctional nanocapsules for both bioimaging and biosensors are discussed.

Monday, February 20, 2017; 15:10

## **3D Printing of Metals: Challenges and Opportunities for Materials Science and Engineering**

**Upadrasta Ramamurty**

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For 3D printing of metallic components, selective laser melting (SLM) of powders is the most commonly used method, which offers a number of technological advantages such as near-net shape forming with zero material loss. Consequently, there is a considerable and recent interest in this new way of manufacturing components for advanced engineering applications. From the scientific perspective, this process offers a number of exciting opportunities, some of which I would like to discuss in this talk. The SLM process not only imparts a substantially finer microstructure but also distinct mesoscale features to them. A complex interplay between these micro- and meso-structural features can lead to property combinations that were hitherto thought as not possible. Some possible additional features that are specific to the SLM process are the presence of considerable residual stresses and microporosity. In this presentation, we will examine as to how all these features will affect the mechanical properties through a comprehensive microstructural and mechanical property characterization of several different alloy components made through SLM, with particular emphasis on understanding their quasi-static tensile, fracture, fatigue crack growth, and unnotched fatigue properties. We will demonstrate that while the SLM process offers new avenues for material design that can exploit the micro- and meso-structures generated by the process for simultaneous enhancement in strength and toughness, their fatigue resistance is a big concern due to the porosity.

Monday, February 20, 2017; 15:50

# **Magnetocaloric Materials: Function, Rapid Preparation, and Rational Screening**

**Ram Seshadri**

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Changes in the temperature of magnetic materials due to applied magnetic fields have been known at least since the report in 1881 by Warburg and were further developed into techniques to reach temperatures below 1 K by Giauque and MacDougall in 1933. The huge interest in the utility of this effect for cooling near room temperature is relatively recent. Recent advances have yielded relatively low-cost and efficient materials that could potentially see widespread application in domestic refrigeration and air-conditioning.

In this talk, I will discuss magnetic refrigeration, and describe routes that allow the rapid preparation of magnetocaloric materials. The material property of interest in finding candidate magnetocaloric materials is their gravimetric entropy change upon application of a magnetic field under isothermal conditions. We have proposed a simple computational proxy based on carrying out non-magnetic and magnetic density functional theory calculations on magnetic materials. This proxy, which we refer to as the magnetic deformation  $\Sigma_M$ , is a measure of how much the unit cell deforms when comparing the relaxed structures with and without the inclusion of spin polarization.  $\Sigma_M$  appears to correlate very well with experimentally measured magnetic entropy change values.<sup>1</sup>

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Monday, February 20, 2017; 17:30

## **PEI Functionalized Multiwall Carbon Nanotubes for Uranium Adsorption**

**Muna Alrebaki, Mohammad Al-Harabsheh and Mohannad Al-Jarrah**

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Adsorption techniques have been found to be superior for water treatment due to simplicity of design, selectivity, low cost, flexibility, ease of operation, efficient technology, and wider applicability for removal various types of pollutants. Nanoscale adsorbents have better efficiency in removing contaminants from wastewater, due to their high surface area to volume ratio and improved dispersion on aqueous solutions. Further research is needed to improve capacity, selectivity, and kinetics, and secondly, the adsorbent reusability for multicycle use.

Natural sorbents under ambient conditions exhibit either low adsorption capacity or weak affinity for sorbate. The use of chemical modification to produce nanocomposite material increase their adsorption capacity and selectivity toward heavy metal ions, which have functional groups such as amine, amide, carbonyl, amidoxime, chitosan etc.

In this work multiwall carbon nanotube (MWCNTs) functionalized with polyethyleneimine (PEI) are used for separation of U (VI) from aqueous solutions. MWCNTs have a strong affinity to  $\text{UO}_2^{2+}$  but with low capacity and selectivity. MWCNTs-PEI would have an excellent, fast and high adsorption capability for  $\text{UO}_2^{2+}$  from aqueous solutions. The tolerance of this novel adsorbent for high salinity and its reusability properties can be removal of trace  $\text{UO}_2^{2+}$  ions from aqueous solution and also the recovery of  $\text{UO}_2^{2+}$  from leaching solution are being tested.

MWCNTs-PEI nanocomposites were synthesized by self-heal coating on acid treated MWCNTs outer surfaces with 1700 rpm agitation rate, modified by sonication to achieve submicron nanocapsules. The morphology and structure of the MWCNTs and MWCNTs-PEI were characterized by FTIR, SEM, TGA, and batch experiments for U adsorption on the produced material were carried out. The effects of process parameters, such as MWCNTs/PEI ratio, solution properties ionic strength, pH, initial sorbate concentration and temperature, on the performance of MWCNTs-PEI are being studied. The concentration of uranium was determined by (ICP-MS). The initial results suggest excellent adsorption of MWCNTs-PEI toward uranium.

Monday, February 20, 2017; 17:40

## **Evaluating Performance of Newly Synthesized ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S Nanophotocatalyst for Degradation of Organic Pollutants and Enhanced Biogas Production from Sludge**

**Muzammil Anjum, Rajeev Kumar, and M. A. Barakat**

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In this study a visible light active ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S nanocatalyst was fabricated by successive precipitation reaction. The obtained catalyst was analysed for its structure, phase, morphology and elemental fraction using XRD, SEM and EDX analysis respectively. Whereas, the valance state and surface properties of the catalyst were determined by using FTIR, Raman and UV-visible spectroscopic analysis. The ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S catalyst was tested for two important environmental applications; (1) the degradation of toxic pollutant (2-Chlorophenol) in wastewater through combine adsorption and photocatalysis under the influences visible light, (2) solubilization of intractable sludge using photocatalysis as pre-treatment method to enhance anaerobic digestion and biogas production. The results indicated that the ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S significantly enhance the removal efficiency of 2-Chlorophenol in adsorption-photocatalysis series reaction. The main reason for enhanced photocatalytic performance was due to the formation of ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S well contacted interface that has improved its visible light response. Furthermore, the ZnO-ZnS/Ag<sub>2</sub>O-Ag<sub>2</sub>S photocatalytic pretreatment showed a promising significance in sludge solubilization where sCOD was increased by 24 % from respective initial concentration. This increased the amount soluble organic matter in the system and thereby boost up subsequent anaerobic digestion of sludge. Biogas production as a whole was improved by 24% as compared in raw sludge due to photocatalytic pretreatment. Overall, this study provides an excellent insight in wastewater treatment and solubilization of sludge for enhance biogas production as an alternate source of energy.

Monday, February 20, 2017; 17:50

## **Amorphous Mixed Metal Hydroxide of Co and La as an Excellent Co-Catalyst for Photoelectrochemical Oxygen Evolution Reaction**

**Manjeet Chhetri, Sunita Dey, and C. N. R. Rao**

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Coupling the solar energy and electrical energy to amplify the production of Hydrogen without compromising the cost is being tried presently.  $\text{BiVO}_4$  (n-type) owing to its suitable band structure ( $E_g=2.5$  eV) and conduction band minimum (CBM) position near the thermodynamic hydrogen reduction potential, is effective for photoelectrochemical (PEC) water splitting. However,  $\text{BiVO}_4$  gives a low water oxidation photocurrent because of the low photogenerated carrier separation efficiency, meager light harvesting ability and surface carrier transport efficiency. These limiting effects can be minimized by the use of suitable co-catalyst for water oxidation. Most of the active oxygen evolution catalysts (OECs) with the highest activity are amorphous. The short range order in amorphous OECs, it creates abundant active sites and their structural flexibility leads to the long term photo-electrochemical stability. However, amorphous catalysts have limited mobility of protons causing the slow kinetics of water oxidation. Amorphous mixed metal hydroxide (MDH) is thus assumed to be important. The OER activity by these amorphous MDH is sensitive to the film thickness over  $\text{BiVO}_4$ . Electrochemical deposition of MDH is therefore suitable method to have good control over the thickness of film and on the relative quantity of the MDH. We have employed a new strategy to deposit Co and La MDH by controlled pulse plating technique. The optimized Co and La MDH co-catalyst over  $\text{BiVO}_4$  shows superior activity in terms of photocurrent onset (0.19 V, RHE), charge transport efficiency ( $\eta_{\text{trans}}$ , 79%), photogenerated e-h separation efficiency ( $\phi_{\text{sep}}$ ) and IPCE values. Fill factor calculated for the water oxidation half reaction was  $\sim 0.36$  which competes with the best known Ni-Fe based co-catalyst.

## **Defect Order and Disorder in Group 4 MOFs**

**Matthew Cliffe and Clare Grey**

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It is becoming increasingly clear that defects are crucial to the chemistry of metal-organic frameworks (MOFs), with recent studies demonstrating the prevalence of defects, especially ligand vacancies, in MOF chemistry. These defects can drastically improve sorption properties,<sup>1,2</sup> catalytic activity<sup>2</sup> and ionic conductivity.<sup>3</sup> In many functional materials, however, it is not just the presence of defects but their interactions and correlations that determine their properties. We have demonstrated, for the first time, that correlated defects can be accommodated in a MOF, by including ‘modulators’ (i.e. ligands able to bind to clusters but not form part of the network structure), for the canonical MOF UiO-66 (Hf).<sup>1,2,4</sup> We further showed, by using a combination of anomalous powder X-ray diffraction, total scattering, and electron diffraction measurements, that these defects are not just of ligand vacancies, but also include Hf cluster absences.

Just as in oxide frameworks, the presence of defects leads to huge variety in the range of structures formed. We have found a new mechanism for the accommodation of compositional flexibility in MOFs: cluster condensation. This is analogous to the formation of edge- or face-sharing polyhedra in oxides, e.g. the Magneli phases. We demonstrate using a combination of in situ and ex situ crystallization experiments that the formation of these new phases depends not just on the concentration of defect-promoting modulators, but also the reaction temperature and evolves over time. Control over the defects allows us to, in turn, tune the unusual thermomechanical properties of UiO-66, in particular allowing us to exercise control over its very large isotropic negative thermal expansion.<sup>5</sup> This provides proof of principle of the use of defects and disorder as design elements for MOF materials.

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## **Topology – From the Materials Perspective**

**Claudia Felser**

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Topological insulators (TIs), Weyl and Dirac Semimetals are a new quantum state of matter, which have attracted interest of condensed matter science. Materials can be identified based on the topology of the band structure via density functional materials. Theoretical predictions work very well and therefore hundreds of materials were identified and some were experimentally verified via Angle resolved photoemission and transport measurements. Large families of materials are of special interest because of their tunability. Heusler compounds are a remarkable class of materials with more than 1,000 members and a wide range of extraordinary multifunctionalities<sup>1</sup> including tunable topological insulators (TI).<sup>2</sup> Additional properties ranging from superconductivity (for example LaPtBi) to magnetism (for example GdPtBi) and heavy fermion behavior (for example YbPtBi) can be realized. These properties can open new research directions in realizing the quantized anomalous Hall Effect and topological superconductors. C1b Heusler compounds have been grown as single crystals and as thin films. The topological signature, the band inversion is proven by ARPES.<sup>3</sup> Dirac cones and Weyl points can occur at the critical points in the phase diagrams of TI, first Heusler compounds were identified. Weyl points, a new class of topological phases were first predicted in NbP, NbAs and TaP. The magneto-transport properties of NbP show a large magnetoresistance of 850,000% at 1.85 K (250% at room temperature) in a magnetic field of up to 9 T, without any signs of saturation, and an ultrahigh carrier mobility of  $5 \cdot 10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  that accompanied by strong Shubnikov–de Haas (SdH) oscillations. We found also ultrahigh magneto resistance, mobilities and Fermi arcs in NbP TaAs and TaP.<sup>4,5</sup> GdPtBi is a magnetic Heusler compounds with magnetically induced Weyl points.<sup>6</sup> More emerging quantum properties and potential applications will be discussed.

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Tuesday, February 21, 2017; 09:40

# **Carbon Nanotubes Dispersed Coating System and its Applications**

**Takashi Yanagisawa**

Nanotechnology Development  
GSI Creos Corporation  
Tokyo, Japan

Tuesday, February 21, 2017; 11:00

## **Production of H<sub>2</sub>S Sensors Based on CuO Nanoparticles and Semiconducting Organic Membranes**

**Ahmad I. Ayesh, Ayah F. S. Abu-Hani, Saleh T. Mahmoud, and Yousef Haik**

Department of Mathematics, Statistics and Physics  
Qatar University  
Doha, Qatar  
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This work reports on H<sub>2</sub>S gas sensors based on CuO nanoparticles that are embedded within polymer membranes of poly-vinyl-alcohol (PVA) and glycerol ionic liquid (IL). The nanoparticles were fabricated by the colloid microwave assisted hydrothermal method that enables a precise control of nanoparticle size. Polymer solutions of PVA and 5% IL were prepared with different concentrations of nanoparticles. Next, the solutions were used to fabricate polymer membranes by the solution casting method. The produced membranes were flexible and they hold semiconducting properties. Each membrane was encapsulated between two electrical electrodes where the top and bottom electrodes were made of stainless steel grid and copper sheet, respectively. A constant voltage was applied across the electrodes, and the electrical current response signal was measured. The measurements revealed that those sensors were sensitive to H<sub>2</sub>S gas with concentrations as low as 10 ppm, and they functioned at low temperatures. In addition, their sensing behavior was reversible which enabled repeatable use of those sensors. Those sensors were also selective to H<sub>2</sub>S, and they exhibited fast response of  $20.4 \pm 12.8$  s. Moreover, the sensors were easy to manufacture, thus, they have potential to be used for practical field applications.

Tuesday, February 21, 2017; 11:30

## **Additive Technologies for Fluid Catalytic Cracking**

**Natalie Herring**

Johnson Matthey Process Technologies  
Savannah, Georgia, USA

Fluid catalytic cracking (FCC) relies on a variety of catalysts to convert crude oils into high value products. In addition to the base catalyst, additives are used to improve FCC efficiencies, increase product selectivity, and reduce environmental emissions. These additives are complex, multicomponent particles combining active components with supports and binders. Each component plays a critical role in the overall performance of the catalyst. Development of FCC additives, including performance testing, is generally unlike that of research catalysts. This presentation will focus on various aspects of designing and effectively testing additives for FCC applications.

Tuesday, February 21, 2017; 14:30

## **Designer Porous Materials for Clean Energy and Water**

**Mircea Dinca**

Department of Chemistry  
Massachusetts Institute of Technology  
Cambridge, Massachusetts, USA

Owing to their extraordinary porosity, metal-organic frameworks have been widely employed for gas storage and storage applications, including natural gas and carbon dioxide. However, their application in devices related to water production or purification has been hampered by their relative sensitivity to moisture or low water uptake. Here we show how engineering pore size can lead to materials that adsorb record amounts of water and thus show promise for energy-efficient cooling applications and water production in arid areas. Similarly, we will show how imbuing MOFs with electrical conductivity produces an entirely new set of materials for electrical energy storage, which led to the fabrication of world's first non-carbon based supercapacitor.

# Tuning Structure and Connectivity of Zinc Phosphate MOFs through SBU Engineering

**Ramaswamy Murugavel**

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Our laboratory has been employing an organic soluble organophosphate (ArO)P(O)(OH) (Ar = 2,6-diisopropylphenyl) as the primary building unit (PBU) to assemble polyhedral molecules that resemble one or more zeolite secondary building units (SBUs).<sup>1-4</sup> Reaction of this phosphate with a divalent metal ion (e.g. Zn<sup>2+</sup>) in a donor solvent predominantly leads to the isolation of stable tetranuclear metal phosphates [(ArO)PO<sub>3</sub>Zn(L)]<sub>4</sub> which possess a Zn<sub>4</sub>O<sub>12</sub>P<sub>4</sub> inorganic core resembling D4R SBU. In recent times, however, we have unraveled that we can also isolate other SBUs from the same set of reactants, but by making small variations in the reaction conditions.<sup>1-5</sup> It is now possible to isolate hitherto unknown discrete D6R and D8R SBUs (which possess Zn<sub>6</sub>O<sub>18</sub>P<sub>6</sub> and Zn<sub>8</sub>O<sub>24</sub>P<sub>8</sub> cores, respectively) by switching the solvent from methanol to acetonitrile and the co-ligand from DMSO to either 4-formylpyridine or 4-cyanopyridine.<sup>5b</sup> From a series of experimental observations it has now become apparent that, irrespective of the conditions employed, S4R SBUs are formed as the initial products.<sup>3</sup> Hence, it is quite intuitive to conclude that a face-to-face fusion of two S4R blocks will lead to the formation of a D4R SBU.<sup>3a</sup> The explanation for the formation of larger SBUs such as D6R and D8R from a S4R however would need a different two-stage mechanism involving (a) side-by-side fusion of two or more S4Rs and (b) a constructive folding to close up the double-n-ring (n = 4, 6, or 8) SBUs.<sup>3a,5b</sup> One cannot discount the possibility of misfolding in step (b), which will lead to the isolation of polymeric chains with a staircase conformation.<sup>3a</sup> Similarly, formation of larger S6R and S8R SBUs in the initial phase of the reaction cannot be ruled out. A rationalization of these building principles and application of these compounds as molecular magnets<sup>4,6</sup> will be presented in this lecture.

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## Hybrid Organic-Inorganic Perovskite Halides

**Anthony K. Cheetham**

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Hybrid organic-inorganic perovskites are found in a number of families, particularly the halides (e.g.  $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) and formates (e.g.  $[(\text{CH}_3)_2\text{NH}_2]\text{Zn}(\text{HCOO})_3$ ).<sup>1</sup> The talk will focus on the halides, which are attracting a great deal of attention on account of their excellent performance as active layers in photovoltaic cells. Our work in this area has explored the use of Tolerance Factors to rationalise known structures and predict new ones.<sup>2</sup> We have also examined the role of hydrogen bonding in hybrid perovskite halides,<sup>3</sup> as well as their mechanical properties.<sup>4</sup> Our on-going research focuses on the search for *lead-free* hybrid perovskites, including layered bismuth-containing phases<sup>5</sup> and hybrid double perovskites such as  $(\text{CH}_3\text{NH}_3)_2\text{KBiCl}_6$ ,<sup>6</sup>  $(\text{CH}_3\text{NH}_3)_2\text{TlBiBr}_6$ <sup>7</sup> and  $(\text{CH}_3\text{NH}_3)_2\text{AgBiBr}_6$ .<sup>8</sup>

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**Poster Session I**  
*Al Hamra Convention Center*  
**Sunday, February 19, 2017 18:30-20:30**

## **I.1 Humidity-Responsive Luminescent Switching in Oxyluciferin-agarose Thin Films as a Basis for Optical Humidity Sensors**

**Nathan Lui**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, UAE

## **I.2 Numerical Simulation of the Femur Fracture for Different Cemented Hip Prostheses Under Forces during Stumbling**

**Zagane Mohammed El Sallah, Benbarek Smail, Benouis Ali, Sahli Abderahmen, Bachir Bouiadjra, and Serier Boualem**

Department of Mechanical, University of Sidi Bel Abbes, Cité Ben M'hidi, Algeria

## **I.3 Stable Molecular Rectifiers Based on Tetrathia-Rubyrin Monolayers Electrografted on Silicon**

**Kavita Garg and Praveen C Ramamurthy**

Department of Material Engineering, Indian Institute of Science, Bangalore, India

## **I.4 Impedance and Dielectric Study of L-arginine Modified Nano Hydroxyapatite**

**Bhoomika Jogiya, Karan Rathod and M. J. Joshi**

Department of Physics, Saurashtra University, Rajkot, India

E-mail: bhoomika.cpi@gmail.com

## **I.5 Influence of Brønsted/Lewis Acidity on Nickel and Cobalt Promoted Heteropolyacid Catalyst Supported on Silica for the Hydrodesulfurization of Thiophene**

**Nabil Al-zaqri, Ali Alsalmeh and M Rafiq H Siddiqui**

Department of Chemistry, King Saud University, Riyadh, Kingdom of Saudi Arabia

## **I.6 The Possible Role of Ni<sup>2+</sup> based Entities in Enhancing the Photocatalytic Activity of ZnO in Natural Sunlight Exposure**

**M. T. Qamar, M. Aslam, Ikram Ahmad, Z. A. Rehan, I. M. I. Ismail, and A. Hameed**

Centre of Excellence in Environmental Studies (CEES)

King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

## **I.7 Facile Microwave Synthesis of Porous CuO Catalysts for CO Oxidation**

**Abdallah F. Zedan, Assem T. Mohamed, Amina S. AlJaber and Siham Y. AlQaradawi**  
Department of Chemistry and Earth Sciences, Qatar University, Doha, Qatar

## **I.8 Tailoring the CO Oxidation Performance of Microwave Prepared Ceria-Nanoparticles through the Simultaneous Doping with Transition and Rare Earth Metals**

**Ayesha AlKhouri, Maitha AlKetbi, Abdallah. F. Zedan, M. A. Baker, Siham Y. AlQaradawi, S. J. Hinder, and K. Polychronopoulou**  
Department of Mechanical Engineering,  
Khalifa University of Science, Technology and Research, Abu Dhabi, United Arab Emirates

## **I.9 The Combined Effect of Transition Metal and Rare Earth Metal Doping of CeO<sub>2</sub> under Microwave Conditions Towards Enhancement of CO Oxidation Reaction**

**Maitha AlKetbi, Abdallah. F. Zedan, M. A. Baker, Siham Y. AlQaradawi, S. J. Hinder, and K. Polychronopoulou**  
Department of Mechanical Engineering  
Khalifa University of Science, Technology and Research, Abu Dhabi, United Arab Emirates

## **I.10 Solid Waste Management in UAE Recycling of Poly(ethylene terephthalate) Water Bottles**

**Mahmoud Allawy Mohsin**  
Department of Chemistry, University of Sharjah, Sharjah, United Arab Emirates

## **I.11 Synthesis of MnBi-Fe-Core-Shell- and Cu@ZnO-Nanoparticles**

**Stephanie Dolique and Barbara Albert**  
Eduard-Zintl-Institute of Inorganic and Physical Chemistry  
Technische Universität Darmstadt, Darmstadt, Germany

## **I.12 Easily Recoverable Nanocatalysts Based on Silver Supported by Different Polymeric Materials**

**Ikram Ahmad, Sher Bahadar Khan, Tahseen Kamal, and Abdullah M. Asiri**

Department of Chemistry

King Abdulaziz University Jeddah, Jeddah, Kingdom of Saudi Arabia

## **I.13 Modified Gamma-Alumina Catalysts for the Dehydration of Methanol to DME**

**Abbas Khalil, Rawad Bou Jaber, and Maliha Parvin**

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

## **I.14 Green Synthesis of Iron Oxide Nano Particle by Phyllanthus niruri Extract and their Applications**

**C S. Karthik<sup>†</sup>, L. Mallesha<sup>‡</sup>, H N. Shankar<sup>†</sup>, S.Nagashree<sup>†</sup>, and P. Mallu<sup>†</sup>**

<sup>†</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, Mysuru, India

<sup>‡</sup>PG Department of Chemistry, JSS College of Arts, Commerce and Science, Mysuru, India

## **I.15 Degradation of Ciprofloxacin Antibiotic in Aqueous Solution by SnS<sub>2</sub> Photocatalyst under UV Irradiation**

**Anas A. Alaidaros, Selvaraj Rengaraj, and Mohammed Meetani**

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

## **I.16 Sun Light Driven Photocatalysis for Degradation of Levofloxacin Drug using CdS Catalyst: An Investigation of Reaction Kinetics and Intermediates**

**Nada A. Elmerhi, Noor I. Albadawi, Anas Alaidaros, Ahmad alhamdat, Selvaraj Renga, and Mohammed Meetani**

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

## **I.17 Photocatalytic Degradation of Levofloxacin in Aqueous Solution by ZnCdS Catalyst under Sunlight Radiation**

**Salwa H. Ahmed, Aysha K. Alraeesi, Anas Alaidaros, Ahmad Alhamdat, Selvaraj Renga, and Mohammed Meetani**

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

## **I.18 Chemical Modification of Activated Carbon with 1,10-phenanthroline-5-amine and its Application for Solid Phase Extraction of Trace Elements from Groundwater**

**Nawader F. AlQadi and Awadh O. AlSuhaimi**

Department of Chemistry, Taibah university, AlMedinah, Kingdom of Saudi Arabia

## **I.19 Redox-Tunable Polycationic Polymers for Environmental Applications**

**Tina Skorjanc, Das Gobinda, Selbi Nuryyeva, Thirumurugan Prakasam and Ali Trabolsi**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates

## **I.20 Production of Anti-Corrosion Material from Lignocelluloses Waste of Palm Tree**

**Nour Abdel Rahman and Ali H. Al-Marzouqi**

Department of Chemical Engineer, UAE University, Al Ain, United Arab Emirates

## **I.21 Breaking Hearts: Indirect Evidence for Cholesterol Crystallization as Possible Cause of Cardiac Arrest**

**Marieh Al Handawi, Patrick Commins, Durga Prasad Karothu and Panče Naumov**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates

## **I.22 New Series of Guanidine/NTA Ternary Complexes as Antimicrobial and Antiproliferative Agents as well as Novel Approach to the Synthesis of their Nanosized Analogues**

**Najla Al-Shaikh, Eman Ismail, and Rawda Okasha**

Department of Chemistry, Taibah University, Medina, Kingdom of Saudi Arabia

## **I.23 Stress Distribution Analysis in the Dental Implants**

**M. Bettayeb and M. Benlebna,**

Department of Mechanical Engineering, University of Mostaganem, Mostaganem, Algeria

## **I.24 Improved Resistance to Cracking of a Cement Mortar through the Incorporation of Crumb Rubber**

**Moulay Smaine Ghembaza and Mbaye Seck**

Department of Civil Engineering, University of Djillali Liabes, Sidi Bel Abbes, Algeria

## **I.25 Mechanical Properties of Concrete-Reinforced Fibers and Powders with Crushed Thermoset Composites: The Influence of Fiber/Matrix Interaction**

**Yahya Sebaibi and Nassim Sebaibi**

Department of Civil Engineering, University of Djillali Liabes, Sidi Bel Abbes, Algeria

## **I.26 The Effect of Calcined Muds on the Properties of Self-Compacting Concrete in Spawning and Hardened State**

**Zoulikha Boukhelif, Bouhamou Nasreddine, and Mostifa Fouzia**

Department of Civil Engineering, Mostaganem University, Mostaganem, Algeria

## **I.27 Strengthening of Metallic Structures using Composite Materials**

**Abbas Soufiane and Larbi Chaht Fouzia**

Department of Mechanics, University of Djillali Liabes, Sidi Bel Abbes, Algeria

## **I.28 Effect of Various Concentration of Zinc Monoxyde on Duckweed (Lemna giba)**

**Sabrina Bouchelaghem**

Department of Biology, University Chadli Bendjedid el Tarf, el Tarf, Algeria

## **I.29 Selective and Sensitive Hydrazine Sensor based on SrO.CNT Nanocomposites for Environmental Safety**

**Mohammad Musarraff Hussain, Mohammed M. Rahman, and Abdullah M. Asiri**

Department of Chemistry, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

### **I.30 Electrochemical Detection of L-Dopa using Crude Polyphenol Oxidase Enzyme Immobilized on Electrochemically Reduced RGO-Ag Nanocomposite Modified Graphite Electrode**

**Sandeep S<sup>†</sup>, Santhosh A S<sup>†</sup>, Kumara Swamy N<sup>†</sup>, Suresh G S<sup>‡</sup> and Melo J S<sup>§</sup>**

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<sup>§</sup>Nuclear Agriculture and Biotechnology Division, Bhabha Atomic Research Centre, Mumbai, India

### **I.31 Biosensor Based on Polyphenol Oxidase and Biosynthesized Silver Nanoparticles for the Detection of Catechol in Green Tea Samples**

**Santhosh A S<sup>†</sup>, Sandeep S<sup>†</sup>, Kumara Swamy N<sup>†</sup>, Suresh G S<sup>‡</sup>, Melo J S<sup>§</sup>**

<sup>†</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, Mysuru, India

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### **I.32 Highly Efficient Co<sup>2+</sup> Ions Sensor based on N,N'-(ethane-1,2-diyl)bis(2,5-dimethoxybenzenesulfonamide) (EBDMBS) Fabricated Glassy Carbon Electrode**

**Tahir Ali Sheikh, Muhammad Nadeem Arshad, Mohammed M. Rahmana, Abdullah M. Asiria, and Khalid A. Alamry**

Department of Chemistry, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

### **I.33 Self-healing Molecular Crystals**

**Patrick Commins, Hideyuki Hara, and Pance Naumov**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates

### **I.34 Mechanically Robust, Chemically Inert, Ultrahydrophobic Charcoal Surfaces**

**Jian-Bo Xie, Liang Li, Anastassiya Knyazeva, James Weston, and Pance Naumov**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates

### **I.35 Preparation and Characterization of Activated Carbon Supported Nano-Bimetallic Composite Catalyst (ANBCC-AC/Cu<sub>2</sub>O/ZnO) for Catalytic Ozonation of Environmental Pollutants**

**P. Hariprasad and M. Muthukumar**

Department of Environmental Sciences, Bharathiar University, Coimbatore, India

### **I.36 Removal of Cr(IV) from Polluted Water Using Carbon Nanofibers and Activated Carbon Prepared from Low Cost Resources**

**Ahmed M. Soliman<sup>†§</sup>, Dalal Al- Shamse<sup>‡</sup>, Ahmed A. Murad<sup>‡</sup>, Ala Aldahan<sup>‡</sup>, Efstratios Svinterikos<sup>‡</sup>, Ioannis Zuburtikudis<sup>‡</sup> and Thies Thiemann<sup>†</sup>**

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### **I.37 Growth and Characterization of Zinc (tris) Thiourea Sulphate (ZTS) Crystals**

**K. P. Dixit, J. H. Joshi, and M. J. Joshi**

Department of Physics, Saurashtra University, Rajkot, Gujarat, India

### **I.38 Functionalized Graphene Nanocomposites with Steroidal Diamine Dimers**

**Khaled Shawakfeh<sup>†</sup>, Edreese H. Alsharaeh<sup>‡</sup> and Sally Butros<sup>†</sup>**

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## **Humidity-Responsive Luminescent Switching in Oxyluciferin-agarose Thin Films as a Basis for Optical Humidity Sensors**

**Nathan Lui**

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The chemistry of bioluminescent systems is important for applications in biochemistry and materials science. The emitter of the bioluminescent reaction by which the fireflies generate light, firefly oxyluciferin, is stable in acidic and neutral solutions, but it is highly labile species due to the coexistence of both the keto- and enol- forms in basic solution. The keto-/enol-tautomerism combined with the additional phenol group yields a complex triple equilibrium that is strongly affected by solvent and pH. Ghose, et al.<sup>1</sup> reported the pH-dependent absorption and emission spectra of oxyluciferin and several derivatives in solution. Using multivariate curve resolution, they assign absorption and emission spectra of individual chemical forms of oxyluciferin. This project seeks to take advantage of the established pH-dependent, solution-state photochemistry of oxyluciferin to develop the active component (indicator) of a solid-state optical humidity sensor.

Towards this goal, self-supporting oxyluciferin-agarose thin films were synthesized at concentrations from 0.2% to 1.0% through an organogel casting process. Next, the conservation of the solution-state pH-dependent photochemical properties in the solid state was established by recording absorption and emission spectra at different pH. The absorbing species were determined using the absorption spectra, and equilibrium constants calculated from isosbestic points. To explore their use as humidity sensors the films were exposed to low (20%), medium (57%), and high (99%) humidity environments, and their absorption and emission spectra recorded, establishing an optical standard curve.

We expect that the continuation of this research will lead to functional water sensors which could serve a range of applications such as sensing for groundwater. Groundwater presents one of few viable alternatives to energy intensive desalination in the region. As such, the looming threat of water scarcity in the UAE and the depletion of the Emirate's ground water resources makes the detection of water, even at low concentrations, of paramount importance.

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## **Numerical Simulation of the Femur Fracture for Different Cemented Hip Prostheses Under Forces during Stumbling**

**Zagane Mohammed El Sallah, Benbarek Smail, Benouis Ali, Sahli Abderahmen, Bachir Bouiadjra, and Serier Boualem**

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Biomechanics is the study of the structure and function of biological systems by means of the methods of mechanics. Hip prostheses were used for patients who have hip fractures, and are unable to recover naturally. To design highly durable prostheses, one has to take into account the natural processes occurring in the bone. Finite element analysis is a computer based numerical analysis method, which can be used to calculate the response of a model to a set of well defined boundary conditions. In this paper, the static load analysis is based, by selecting the peak load during the stumbling activity. Two different implant materials have been selected to study appropriate material. The results showed the difference of maximum von Mises stress and detected the fracture of the femur shaft for different model (Charnley and Osteal) implant with the extended finite element method (XFEM), and after the results of the numerical simulation of XFEM for different was used in determining the stress intensity factors (SIF) to identify the crack behavior implant materials for different crack length. It has been shown that the maximum stress intensity factors were observed in the model of Charnley.

**Keywords:** Total Hip Prosthesis (THP); Extended finite element method (XFEM); Bone fracture; Femur; Stumbling; Stress intensity factor (SIF).

## **Stable Molecular Rectifiers Based on Tetrathia-Rubyrin Monolayers Electrografted on Silicon**

**Kavita Garg and Praveen C Ramamurthy**

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Molecular electronics is being proposed as an alternative to the silicon based microelectronics. An intense research carried worldwide during last couple of years has demonstrated that molecules exhibit a unique electronic functions, e.g. rectification, negative differential resistance, memory, etc. and many more new molecules with desired properties are being synthesized by the chemists around the world [1,2]. Building electronics solely using molecules might take a much longer time (may be several decades!). Thus, a medium term solution, say for next 10–15 years, is to make molecules compatible to the silicon, so that the nanoscale electronic functionality of molecules can be utilized in silicon based microelectronics, and this research field is termed as hybrid nanoelectronics [1,2]. The advantage of molecule/Si hybrid concept is that the inputs available from an already existing powerful silicon- based integrated circuit industry can be used effectively for the development of integrated hybrid devices. We are actively engaged in the development of the hybrid nano-electronics and demonstrated that organic molecules exhibiting different electronic functionalities can be deposited on Si substrates by self-assembly process [1,4–6]. Porphyrin molecule and its derivatives have been found to be a good candidate for charge storage devices [7]. The electronic properties of porphyrin molecules can be altered through modification of the basic “tetra” pyrrole macrocycle system and by replacing pyrrole with other heterocyclic systems. Since, these molecules possess two stable and reversible oxidation and reduction states, they are ideal candidates for the development of memory elements. For making hybrid nanoelectronic memory devices, grafting of these molecules on Si substrates is essential. Here, we demonstrate, for the first time, that a specifically designed alkenyl terminated derivative of dithiaporphyrin molecule, that is, 5-(4-undecenyloxyphenyl)-10,15,20-tri(phenyl)-21, 23-dithiaporphyrin ( $N_2S_2-C_{11}$ ) can be easily grafted on doped n-Si substrates by an electrochemical process via formation of Si–C bonds. Monolayers were characterized by various spectroscopic techniques. The current– voltage characteristics of these molecules exhibit a pronounced hysteresis and demonstrated that such electrical bistability can be utilized for the resistive molecular memory devices.

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Keywords: Molecular electronics; rubyrin; rectifier

## **Impedance and Dielectric Study of L-arginine Modified Nano Hydroxyapatite**

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Hydroxyapatite,  $\text{Ca}_{10}(\text{PO}_4)(\text{OH})_2$ -HAP, has a number of applications in industrial and clinical fields. It is an excellent bio-compatible material owning similarities to inorganic content of bone and teeth. As amino-acid having synergetic effect on structure and morphology of HAP, the present authors have synthesized L-arginine modified nano HAP by using surfactant mediated approach and characterized by impedance and dielectric studies within the frequency range of 100 Hz to 20 MHz at room temperature. The variation of dielectric constant, dielectric loss and a.c. conductivity were studied as the concentration of L-arginine increases. The Nyquist plots were drawn. The typical behaviour of the Nyquist plot was represented by equivalent circuit having two parallel R-C combinations in series.

Keywords: L-arginine; Nano-Hydroxyapatite; Impedance spectroscopy; Dielectric studies

## **Influence of Brønsted/Lewis Acidity on Nickel and Cobalt Promoted Heteropolyacid Catalyst Supported on Silica for the Hydrodesulfurization of Thiophene**

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Phosphomolybdic acid (PMoA), Phosphotungstic acid (PWA) supported on silica and nickel, cobalt substituted were prepared with different loadings. All catalysts have been characterized using thermogravimetric analysis (TGA), BET surface area, solid-state  $^{31}\text{P}$  NMR spectra, FT-IR, Diffuse Reflectance Infrared Fourier Transform (DRIFT), powder X-ray diffraction and thermogravimetric analysis. The surface areas of the catalysts are slightly lower than the surface area of the silica used in making these catalysts.

All catalysts were tested for their activity in the hydrodesulfurization of thiophene in the temperature range of 300 – 500 °C. Under similar conditions silica supported PMoA, PWA showed lower hydrodesulfurization activity. The catalytic activity increased with substitution of nickel and cobalt on PMoA and PWA. The nickel substituted Catalysts showed higher activity than the cobalt-substituted ones. At 500 °C, Ni(HPMo) gave a HDS conversion of thiophene of 99.6% whereas the Co(HPMo) gave a HDS conversion of thiophene of 98.3%. Ni(HPWA) gave a HDS conversion of thiophene of 95.2%, whereas Co(HPW) gave a HDS conversion of thiophene of 87.2%. Although the catalysts lose all the acidity after hydrodesulfurization, Brønsted/Lewis acidity of the catalyst precursor appear to be essential for the catalytic hydrodesulfurization.

Keywords: Hydrodesulfurization; Thiophene; Catalyst

## **The Possible Role of Ni<sup>2+</sup> based Entities in Enhancing the Photocatalytic Activity of ZnO in Natural Sunlight Exposure**

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The photocatalytic activity of ZnO was improved by the gradual deposition of nickel based oxides at its surface. The absorption and photoluminescence spectra revealed the formation of visible light receptive entities with the quenching abilities of the exciton recombination process whereas the multiple absorption edges exposed the composite nature of the synthesized materials. The existence of surface Ni<sup>2+</sup> and Ni<sup>3+</sup> in XPS analysis revealed the formation of mixed oxides and the variations in the oxidation state of the precursor Ni<sup>2+</sup> during the slow deposition process. The structural and morphological characterization of the synthesized powders was performed by XRD and FESEM. The Mott-Schottky analysis of the materials revealed the n-type nature of the deposited mixed oxides. A mild p-type character of the deposited oxides was witnessed at higher loading. The effect of the surface mixed Ni (2+, 3+) oxides on the charge transfer and retention was estimated by electrochemical impedance spectroscopy and chronopotentiometry. In comparison to pure ZnO, the photocatalytic activity of the synthesized powders was investigated for the removal of a variety of pollutants such as chlorophenol and chloroacetic acid derivatives in the natural sunlight exposure. The kinetics of the degradation as well as mineralization process was evaluated and the validity of the Langmuir-Hinshelwood kinetic model was also assessed. The Ni modified catalysts exhibited substantially higher activity as compared to the pure ZnO. The stability of the catalysts under illumination was examined by measuring the release of Zn<sup>2+</sup> and Ni<sup>2+</sup> whereas the reusability was examined for five consecutive cycles using the same catalyst.

Keywords: Sunlight photocatalysis, chlorophenols, chloroacetic acids, mixed nickel oxides

## **Facile Microwave Synthesis of Porous CuO Catalysts for CO Oxidation**

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Among the diverse catalytic processes, the heterogeneous catalytic CO oxidation is an important reaction for removal of small amounts of poisoning CO in fuel cell applications and environmental remediation. Therefore, there is a great need to develop active, stable and low-cost catalysts for CO oxidation at low temperature. Copper oxide (CuO) nanostructures have received a great deal of attention as inexpensive and non-plasmonic catalysts for gas-phase oxidation reactions, gas sensing and gas adsorbents. In this work, we have developed a facile microwave-assisted method to synthesize porous CuO nanocatalysts with high activity and stability for CO oxidation at low temperature window between 60-150 °C. The CuO nanocatalysts were prepared by microwaving an aqueous mixture of the copper salt and the precipitating agent followed by drying and annealing of the reaction product in ambient air. We studied the morphological and structural properties of the prepared CuO nanocatalysts using standard physical techniques including SEM, EDX, XRD, TGA, FT-IR and XPS in order to understand the structure-property relationship. We carried out multiple catalytic CO oxidation cycles in a continuous flow fixed-bed reactor at low temperature range (25-200 °C) and studied the catalytic activity and the stability of the microwave-synthesized CuO nanocatalysts and we further compared their activity to CuO prepared with traditional deposition precipitation. The experimental results revealed that the unsupported CuO nanoparticles prepared by microwave-assisted synthesis exhibited higher activity and enhanced CO conversion rates at lower temperature, compared to CuO nanoparticles prepared by deposition precipitation or by conventional heating. The CO is completely oxidized to CO<sub>2</sub> over microwave-synthesized CuO at temperature as low as 120-150 °C, depending on the WHSV (Weight-Hourly Space Velocity) value. The enhanced CO conversion rates are probably due to the increased porosity and readily-available oxygen vacancies in the porous copper oxide nanostructures. The CuO nanocatalysts demonstrated a high stability for CO oxidation for test periods of up to 50 h under stream at 150 °C. Moreover, the CuO catalysts demonstrated high activity for CO oxidation in absence and in presence of smoke which could raise the potential application of the developed catalysts in hydrogen purification in fuel cell systems, CO removal in carbon dioxide lasers, in air quality industries and for efficient CO removal in carbon dioxide atmosphere during fires.



Keywords: CO Oxidation, Porous CuO, Heterogeneous Catalysts, Microwave Synthesis

## **Tailoring the CO Oxidation Performance of Microwave Prepared Ceria-Nanoparticles through the Simultaneous Doping with Transition and Rare Earth Metals**

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Ceria-based metal oxides have been attracting a great deal of attention in many portable and stationary power applications due to its unique properties in various fields. Among them, the hydrogen fuel cells which are on high demand, due to their high efficiency and environmentally friendly advantages in generating electricity with zero emissions. For conditioning the fuel hydrogen gas, selective CO oxidation processes are introduced. Doping ceria with transition (e.g.  $\text{Cu}^{2+}$ ,  $\text{Mn}^{4+}$ ) and rare earth (e.g.  $\text{La}^{3+}$ ,  $\text{Sm}^{3+}$ ) metals it is anticipated to enhance the oxygen storage capacity (OSC) of pure ceria. The introduction of samarium and copper cations into ceria-based materials, which have different sizes and charges will create imperfections that indeed will lead to the improvement of the oxygen mobility in the structure. In the particular study, microwave radiation synthesis was adopted to facilitate the formation of nanocrystalline cerium-samarium-copper ternary metal-oxides (Ce-Sm-Cu-O), which were prepared by coupling microwave heating with sol-gel method. The Ce-Sm-Cu-O catalysts were studied as promising candidates for the CO-cleanup process. The effect of Cu composition in the 5-20 at.% range and solvent polarity and coupling with the microwave radiation (water, ethanol, and propanol) was studied on the microstructure properties (i.e. particle size, pore volume, and morphology) and on the catalytic performance (CO oxidation activity). Different characterization analytical tools were employed in order to study the microwave prepared materials microstructure (XRD, TEM), morphology (SEM), porosity (BET), thermal behavior (TGA), and surface properties (XPS,  $\text{CO}_2$ -TPD,  $\text{NH}_3$ -TPD), whereas the CO catalytic activity was studied as well. The SEM results demonstrated that there is no significant impact of Cu concentration on the morphology of the catalysts. X-ray diffraction (XRD) studies showed that all the catalysts present cubic fluorite structure, while Scherrer calculations gave a small crystallite size in the 9-12.5 nm range.

The thermal stability of Ce-Sm-Cu catalysts was further investigated in an inert atmosphere ( $\text{N}_2$ ) using thermogravimetric analysis (TGA), which allowed the monitoring of the decomposition process of the catalysts precursors. Furthermore,  $\text{N}_2$  adsorption at 77 K allowed us to study the surface area of the catalysts that ranges between 2.5-9  $\text{m}^2/\text{g}$  and generally decreases as the Cu content increases. Strong effect of the Cu concentration on the acidic/basic properties of the catalysts surface was found which concomitantly affects the catalyst's sites activity regarding the CO oxidation reaction.

Keywords: microwave, sol-gel, doping,  $\text{CeO}_2$ , ternary oxides, CO oxidation

## **The Combined Effect of Transition Metal and Rare Earth Metal Doping of CeO<sub>2</sub> under Microwave Conditions Towards Enhancement of CO Oxidation Reaction**

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Contrasting to burning fossil fuels for power generation, zero emission H<sub>2</sub> fuel cells are a very promising alternative. Fuel cells such as proton exchange membrane (PEM) and solid oxide fuel cells (SOFC) can generate electricity by electrochemical reactions with water as the only waste. Toward reaching the optimal fuel cell performance, the conditioning of hydrogen fuel is essential. Hydrogen mixture that contains carbon monoxide will affect the performance of the fuel cell negatively, as CO acts as poison to the Pt electrode. CO clean-up processes are used to solve the issue with various catalysts such as platinum, gold and ceria. The properties of ceria catalyst can be enhanced by metal doping. In the present work, the microwave prepared cerium-lanthanum-copper oxides catalyst was synthesized with a wide range of Cu percentages (3-20%) and with varying the solvent system e.g. water, ethanol and propanol as per their different microwave absorption capacity. Different techniques were applied on the materials during the microwave synthesis such as simultaneous cooling and reflux so to prolong the reaction time and interfere with the nucleation and growth of the nanoparticles. By altering the morphology of the catalyst, the properties (porosity, oxygen storage capacity and particle size) and the performance (selectivity and activity) can be changed as well. The synthesized samples are then characterized using different analytical tools. In particular, XRD was used for investigating the crystalline structure and then crystal size was calculated using Scherrer equation. In addition TGA was used for evaluating the thermal stability and decomposition of the precursor material in inert atmosphere.

The SEM studies showed that there is no profound effect of Cu concentration on the morphology of the catalysts. X-ray diffraction (XRD) studies showed that all the catalysts present cubic fluorite structure, while Scherrer calculations gave a small crystallite size in the 8-15 nm range depending on the Cu content. Furthermore, N<sub>2</sub> adsorption at 77 K allowed us to study the surface area of the catalysts that ranges between 5-20 m<sup>2</sup>/g and generally decreases as the Cu content increases. Strong effect of the Cu concentration on the acidic/basic properties of the catalysts surface was found which concomitantly affects the catalyst's sites activity regarding the CO oxidation reaction.

Keywords: microwave, sol-gel, CeO<sub>2</sub>-doping, CO-oxidation

## **Solid Waste Management in UAE Recycling of Poly(ethylene terephthalate) Water Bottles**

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A maximum of 12.5% of waste water bottle is recycled at different recycling plants in UAE. Waste plastics in general is posing an ecological problem as it is not easily degrade, and is filling the wasteland fields fast. Polyethylene terephthalate (PET) waste is one of many sources of environmental pollution that can cumulatively have big impact if left unmanaged. The proposed technique that uses ionic liquid and nano-materials to produce added-value products from plastics waste, not only will benefit the economy, and conserve valuable energy, but also to save the environment from waste plastics scattered around the costal lines and to minimizes the plastic waste being sent to landfill sites. The UAE municipalities are currently facing a huge amount of (PET) waste as a result of the consumption of bottled water, cosmetics containers, and food packages. UAE is leading the world in drinking bottled water per capita consuming an estimated 272 liters per person annually. The current physical processes to recycle PET at UAE are not addressing the growing demand for functional reuse of PET waste. This research focused on using different classes of ionic liquids and nano-materials to produce new value-added material with modified mechanical, thermal and electrical properties that can be incorporated by different local industries.

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Keywords: Recycling of plastics; poly(ethylene terephthalate); waste water bottles; ionic liquids; nano-materials;

## **Synthesis of MnBi-Fe-Core-Shell- and Cu@ZnO-Nanoparticles**

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The properties of nanoparticles are quite different from those of single atoms or bulk materials. Because of their large surface-to-volume ratio nanomaterials have specific chemical and physical properties depending on the particle size and shape. By synthesizing bimetallic nanoparticles the electronic transfer of one metal to another or even magnetic coupling can be modified. The development of bottom-up synthesis procedures is highly desirable to produce new functional (core-shell) nanoscale powders. Reactions in different solvents while applying capping agents like oleylamine and oleic acid allow for the generation of shape- and size-controlled nanoparticles.

Nearly monodisperse nanoparticles of Cu, Mn, Bi and MnBi were synthesized and characterized via X-ra powder diffraction and transmission electron microscopy (TEM). Such MnBi nanoparticles were now used as a precursor to produce core-shell nanoparticles. We expect core-shell particles of Fe@MnBi to exhibit hard-soft magnetic properties.

Furthermore, nanostructured ZnO@Cu was synthesized. By varying the solvent, capping agents, temperature and the organometallic precursor monodisperse nanoparticles could be produced. Nanoparticles of ZnO@Cu will be tested for catalytic properties and compared to bulk ZnO-Cu-Al<sub>2</sub>O<sub>3</sub> catalyst.

Keywords: Nanoparticles, Catalysis

## **Easily Recoverable Nanocatalysts Based on Silver Supported by Different Polymeric Materials**

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Retrievability of a catalyst is an important task, which is commonly achieved by loading it on easily separable supports such as magnetic substrates. However, we demonstrate here the process of easy and fast catalyst separation from a reaction medium by loading it onto an economically feasible and microscopically high surface substrate of filter paper (FP) made up of cellulose microfibrils and Cellulose acetate fibers (CAfiber), and sheets (CASheet) as catalyst support. To prepare FP support, we coated chitosan (CH) on filter paper (CH-FP) to impart a high affinity of the substrate for metal ion absorption. And for Cellulose acetate fibers (CAfiber), and sheets (CASheet) we prepared these by wet-spinning, and doctor blade methods, respectively. For CA-fiber, the CA-acetone solution was pushed through narrow orifice of the medical syringe into a coagulating bath containing water. Then for all FP, (CAfiber) and (CASheet) AgNO<sub>3</sub> dissolved in water with a 0.1 M concentration was used as the Ag ion carrier solution, and CH-FP strips, (CAfiber) and (CASheet) with known dimensions were submerged into it for the metal ion absorption. The metal ion-loaded CH-FP strips, (CAfiber) and (CASheet) were dip treated with sodium borohydride (NaBH<sub>4</sub>) aqueous solution to prepare Ag-nanoparticle loaded CH-FP (CAfiber) and (CASheet) (Ag/CH-FP, Ag/CAfiber and Ag/CASheet). X-ray diffraction and energy dispersive X-ray spectroscopy confirmed the formation of the Ag/CH-FP, Ag/CAfiber and Ag/CASheet. The morphology was examined through scanning electron microscopy analysis (SEM), which showed the presence of Ag nanoparticles attached to the cellulose microfibrils. The prepared Ag/CH-FP, Ag/CAfiber and Ag/CASheet were employed as a dip catalyst for the degradation of nitroarene compounds of 2-nitrophenol (2-NP) and 4-nitrophenol (4-NP) and 2,6-dinitrophenol by NaBH<sub>4</sub>. Remarkable reaction rates and reusability of materials was found.

Keywords: Ag/CH-FP, Ag/CAfiber, Ag/CASheet, Nanomaterials

## **Modified Gamma-Alumina Catalysts for the Dehydration of Methanol to DME**

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Solid Acid catalysts, such as  $\gamma$ -alumina, are important materials in different applications especially in the petroleum industry and energy-related processes. They are known, as an example, for their catalytic activity in the dehydration reactions of alcohols due to their significant surface Lewis acidity. Methanol is one of the most important intermediates that can be obtained from natural gas and can be further converted to other efficient fuels and chemicals. Dimethyl ether, which can be obtained from methanol, is being considered as a promising future fuel besides being the building block for several industrially important chemicals. Although  $\gamma$ -alumina has shown significant activity for the dehydration of methanol to dimethyl ether, improving the conversion and the selectivity is still a major concern.  $\gamma$ -Alumina, which is a cost-effective material, can be further modified by doping with other elements and hence its textural properties and catalytic performance can be enhanced. The aim of the present work is to modify  $\gamma$ -alumina by doping with gallium ions and to study the dopant effect on the textural properties, surface acidity, and the performance in the methanol dehydration to DME. Ga-doped alumina was compared with other catalysts including a zeolite material and alumina doped with other metal ions. The catalysts were prepared in different compositions using the sol-gel method and different preparative parameters were studied and correlated with the final properties of the catalysts. The catalytic activity and selectivity were evaluated and were correlated with other properties of the catalysts. catalytic activity of selected promising catalysts was studied at different reaction temperatures. In addition, adsorption of methanol was studied in attempt to elucidate the reaction mechanism.

Keywords: DME, Dimethylether



## **Green Synthesis of Iron Oxide Nano Particle by Phyllanthus niruri Extract and their Applications**

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A facile, efficient and eco-friendly method has been followed for the green synthesis of iron oxide nano particles by phyllanthus niruri extract. Phyllanthus niruri extract act as mild, reducing and stabilizing agent. The synthesized iron oxide NPs were characterized with X-ray diffraction (XRD), ultraviolet-visible spectroscopy (UV-Vis), Fourier transform infrared (FT-IR), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) techniques. More importantly, the green synthesized iron oxide NPs presented excellent catalytic activity for the synthesis of the ureas and thioureas derivatives. The catalyst was easily separated and recovered catalyst can be used several times without any significant loss of the catalytic property. The electrochemical behaviour of iron oxide NPs was studied by cyclic voltammetric techniques. As observed in this study, iron oxide NPs can be used as a matrix in sensors.

Keywords: Phyllanthus niruri, Green synthesis, Iron oxide NPs, Catalytic property, Sensors

## **Degradation of Ciprofloxacin Antibiotic in Aqueous Solution by SnS<sub>2</sub> Photocatalyst under UV Irradiation**

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Antibiotics are one of the most important pharmaceutical groups widely used by humans as well as in veterinary medicine and aquaculture. Between 2000 and 2010, consumption of antibiotic drugs increased by 40% - from 50 million standard units to 70 million standard units. With the over prescription of antibiotics, a significant of antibiotic wastewater discharge into groundwater. Antibiotic pollution has become a serious problem and present a hazardous risk to the environment. In this study, three Tin (IV) sulfide (SnS<sub>2</sub>) was prepared for photocatalytically degrade the antibiotic ciprofloxacin in aqueous solution using both UV-C and sunlight irradiation. In UV-C tests, approximately 90% degradation of the drug solution was achieved in 270 min, while in sunlight photo catalysis, ciprofloxacin solution was only partially removed. The kinetic studies showed that photo degradation of ciprofloxacin follows first order reaction kinetic model. Effective parameters such as pH, photo catalyst dose and contact time were optimized and well investigated. Furthermore, the identification of ciprofloxacin intermediates during photocatalytic degradation was analyzed using high performance liquid chromatography and tandem mass spectrometry (HPLC-MS/MS) and the reaction pathway based on them was proposed.

Keywords: Photocatalytic, degradation , SnS<sub>2</sub>, ciprofloxacin , UV irradiation.

## **Sun Light Driven Photocatalysis for Degradation of Levofloxacin Drug using CdS Catalyst: An Investigation of Reaction Kinetics and Intermediates**

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Large amounts of antibiotics, notably fluoroquinolones, tetracyclines, sulfonamides and macrolides are applied in both human and veterinary medicine worldwide. However, as much as 30 – 90% of administered antibiotics can enter the environment via excretion because they are not fully metabolized in the body. Levofloxacin is a synthetic antibacterial which has broad spectrum activity against various bacteria. It usually escapes intact from conventional treatment plants, and consequently gets into the environment. In this study, Cadmium sulfide nanoparticles (CdS) were prepared for photocatalytically degrade the antibiotic levofloxacin in aqueous solution using sunlight irradiation. Approximately 70% degradation of the drug solution was achieved in 60 min. The kinetic studies showed that photocatalytic degradation of levofloxacin follows first order reaction kinetic model. Effective parameters such as pH, photo catalyst dose and contact time were optimized and well investigated. Furthermore, the identification of levofloxacin intermediates during photo catalytic degradation were analyzed using high performance liquid chromatography and tandem mass spectrometry (HPLC-MS/MS) and the reaction pathway based on them is proposed d discussed.

Keywords: Sun Light, Photocatalysis, Degradation ,Levofloxacin drug, CdS catalyst, kinetics, intermediates

## **Photocatalytic Degradation of Levofloxacin in Aqueous Solution by ZnCdS Catalyst under Sunlight Radiation**

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Antibiotics belong to the class of pharmaceuticals whose consumption has increased considerably over the years. Between 2000 and 2010, consumption of antibiotic drugs increased by 40% - from 50 million standard units to 70 million standard units. Their presence in wastewater is an imperative issue and has been acquiring increasing interest because of unidentified environmental effects and probable damage to aquatic life. Levofloxacin is a synthetic antibacterial which has broad spectrum activity against various bacteria. It usually escapes intact from conventional treatment plants, and consequently gets into the environment. In this study, three zinc cadmium sulfide (ZnCdS) were prepared -  $Zn_{0.2}Cd_{0.8}S$ ,  $Zn_{0.5}Cd_{0.5}S$  and  $Zn_{0.8}Cd_{0.2}S$  - to photocatalytically degrade the antibiotic levofloxacin in aqueous solution using sunlight irradiation. Approximately 80% degradation of the drug solution was achieved in 60 min. The kinetic studies showed that photo degradation of levofloxacin follows first order reaction kinetic model. Effective parameters such as pH, photo catalyst dose and contact time were optimized and well investigated. Furthermore, the identification of levofloxacin intermediates during photocatalytic degradation was analyzed using high performance liquid chromatography and tandem mass spectrometry (HPLC-MS/MS) and the reaction pathway based on them was proposed.

Keywords: Photocatalytic, degradation, Levofloxacin, ZnCdS catalyst, Sunlight radiation

## **Chemical Modification of Activated Carbon with 1,10-phenanthroline-5-amine and its Application for Solid Phase Extraction of Trace Elements from Groundwater**

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Post synthesis chemical modification is a versatile approach for the production of materials with desirable functionalities. It has been used widely to fabricate chelating resins; the most preferable materials for solid phase extraction (SPE) materials for trace metals. In this work, a straightforward chemical modification process for the attachment of 1,10-phenanthroline-5-amine onto activated carbon has been reported. The successfulness of the synthesizes procedure was confirmed using ATRIR and XPS. The efficiency of the synthesised resin as SPE materials for sample preparation of trace metals was established by its application to pack standard SPE cartridges for SPE vacuumed manifold. At optimized conditions, the resin capacity exchange Zn, Cd, Ni, Mn and pb ions, were 0.303, 0.181, 0.302, 0.355 and 0.089 mmol/g receptively. The chelating resin was tested for matrix elimination prior to the determination of these metals by ICP-MS. The resin-SPE cartridge, was demonstrated a potential applicability for the analysis of Zn, Cd, Ni, Mn and pb in groundwater reference materials and real samples from several locations in Almedinah Almunwarah, Saudi Arabia.

Keywords: Chelating resin, Activated Carbon, 1,10-phenanthroline-5-amine, solid phase extraction, groundwater, and matrix elimination

## **Redox-Tunable Polycationic Polymers for Environmental Applications**

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Toxic pollutants released by industry and nuclear waste from power plants pose a serious risk to the environment.[1] Therefore, it is essential to develop efficient materials that are able to remove toxic compounds rapidly from the polluted sources. While materials such as activated carbon have been reported as very effective dye and iodine sorbents, their use is limited by their high cost,[2] so cheaper and equally efficient sorbents need to be designed. Here, we present the design, synthesis and characterization of a series of polycationic 4,4'-bipyridine (viologen)-containing covalent organic polymers (COPs), which we tested for their ability to remove toxic dyes and iodine capture. These materials were synthesized by either the Menshutkin[3] or the Zincke[4] reactions. The viologen units of one of the COPs were reduced to evaluate the effect of overall charge on the dye adsorption abilities. We found that the polymer's preference for the adsorption of hydrophobic and hydrophilic toxic organic dyes can be altered by changing the redox state of the viologen units: polycationic COPs showed a higher affinity for hydrophilic dyes such as fluorescein whereas reduced (neutral) COPs had a preference for hydrophobic dyes such as Nile red. In particular, the rate of fluorescein adsorption by the polycationic COP was one of the fastest reported till date. The remaining polymers in the series were used for solid and solution state iodine capture. We found that by changing the central core unit of the 4,4'-bipyridinium-linked COPs distinct morphologies can be obtained, and these show different affinities for iodine capture. For example, pyrene- and alkyne bond-containing COPs were the most effective in removing iodine from solution as 100% was removed in ten minutes, which can be attributed to the presence of the triple bonds and phenyl rings. In solid state, however, the triazine-containing COP proved to be the most promising as it adsorbed 200% of its weight in iodine over the course of 22 hours. We trust that in the future, the development of polycationic COPs with tunable redox states will result in even more versatile materials with customized ability to adsorb several classes of pollutants.

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Keywords: Polycationic polymers, viologen, dye adsorption, iodine capture

## **Production of Anti-Corrosion Material from Lignocelluloses Waste of Palm Tree**

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The main idea of this project is to solve two current problems with simple and useful solution that benefit both environment and industrial field equally. In our country we are blessed with a huge number of date palms tree (*Phoenix dactylifera* L.) Since our ancestors start living in this welfare land and the uses of the palms tree varies in different shapes such as nourishment, building and daily tools. Given that the increase of using palm tree multiplied, which leads in increasing in palm treeswaste. Date palm tree produces approximately 20 kg of waste leaves annually. UAE has over 40 million date palm tree. Most components included in date palm tree wastes are lignin, cellulose and hemicelluloses. On the other hand, corrosion plays a very important role in diverse fields of industry and, consequently, in economics. In the present work, we studied the potential of date palm waste as an anti-corrosion material from the extracted lignin after converting it to lignosulphonate. First, the chemical composition of the waste was studied to find the best extracting method of lignin. Then two main methods were selected for the laboratory work. The extracted lignin was converted to sodium lignosulphonate. This product was used in the corrosion test. Preliminary results are very promising. These preliminary results will allow focusing on the potential of having a lignosulphonate as replacement of the current technology used in the marine environment. A commercial scale plant process was also designed.

Plant extracts can serve as non-toxic and cost-effective corrosion inhibitors to prevent the corrosion before happening in the surface of ship body and most type of pipe line and storage tanks in industrial field. Using this product can be enough to reduce corrosion effect before it accrue in the surface of the steels which save money from the maintenance cost until the next coat. Moreover using an organic solution is more efficient to the environment to save our plant from harm chemicals.

Keywords: non-toxic corrosion inhibitors



## **Breaking Hearts: Indirect Evidence for Cholesterol Crystallization as Possible Cause of Cardiac Arrest**

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Heart disease is the leading causes of death around the world and research into its origins and prevention are immediately valuable to hundreds of millions of people. What occurs during a heart is well documented and known; a coronary artery becomes blocked, blood flow to the heart stops and this is followed by cardiac arrest. However, the source of the initial blockage, and what ultimately causes the heart attack remains a point of discussion. One theory is that cholesterol found in the plaques in arteries reaches a critical concentration, crystallize and the resulting sharp needle-like crystals puncture the plaque and spur the subsequent blockage . Previous studies have demonstrated that cholesterol expands during crystallization and the sharp-needle crystals that were formed were able to puncture a heart membrane tissue. Additionally, ex-vivo studies on humans have found crystals of cholesterol in the arteries of people who experienced cardiac arrest. In this study we aimed to elucidate the mechanism of plaque rapture by simulating the crystallization conditions of cholesterol in the plaque and reproducing the formation of acicular cholesterol crystals in vivo using various non-polar solvents and natural oils. Crystals of a cholesterol hydrate were grown from octanol, Thermal and mechanical analysis on cholesterol crystals were also performed and the crystals were found to puncture through the lamb heart pericardium with forces ranging from 1 to 11 MPa. The result confirms that hydrated cholesterol crystals are sufficiently rigid to cause the infarction.

Keywords: cholesterol monohydrate

## **New Series of Guanidine/NTA Ternary Complexes as Antimicrobial and Antiproliferative Agents as well as Novel Approach to the Synthesis of their Nanosized Analogues**

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Development of novel mixed ligands metal complexes is a major goal in material science due to their chemical, biological, environmental and catalytic importance. For instance, the stability of these complexes plays an important role in many metabolic and toxicological functions. In this work, we introduce a new family of mixed ligand transition metal complexes, M (II & III) sulfate, with nitrilotriacetic acid as a primary ligand and guanidine as a secondary ligand. The new complexes were prepared in bulk and nanosized structures. Controlling the structure of these complexes has been achieved using different capping agents (CTAB or PVA). The sizes of the nanocomplexes have been confirmed using transmission electron microscope (TEM) and were found to be in the range of 2-15 nm diameter. This methodology considers a novel approach of preparing nano ternary complexes. All complexes displayed octahedral structure with the formation of polymeric chains due to the presence of the sulfate bridged ligand. The biological activity of these complexes as well as their tumor inhibitory activity has also been examined.

**Keywords:** Ternary mixed ligand complexes, nitrilotriacetic acid, guanidine , nanosized metal complexes, coordination polymer, antimicrobial activity, antitumor Activity.

## **Stress Distribution Analysis in the Dental Implants**

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This study is interested in mechanics of a dental prosthesis subjected to dynamic loads masticatory behavior. It relates to a three-dimensional analysis by the finite element method, the level of the distribution of equivalent stresses induced in the bone between the implants (depending on the number of implants). The studied structure composed of a dejection, implant and mandibular bone is subjected to dynamic loading of variable amplitude in the three directions coronal, apical, mesial and distal-bucco-lingual. These efforts those simulate of mastication. We show that compared to the implementation of a single implant, implantology using two implants promotes the embrittlement of the bone. This embrittlement is all the more likely that the implants are located the vicinity in close one another.

Keywords: Implant, stress, abutment, dynamic, effort, prosthesis, dental, distribution, level, bone

## **Improved Resistance to Cracking of a Cement Mortar through the Incorporation of Crumb Rubber**

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Within a context of sustainable development, innovative processes for various application to recycles rubber are put in place to make aggregates or crumb rubber. These uses include sports floor coverings, to manufacture of sealants, sound absorbing walls, to make roads, as an alternative fuel in cement kilns, etc. In this study, the addition of crumb rubber to mortar was investigated through optical and mechanical tests. The results showed that the incorporation of crumb rubber from used tires into mortar produced a better resistance to shrinkage cracking, but a compressive strength/ tensile is reduced. This feature could lend itself to making play-grounds and sports grounds more absorbing and flexible, which would allow a more significant fall to be withstood without injury and consequently enhance the safety of playgrounds.

Keywords: Resistance, Cracking, Cement mortar, Crumb rubber

# **Mechanical Properties of Concrete-Reinforced Fibres and Powders with Crushed Thermoset Composites: The Influence of Fibre/Matrix Interaction**

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This work focuses firstly on the formulation and mechanical behavior of concrete reinforced fiber and powder (CRFP). Secondly, we present the effect of silane treatment on the bond characteristics of the fiber–matrix of ultra-high-performance concrete (UHPC). The initial objective of the study was to optimize the incorporation of fibers and powders in high performance concrete (HPC). Two materials were investigated. The first involved replacing a volume of sand by an equivalent volume of fibers and powders. The second type was obtained by replacing an equivalent volume of silica fume with powders. Testing of the first material showed that the incorporation of fibers and powders by sand substitution increased the bending and tensile strength by 32%. In the second material, the substitution of silica fume by the powder led to an increase of 37% in flexural and tensile strengths.

The second section of this paper focuses on silane-treated fibres. The experimental results on fiber pullout tests under different conditions are reported. Various silane treatment contents ranging from 0% to 1% were studied. Fiber pullout tests were conducted to measure the bond characteristics of fibers in the UHPC matrix. The treatment by vinyl trimethoxy silane (VTMO) can effectively enhance the fiber–matrix interfacial properties, especially the fiber pullout energy. It was concluded that in terms of the bond characteristics, the optimal silane content is 0.5% under these conditions. Thermoset composite materials are used in a wide range of applications in industries such as the automotive sector and construction.

Fiber-reinforced concrete provides advantages such as lightness, less frequent repair, and improved ductility and uniaxial tensile strength . In Europe, approximately 1 million tonnes of polymer composites are produced each year, and most are glass-fiber-reinforced unsaturated polyester. Although there are many successful uses for thermoset composite materials, recycling at the end of the life cycle is a difficult issue.

Today, more than 90% of production waste thermoset composites currently end up in landfills, at a high cost and with the increasing threat regulatory prohibition. To ensure the sustainability of the polymer composite industry, alternatives to the land filling of production waste should be quickly identified. A great number of recycling technologies have been proposed and developed for thermoset composite materials, and these are summarized. There are mainly two process categories: (1) Those involving mechanical comminution techniques to reduce the size of the

scrap to produce recyclates, and (2) those using thermal processes to break the scrap down into materials and energy. Each will be studied. The incineration process, which is currently the most used, will not be feasible in the near future. Indeed, a recent EU Directive on Landfill of Waste (Directive 99/31/EC) will result in a reduction in the amount of organic material that is landfilled.

Keywords: UHPC; UHPFRC; Thermoset composite; Waste recycling ;Ductility; Interfacial transition zone.

## **The Effect of Calcined Muds on the Properties of Self-Compacting Concrete in Spawning and Hardened state**

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In recent years the use of self-compacting concrete in the area of construction is gradually increasing, in parallel scientific research about this concrete seeks to improve this concrete and use addition in this concrete and study its behavior.

The mineralogical composition of the muds makes it possible to consider the transformation of the stable argillaceous structures to amorphous structures. This transformation giving it the pozzolanic reactivity desired for the proposed substitution. Knowing that the performance due to pozzolanic properties gradually acquire over time. The substitution of a certain quantity of mud calcined (with pouzzolanique character). The substitution of a certain quantity of vase calcined (in pozzolanic matter) with the Portland cement whose hydration releases from lime (salt of Candlot), would make it possible to obtain binders with almost similar characteristics that those of Portland cement alone. While saving the same quantity of cement. Indeed released lime will be fixed by added pozzolana.

This research consists to valuing the mud resulting from dredging of dams in self-compacting concrete and even its effect on the physico-mechanical properties in fresh and hardened state of the self-compacting concrete. Seven formulations were studied: a control concrete without substitution of the mud, six with substitution of 10, 15 and 20% of the muds of two dams, the tests to the state abrasion and hardened were carried out on these concretes to determine their physico-mechanical properties.

According to this study we find that the results obtained show that the self-compacting concrete bases of the treated muds have good properties in the fresh state, it was noted that the mechanical compressive strength and tensile strength are acceptable for concrete especially with addition of mud which has a lower resistance loss of 2% for addition of 10% of the mudsl to 90 days.

Keywords: Calcined mud, pozzolanic reactivity, self-compacting concrete, physico-mechanical properties

## **Strengthening of Metallic Structures using Composite Materials**

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A reinforcing technique developed in recent years, using the bonding and composite materials. Strengthening based composites can be more competitive in practice than conventional methods, thanks to the simplicity of the implementation, this limits the operating interruptions, often determining factor. The ease of implementation comes from the fact that the reinforcement is simply glued onto the structure to be repaired or reinforced. The buckling is generally the mode of destruction of metal hulls structures, thin or thick. These structures are very sensitive to any imperfection of form (initial geometrical defects). The sizing is usually based on knowledge of the actual initial state of structures. Strengthening connections with the collage technique improves the strength, keeping in shape and maintain the potential charge and performance of metallic structures. The analyzes of the behavior of composite materials on the reinforcement by bonding improve the life of the structures. Thanks to the calculation by the finite element method, we get to have results that prove necessary in order to use these materials to their full potential.

Keywords: adhesive bond, adhesion, modeling, composite materials, cylindrical shells



## **Effect of Various Concentration of Zinc Monoxyde on Duckweed (*Lemna giba*)**

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This study aims to highlight the efficiency of use of biological processes to remove industrial pollutants that contaminate the biogeochemical cycle of natural substances, and those to reduce the level of pollution in the air, the water or soil. The present study aimed to investigate the effects of different concentrations of zinc oxide on fresh duckweed (*Lemna giba*.) Over a period of 15 days. High bioaccumulation of zinc oxide has been accompanied by an increase in fresh weight in treatment of metals. Thus an increase in the rate of increase. Metabolically, zinc oxide causes a significant increase of the mean levels of proline and soluble sugars as inhibition of chlorophyll synthesis.

Keywords: *Lemna giba*; ZnO; PF; DNF; protein; proline; chlorophyll

## **Selective and Sensitive Hydrazine Sensor based on SrO.CNT Nanocomposites for Environmental Safety**

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Nanocomposite of Strontium oxide nanoparticle decorated on carbon nanotube (SrO.CNT NCs) was synthesized in basic medium by wet-chemical method. The SrO.CNT NCs were characterized using FT-IR, UV/Vis., FESEM, XEDS, XPS, and XRD techniques. A selective hydrazine sensor onto glassy carbon electrode (GCE:  $0.0316 \text{ cm}^2$ ) was fabricated with a thin-layer of NCs. Enhanced electrochemical responses, higher sensitivity, large dynamic range, and long-term stability towards hydrazine were achieved using the fabricated chemical sensor. The calibration curve was found linear over a wide range of hydrazine concentration ( $0.2 \text{ nM} \sim 0.2 \text{ M}$ ). The detection limit and sensitivity were calculated as  $0.036 \text{ nM}$  and  $\sim 26.37 \mu\text{AmM}^{-1}\text{cm}^{-2}$ , respectively. It is the first time to report that hydrazine was determined by current vs voltage (I-V) technique using SrO.CNT NCs modified GCE electrode with very high sensitivity compared to various nanomaterials. It is also commenced a potential sensitive hydrazine sensor development using SrO.CNT NCs by a facile and reliable I-V technique for the prospective application for hazardous compounds in environmental remediation.

Keywords: SrO.CNT NCs; Electrochemical characterization; Fabrication; Sensitivity; Hydrazine; I-V technique; Environmental safety.

## **Electrochemical Detection of L-Dopa using Crude Polyphenol Oxidase Enzyme Immobilized on Electrochemically Reduced RGO-Ag Nanocomposite Modified Graphite Electrode**

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In the present work, we report the selective and sensitive electrochemical detection of L-DOPA using crude Polyphenol oxidase enzyme (PPO) immobilized on electrochemically reduced graphene oxide – silver nanoparticles (RGO-Ag) nano composite modified graphite (Gr) electrode. The modified Gr electrode is first prepared by electrochemical reduction of graphene oxide - silver (GO-Ag) nano composite to RGO-Ag nano composite onto graphite rod. The crude PPO extracted from apple fruit is later used for the immobilization on modified Gr electrode. Modification of Gr electrode at each step is confirmed by cyclic voltammetry (CV) and Electrochemical impedance (EIS) techniques. The surface characterization of modified electrode is performed by Scanning electron microscopy (SEM). The modified electrode exhibited excellent electro catalytic activity towards the detection of L-Dopa in the concentration range of 10 to 140  $\mu$ M with low detection limit and high sensitivity. Further, the practical applicability of the developed biosensor is examined for the detection of L-Dopa in real samples. The study conclude that the RGO – Ag nano composite modified Gr provide excellent matrix platform for the detection of L-DOPA.

Keywords: Bio sensor, L-DOPA, reduced graphene oxide, silver nanoparticles, nanocomposite

## **Biosensor Based on Polyphenol Oxidase and Biosynthesized Silver Nanoparticles for the Detection of Catechol in Green Tea Samples**

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Crude extract of polyphenol oxidase (PPO) is obtained using Manilkara Zapota (sapota) fruit and immobilized on biosynthesized silver nanoparticles (AgNPs) with polypyrrole (PPy) as fabricating material. The morphology of developed Gr/PPy/AgNPs/PPO electrode is characterized by scanning electron microscopy. The electrochemical performance of the developed electrode were evaluated using cyclic voltammetry, differential pulse voltammetry. Under neutral pH and at room temperature, the developed Gr/PPy/AgNPs/PPO biosensor showed excellent electrocatalytic activity towards the detection of catechol. Further it is used for the determination of catechol in the concentration range of 0.001 to 0.015 mM with low detection limit and high sensitivity. The practical applicability of the PPO biosensor for the analysis of catechol in green tea sample is examined. The response of the biosensor is found to be uninfluenced by some common interferences and also it showed good stability and repeatability.

Keywords: Bio sensor, bio synthesis, silver nanoparticles, catechol

## **Highly Efficient Co<sup>2+</sup> Ions Sensor based on N,N'-(ethane-1,2-diyl)bis(2,5-dimethoxybenzenesulfonamide) (EBDMBS) Fabricated Glassy Carbon Electrode**

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Two bis-sulfonamides, N,N'-(ethane-1,2-diyl)bis(2,5-dimethoxybenzenesulfonamide) (EBDMBS) and N,N'-(ethane-1,2-diyl)bis(2-methoxy-5-bromobenzenesulfonamide) (EBMBBS) were synthesized to study their applications as heavy metal sensors. These molecules were prepared via very environment friendly methodology using diaminoethane and respective sulfonyl chlorides as reactants. Aromatic rings were ornamented with electron donating and withdrawing groups for comparison studies and to choose a best ligand for sensor preparation. The synthesized molecules were well characterized using UV/VIS, IR and NMR (<sup>1</sup>H and <sup>13</sup>C) spectroscopic techniques. Finally, single crystal X-Ray diffraction studies prove the structures of our designed molecules. For the selective and sensitive potential sensor application, EBDMBS and EBMBBS were fabricated onto glassy carbon electrode (GCE) with conducting nafion binders to develop a Co<sup>2+</sup> ions sensor in phosphate buffer phase. The fabricated ionic-sensor with EBDMBS/GCE is exhibited higher sensitivity, large-dynamic concentration ranges, long-term stability, and improved electrochemical performances towards cobalt ions. The calibration plot is linear ( $r^2 = 0.9891$ ) over the large Co<sup>2+</sup> concentration ranges (0.35 nM to 3.5 mM). The sensitivity and detection limit is  $\sim 1.87 \mu\text{A}\mu\text{M}^{-1}\text{cm}^{-2}$  and  $\sim 0.17 \text{ nM}$  (signal-to-noise ratio, at a SNR of 3) respectively. This novel effort is initiated a well-organize way of efficient cationic sensor development for toxic pollutants in environmental and health-care fields in large scales.

Keywords: Sulphonamide; EBDMBS; Co<sup>2+</sup> ions; I-V method; Glassy carbon electrode; Sensitivity

## Self-healing Molecular Crystals

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There has been an exponential growth in the interest in self-healing materials over the past 15 years. The materials are robust, flexible and of course, visually impressive. However, interest in this exciting area of research has remained mostly within the soft materials community and has not been explored by solid-state organic chemists. With recent advancements in the understanding of molecular migration in solids and the apparent boon of discoveries of crystals that are able to bend, twist, curl, jump, flip or spiral, solid-state chemistry research has become much more dynamic. With the latest insights into solid-state reactivity we believe it is possible extend the self-healing phenomenon towards molecular crystals.

Here we present our finding towards the first self-healing molecular crystal. Singles crystals of dipyrazolethiuram disulfide are synthesized, grown and its self-healing properties were measured using a modified tensile tester and the material is found to display 6.7% healing. The physical characteristics of the self-healed material was investigated using scanning electron microscopy, confocal fluorescence microscopy and computerized tomography scanning. The three forms of imaging show there was a degree of healing across the cracked region on both the surface and on the interior.

The self-healing event is postulated to occur by a S-S bond shuffling between the two separated halves, as commonly shown in self-healing polymers. This mechanism was rationalized by the close contacts found in the X-ray crystal structure and the electron spin resonance data showing the presence of a R—S· radical under the same conditions as the healing. Additionally, we demonstrate there was molecular migration at the surface of the crystal, which is necessary for healing, using atomic force microscopy and the features dissipated at a rate of 9.4 nm/h.

Keywords: Smart Materials, Crystal Engineering, Self-healing

## **Mechanically Robust, Chemically Inert Ultrahydrophobic Charcoal Surfaces**

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Small-scale superhydrophobic surfaces are accessible via microfabrication techniques and chemical modification, however impediments such as poor scalability and high production costs are prohibitive to large-scale preparation of self-cleaning materials by using these approaches. Here we report a fast-forward and cost-effective strategy to preparation of superhydrophobic composites where a double-sided adhesive tape is paved with charcoal particles. These surfaces are ultrahydrophobic, and have static contact angles with water of  $176.9 \pm 3.4^\circ$  and sliding angle of  $4 \pm 1^\circ$ . The composites are mechanically robust, durable, and resistant to strong chemical agents. The remarkable hydrophobicity is of Cassie-Baxter type, and is attained by a combination of water floating over air bags trapped between the charcoal particles and repulsive interactions with the hydrophobic carbonaceous surface. This inexpensive approach that uses only commonly available materials is scalable and meets the requirements for a variety of practical applications.

Keywords: superhydrophobic surfaces, charcoal particles

## **Preparation and Characterization of Activated Carbon Supported Nano-Bimetallic Composite Catalyst (ANBCC-AC/Cu<sub>2</sub>O/ZnO) for Catalytic Ozonation of Environmental Pollutants**

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The physicochemical properties, nature, and morphology of composite materials involving activated carbon, nano copper oxide, nano zinc oxide, Activated carbon supported Nano-Bimetallic Composite Catalyst (ANBCC) were investigated and compared. Nature and morphology of ANBCC were carried out by using SEM, XRD, FTIR, BET surface area analyzer, DLS particle size analyzer and UV-VIS Spectroscopy. Since Heterogeneous catalytic ozonation using metallic catalyst had gained much attention in these days, the presence of metal oxides on activated carbon surface confidently contributed to catalytic activity of ozonation of environmental pollutants. The sole idea of this study to explore the uses of ANBCC for heterogeneous catalytic ozonation.

Keywords: Nano-Bimetallic Composite Catalyst, nano copper dioxide nano zinc oxide, Activated carbon, Catalytic ozonation



## **Removal of Cr(IV) from Polluted Water Using Carbon Nanofibers and Activated Carbon Prepared from Low Cost Resources**

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Activated carbon and Carbon Nanofibers (CNFs) were prepared from low cost precursors. Activated carbon was prepared from agricultural biomass date palm leaves and stones by chemical activation using different chemical reagents. The chemical reagents used for activation were boric acid, urea, thiourea and sodium phosphate. Also, CNFs were prepared from a mixture of poly(ethylene terephthalate) (PET) waste and lignin. The mixture was dissolved in trifluoroacetic acid. The fibers were prepared from the PET and lignin solution by electrospinning and then, they were carbonized at 1000 °C in nitrogen atmosphere for 5 hours. The Chromium (IV) adsorption capacity of the produced activated carbon and of CNFs were measured. The highest adsorption capacity was obtained with CNFs and activated carbon treated by boric acid (AC-BAA). The measured adsorption capacity was found to be 48 mg/g and 56 mg/g for CNFs and AC-BAA, respectively. The effect of pH, chromium ion concentration, adsorbent quantity, time, and temperature on the adsorption of chromium were investigated.

The results show that the adsorption of chromium is higher at pH lower than 5. The adsorption capacity increases with increasing initial chromium concentration and also increases with increasing temperature. Complete characterization of the prepared activated carbon and CNFs will be carried out using chemical and spectroscopic analyses.

Keywords: Activated Carbon, Carbon nanofibers, Cr(IV), Water purification, Adsorption.

## **Growth and Characterization of Zinc (tris) Thiourea Sulphate (ZTS) Crystals**

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Zinc (tris) Thiourea Sulphate (ZTS) crystals demonstrate nonlinear optical properties like second and third harmonic generation efficiency of pump Nd: YAG LASER. To obtain crystals, slow solvent evaporation method has been used, in which the starting compounds were zinc sulphate and thiourea in molar ratio of 1:3 and stirred well for homogeneity. The supersaturated solution was allowed to evaporate in a controlled manner at room temperature, which yielded ZTS crystals after almost 25 days. The crystals were transparent and colourless with maximum dimension of 10 mm x 9 mm. The powder XRD study indicated orthorhombic structure with unit cell parameters as;  $a=11.1260 \text{ \AA}$ ,  $b=7.7730 \text{ \AA}$  and  $c= 15.4910 \text{ \AA}$  with space group Pca21 and Space group number 29. The FTIR spectrum was recorded in the range of  $400 \text{ cm}^{-1}$  to  $4000 \text{ cm}^{-1}$  in KBr medium. The presences of various functional groups were identified during the analysis of the FTIR spectrum.

Key words: Crystals, Non-linear Optical, Slow solvent evaporation method, Powder XRD, FTIR

## **Functionalized Graphene Nanocomposites with Steroidal Diamine Dimers**

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The functionalization of pristine graphene sheets with organic functional groups has been developed for several purposes. The main purpose is the dispersion of graphene sheets in organic solvents that is a crucial move toward the formation of nanocomposite materials with graphene. In this work, the obtained chemically reduced graphene sheets (RGO) were activated using thionyl dichloride (SOCl<sub>2</sub>) to obtain a graphene derivative that contained acyl chloride groups. These acyl chloride groups reacted with the amine groups of steroidal diamine to form amide groups that anchored steroidal dimine dimer nanofibers onto the graphene sheets. Several steroidal diamine dimers were used and compared with typical diamine. These nanocomposites were characterized using atomic force microscopy (AFM) images, UV-vis spectra, scanning electron microscopy (SEM), Fourier transform infrared (FT-IR) spectra and XRD.

Keywords: graphene, steroidal, nanocomposites, diamine

**Poster Session II**  
*Al Hamra Convention Center*  
**Monday, February 20, 2017 18:30-20:30**

## **II.1 Platform Strategy by Uniting Solar, Thermal, Vibrational and Wind Energy with Maximum Power Point Tracking System**

**Zia Hameed, Adnan Yousaf, and Muhammad Rafay Khan Sial**

Department of Electrical Engineering, Superior University, Lahore, Pakistan

## **II.2 The Race of Phase Change Memory Materials: The Role of Capacitance-Voltage Behavior**

**R. T. Ananth Kumar, Saleh T. Mahmoud, and Naser N. Qamhieh**

Department of Physics, UAE University, Al-Ain, United Arab Emirates

## **II.3 Photochromism of Dihydroazulenes: Investigating the Reaction Mechanism and Thermodynamic Properties in Solid State**

**Ieva Liepuoniute, Patrick Commins, and Panče Naumov**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates

## **II.4 Light Trapping Mechanisms in Nanostructured Thin Film Photovoltaic Devices**

**Jagdish A.K, Sibimol Luke, Kavita Garg, Praveen C Ramamurthy, D Roy Mahapatra, and Gopalkrishna Hegde**

Center for Nano Science and Engineering, Indian Institute of Science, Bangalore, India

## **II.5 Solution Based Fabrication of a Fast Response, Broad-Band, Large Area Photodetector**

**B. Bharath, K. D. M. Rao, K. N. Harish, and G. U. Kulkarni**

Department of Chemistry & Physics of Materials Unit

Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India

## **II.6 Carbon Dioxide Capture at Ambient Conditions by Some Primary Amines**

**Ranganathan Sathishkumar and Munirathinam Nethaji**

Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India

## **II.7 Adenine-functionalized Spongy Graphene for Green and High-Performance Supercapacitors**

**Dalia M. El-Gendy, Nabil A. Abdel Ghany, E. E. Foad El-Sherbini, and Nageh K. Allam**  
Department of Physical Chemistry, The American University in Cairo and  
National Research Centre, Cairo, Egypt

## **II.8 Catalytic Pyrolysis of Plastic Waste with Natural Zeolite**

**R Miandad, M. A. Barakat, Asad S. Aburiazaiza, M. Rehan, I. M. I. Ismail,  
and A. S. Nizami**  
Department of Environmental Sciences  
King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

## **II.9 Boron-Modified Silicon Oxycarbide/Graphene Composite Paper Electrode for Electrochemical Energy Storage**

**Monsuru A. Abass, Muhamed S. Kolathodi, and Gurpreet Singh**  
Department of Mechanical and Nuclear Engineering  
Kansas State University, Manhattan, Kansas, United States of America

## **II.10 Sulfur Polymers for Stable Lithium–Sulfur Batteries**

**Molleigh Preefer, Bernd Oschmann, and Ram Seshadri**  
Department of Chemistry  
University of California Santa Barbara, Santa Barbara, California, United States of America

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**Gourav Tarafdar, Sanchita Sengupta, Upendra Kumar Pandey,  
and Prvaeen C Ramamurthy**  
Interdisciplinary Center for Energy Research, Indian Institute of Science, Bangalore, India

## **II.12 Effectiveness of Bioelectricity Generation from Urine and Its Treatment by Microbial Fuel Cell Using Graphite Electrodes**

**Hanish Mohammed C. H. and M. Muthukumar**  
Department of Environmental Sciences, Bharathiar University, Coimbatore, India

## **II.13 Design and Synthesis of New Thieno[3,4-c]pyrrole-4,6-dione based D-A Type Low Band Gap Conjugated Polymers Having Different $\pi$ -Conjugated Spacers for Organic Photovoltaics**

**Murali M. G., Chandrashekara G. K., Arun D Rao, and Praveen C Ramamurthy**  
Department of Materials Engineering, Indian Institute of Science, Bangalore, India

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**Nagwa Ibrahim**

Department of Physics, Majmaah University, Zulfi, Kingdom of Saudi Arabia

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**Nouf Al-Shaikh, and Eman Ismail**

Department of Chemistry, Taibah University, Medina, Kingdom of Saudi Arabia

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**Nathir A. F. Al-Rawashdeh, Borhan Al Biss, and Moath Yousef**

Department of Chemistry, Jordan University of Science & Technology, Irbid, Jordan

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**Arsalan Haider, Tamara Dewi Jasmine, and Muhammad Anus Hashmi**

Department of Electrical Engineering, Superior College, SU campus, Lahore, Pakistan

## **II.18 Synthesis and Properties of Bi-based Hybrid Double Perovskites for Photovoltaic Applications**

**Fengxia Wei, Zeyu Deng, Shijing Sun, Paul D. Bristowe, and Anthony K. Cheetham**

Department of Materials Science and Metallurgy  
University of Cambridge, Cambridge, United Kingdom

## **II.19 Deciphering the Mechanism of Phase Separation in Organic Photovoltaics**

**Fiyanshu Kaka, Praveen C Ramamurthy, and Abhik Choudhury**

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

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**Yue Wu, Hamish H.-M. Yeung, Richard I. Walton, Dermot O'Hare,  
and Anthony K. Cheetham**

Department of Materials Science & Metallurgy  
University of Cambridge, Cambridge, United Kingdom

## **II.21 Industrial Waste Fly Ash Cenosphere Based Lightweight Microwave Absorber**

**Pritom J. Bora, Mayuri Porwal, K. J. Vinoy, and Praveen C. Ramamurthy**

Interdisciplinary Centre for Energy Research (ICER), Department of Materials Engineering, and  
Department of Electrical and Communication Engineering  
Indian Institute of Science, Bangalore, India

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**Zeeshan Ahmad, Vartika Varshney, and J. P. Tegar**

Department of Civil and Environmental Engineering  
National Institute of Technical Teachers Training and Research, Bhopal, India

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**Sammy Shaker, Stephen Rudisill, and Andreas Stein**

Department of Chemistry  
University of Minnesota-Twin Cities, Minneapolis, Minnesota, United States of America



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**Tholkappian Ramachandran and Fathalla Hamed**

Department of Physics, UAE University, Al Ain, United Arab Emirates

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**Ameen Sadek, Basem AbdelAziz, Sannan Ahmed, Tameem Salah, Khadija Said, and Naser Qamhih**

Department of Physics, UAE University, Al Ain, United Arab Emirates

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**Ashish Tanna and Hiren Joshi**

Department of Physics, School of Science, RK University, Rajkot, India

## **II.27 Antibacterial Activity of Metal Nanoparticles (AgNO<sub>3</sub>, ZnO, CuO) Against Pathogenic Bacteria**

**Grara Nedjoud, Khaldi Fadila, Boumaza Awatif, Belhaoues Farah, and Maaizia Mabrouka**

Department of Biology, University 8 May 1945, Guelma, Algeria

## **II.28 Structural and Vibrational Properties of Bulk and Few-Layer Td-WTe<sub>2</sub>: A Combined Experimental and Theoretical Analysis**

**Manoj K. Jana<sup>†</sup>, Anjali Singh<sup>‡</sup>, Dattatray J. Late<sup>§</sup>, Catherine R. Rajamathi<sup>¶</sup>, Kanishka Biswas<sup>†</sup>, Claudia Felser<sup>¶</sup>, Umesh V. Waghmare<sup>‡</sup> and C. N. R. Rao<sup>†</sup>**

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<sup>§</sup>Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune, India

<sup>¶</sup>Max Planck Institute of Chemical Physics for Solids, Dresden, Germany

## **II.29 *Ab Initio* Statistical Mechanics of Martensitic Phase Transition in NiTi Shape Memory Alloy (SMA)**

**Pawan Kumar and Umesh V. Waghmare**

Theoretical Sciences Unit

Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

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**Suchitra, Caroline Mellot-Draznieks, Anthony K. Cheetham, and Umesh V. Waghmare**

Theoretical Sciences Unit

Jawaharlal Nehru Center for Advanced Scientific Research, Bengaluru, India

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**Xiaoping Han, Nouredine Amrane, and Maamar Benkraouda**

Department of Physics, UAE University, Al Ain, United Arab Emirates

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**Sharifa A. AlMutawa, Reem M. Mohamad, Ahmed Benkraouda, Ahmed A. Altelbani, Omar Benkraouda and N. Amrane**

Department of Physics, UAE University, Al Ain, United Arab Emirates

### **II.33 Structural, Electronic and Thermodynamic Properties of CeO<sub>2</sub> Compound: An *Ab Initio* Study**

**Hadj Baltach, Aicha Bendjdid, Mohammed El Amine Monir, Rabah Khenata, Tarik Ouahrani, and Djamel Rached**

Department of Physics, Mustapha Stambouli University, Mascara, Algeria

### **II.34 Laser Processing of Nano-Crystalline Copper Sulfide Thin Film Prepared by Spray Pyrolysis**

**F. A. Mahmoud, W. Magdy, A. S. Gadallah, Mahmoud Nasr, and I. Azzouz**

Department of Solid State Physics, National Research Center, Cairo, Egypt

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**Pratap Vishnoi, Archana Sampath, Umesh V. Waghmare, and C. N. R. Rao**

New Chemistry Unit, International Centre for Materials Science and Theoretical Sciences Unit,  
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

### **II.36 P-type Mg Doped CuCrO<sub>2</sub> Transparent Conducting Thin Layers**

**E. Chikoidze, M. Boshta, Hagar Mohamed, T. Tchelidze, D. Daraselvia, D. Japaridze, A. Shengelaya, Y. Dumont, Cijy Mathai, and M. Neumann-Spallart**

Department of Solid State Physics, National Research Centre, Cairo, Egypt

### **II.37 Preparation and Characterization of CeO<sub>2</sub>-based Binary Oxides with Divalent and Trivalent Transition Metal Ions by Microwave Process for CO-PROX Applications**

**A. Almutawa, A. F. Zedan, M. A. Baker, S. J. Hinder, M. Abi Jaoude, S. Y. AlQaradawi, and K. Polychronopoulou**

Department of Mechanical Engineering

Khalifa University of Science, Technology and Research, Abu Dhabi, United Arab Emirates

### **II.38 Adsorption of CO<sub>2</sub> on Fe-doped Graphene Nano-Ribbons: Investigation of Transport Properties**

**Wael Othman<sup>†</sup>, Mayar Fahed<sup>†</sup>, Saifeddine Hatim<sup>‡</sup>, Abdullah Sherazi<sup>§</sup>, Golibjon Berdiyev<sup>¶</sup>, and Nacir Tit<sup>†</sup>**

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<sup>§</sup>Department of Mechanical Engineering, UAE University, Al Ain, United Arab Emirates

<sup>¶</sup>QEERI, Hamad bin Khalifa University, Qatar Foundation, Doha, Qatar

### **II.39 Synthesis and Characterization of Mg<sub>1-x</sub>Mn<sub>x</sub>CuP**

**Pascal Lerner, Dennis Henge, and Barbara Albert**

Eduard-Zintl-Institute of Inorganic and Physical Chemistry

Technische Universität Darmstadt, Darmstadt, Germany

## **II.40 Effect of Supercritical Fluid Extraction on the Adsorption Capacity of Date Pits Powder for Lead Removal**

**Haliemeh Sweidan, Naeema Al Darmaki, Yaser Greish, and Ali Al Marzouqi**

Department of Chemical Engineering, UAE University, Al Ain, United Arab Emirates

## **Platform Strategy by Uniting Solar, Thermal, Vibrational and Wind Energy with Maximum Power Point Tracking System**

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This paper presents the power generation through multiple sources where maximum power point tracking system is used to achieve maximum efficiency. The dynamic and static performance is theoretically analyzed and design criteria are provided. DC current is used as a disturbing variable for WECS in MPPT algorithms due to the help of changing in dc voltage the change in wind speed is detected. By using this 15-20% efficiency will be improved of the system.

The system consists of specific several input and several output switching matrixes that associations the energy from four discrete systems of energy harvesting sources such as thermoelectric, wind electric, piezo electric and photovoltaic. The system can be hold input voltages from 50 mV to 6 V and is proficient of removing maximum power and efficiency from all individual combines at that time by using a single inductor and can also be combines using a single capacitor. A projected time base power monitoring system is used for obtain MPPT for the photovoltaic harvester. The control circuits and the switch matrix are executed on a 0.36- m CMOS (Complementary Metal Oxide Silicon) process. This is a peak maximum power point tracking efficiency of 97%. The maximum efficiencies obtained with a inductor sharing or capacitor sharing are 88%, 89%, and 59% for piezoelectric buck-boost converters, photovoltaic and thermoelectric respectively.

Keywords: MPPT, Maximum power point Tracking, efficiency, solar, wind, thermo and piezoelectric harvesters.

## **The Race of Phase Change Memory Materials: The Role of Capacitance-Voltage Behavior**

**R. T. Ananth Kumar, Saleh T. Mahmoud, and Naser N. Qamhieh**

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This work is concerned with the investigation of Capacitance-Voltage (CV) behavior of phase change  $\text{GeTe}_2$  thin films prepared by vacuum evaporation technique. The phase change technology is mainly based on the reversible switching between the crystalline and amorphous states induced by an electric field, light or combination of both. A sufficient knowledge of the thermal crystallization kinetics is necessary for the development of suitable phase-change materials with optimized parameters. In this context, significant progress has been made in binary Ge-Te glass system to investigate the variation of the capacitance by the changing electric field (applied bias), signal frequency, and temperature for possible application in memory devices. The electrical measurements were carried out in the temperature range of 300 – 400 K with a heating rate of 5 K/min with two operating frequencies 100 KHz and 1 MHz. The resistance was found to decrease gradually from 300 K to 335 K and latter it falls steeply until the temperature reaches 370 K and then decreases gradually until the temperature reaches 400 K. At room temperature, a high resistance was noted for  $\text{GeTe}_2$  thin film characterizing the amorphous nature of the film. The sharp drop in resistance at about 350 K is attributed to the amorphous-crystalline phase transition, and this temperature is denoted as TC. The fast transition in the resistivity could be utilized for high-speed memory devices based on electrical switching. The variation of capacitance with temperature can be understood in terms of nucleation and growth process. The structural changes accompanied by the phase change with temperature will occur as the movement of Ge atoms from tetrahedral site in the amorphous phase to octahedral sites in the crystalline phase. In this study a strong correlation is found between the electrical parameters and local structure of the  $\text{GeTe}_2$  alloy. Moreover, the local atomic structure of amorphous materials is discussed in detail by the random covalent network (RCN) model.

Keywords: Phase-change materials , capacitance-voltage measurement, Memory devices

## **Photochromism of Dihydroazulenes: Investigating the Reaction Mechanism and Thermodynamic Properties in Solid State**

**Ieva Liepuoniute, Patrick Commins and Panče Naumov**

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The dihydroazulene–vinylheptafulvene (DHA–VHF) photoswitch is a  $10\pi$ -electron electrocyclic system that undergoes inter-conversion between two molecular states with the aid of external stimuli. When the thermodynamically stable form DHA absorbs UV light, it undergoes a photochemical ring-opening reaction to generate a more intensely colored but thermally unstable form, VHF. The lifetime of the VHF state depends primarily on the physical state, as well as on the electronics of substituents attached to it. Since VHF is converted back to the DHA thermally, the DHA/VHF couple is a positive T-type photoswitch. The exact solid-state kinetics of how the inter-conversion between the two states occurs has remained largely unknown and is a great area of potential research.

One of the interesting applications of the DHA–VHF photoswitch is its potential use as a solar panel alternative, which, if optimized, could be a cheaper way of storing renewable solar energy. As such, it is of a crucial importance to understand the mechanism and kinetics of the DHA–VHF photoswitch and to learn how to effectively manipulate this photochromic system in the solid state.

In this work, we plan to study the effect that different electronic substituents have on the thermal electrocyclic ring opening reaction of dihydroazulene. DHA molecules with phenyl and 4-methyl phenyl substituents were synthesized and the interconversion between the two molecular states of the dihydroazulene–vinylheptafulvene photoswitch was studied using UV-visible spectroscopy, NMR spectroscopy, and X-ray crystallography. The results of the study showed that the materials are photochromic not only in liquid, but also in the solid state— yellow DHA crystals can be irradiated to become deep red. In addition, X-ray diffraction measurements suggested that the DHA–VHF interconversion could be a single-crystal-to-single-crystal conversion as the sample retains its crystallinity; however this conclusion is based upon preliminary results and further investigation is underway using Two-photon excitation experiments. As a result, the study of DHA–VHF photochromic switch can provide insight into the photochromic phenomenon in solid state as well as suggest that this particular photoswitch could operate in a single-crystal-to-single-crystal manner.

Keywords: DHA–VHF, photoswitch, solid state

## **Light Trapping Mechanisms in Nanostructured Thin Film Photovoltaic Devices**

**Jagdish A.K., Sibimol Luke, Kavita Garg, Praveen C Ramamurthy, D Roy Mahapatra, and Gopalkrishna Hegde**

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Employing nanostructured design for light-management and trapping is a promising route to reduce active material thickness and cost in thin film solar cells. These designs are further beneficial if minimal complexity is introduced in the fabrication process. We present a novel nanostructured design for light-management and trapping in thin-film photovoltaic devices. Using simulations, we have made significant advances in understanding mechanistic changes in the coupled phenomena which affect the performance of nano-structured devices, depending on the opto-electronic properties of the materials in the photovoltaic device system. We also highlight, how a mechanistic understanding of coupled working of nanostructure and opto-electronic properties, obtained from simulations can aid in developing generic design rules, which have significantly helped us in phasing out usage of scantily available materials in the fabrication of devices.

In translating this design into scalable fabrication technologies, we have significantly simplified the fabrication of nanostructured devices both in terms of adopting template based fabrication of large area nanostructured platforms. We present our findings on facile fabrication methods to realize a wide range of nano-structures on transparent, light-weight platforms, which can be employed on a range of photovoltaic systems. In particular we present our findings on the mechanisms of light trapping in polymer solar cells, highlighting the importance of nanostructured interfaces in light scattering and trapping.

In summary, we highlight the phenomenological insights we have obtained from design, simulations and experiments which have assisted us in making significant advances towards translation of nano-structured design into up-scalable technologies.

Keywords: Nanostructure, solar cell, light trapping, thin films



## **Solution Based Fabrication of a Fast Response, Broad-Band, Large Area Photodetector**

**B. Bharath, K. D. M. Rao, K. N. Harish, and G. U. Kulkarni**

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High speed, sensitive photodetectors are essential in imaging and optical communication applications. However, the laborious fabrication processes and the costs involved set hurdles for technology realization of such devices. Herein, we report a simple cost effective solution based method of fabricating high performance photodetectors based on Au nanopyramidal structures grown on Silicon substrate by an electroless process. These nanostructures reduce the reflectivity of Si in the infrared region thus enhancing light trapping and absorption. The device exhibits a high on/off ratio of  $10^3$  at room temperature. Its excellent responsivity,  $\sim 310$  mA/W in wide range of wavelengths, and fast response,  $\sim 40$   $\mu$ s, are promising in the context of various optoelectronic applications. The device can be realized on  $\text{mm}^2$  areas while maintaining uniformity of the response. This method enabled us to realize a 5x5 image sensor which displayed appreciable performance.

Keywords: Photodetector, Nanostructure, Responsivity, Image sensor

## **Carbon Dioxide Capture at Ambient Conditions by Some Primary Amines**

**Ranganathan Sathishkumar and Munirathinam Nethaji**

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Industrial processes use the combustion of coal or gas which release a large amount of CO<sub>2</sub> into the atmosphere. In numerous cases, the methods used by industries to prevent emanations of gas consist of CO<sub>2</sub> removal by chemical absorption/desorption processes with alkanolamine solutions concomitant with a regeneration of amines for reuse. Some of the commonly used amines are monoethanolamine (MEA), diethanolamine (DEA), triethanolamine (TEA), diisopropanolamine (DIPA), and methyldiethanolamine (MDEA). Recently, metal organic frameworks (MOFs) were reported to play a vital role in the CO<sub>2</sub> absorption, transportation and storage. However, in both these cases a lot of challenges like, tuning the pore size in MOFs, CO<sub>2</sub> reactivity, and requirement of non-ambient conditions like high pressure and high temperature, cost effectiveness, etc. need to be addressed.

CO<sub>2</sub> is acidic, we anticipated that in principle it can react with amines to form carbamate salts. Accordingly we have selected several primary amines (Benzyl amine, Phenylethyl amine, 3-Phenylpropyl amine, 4-Phenylbutyl amine and Ethylene diamine) and exposed them to ambient atmospheric conditions in a fume hood. All the selected amines, which are liquid at room temperature, have become crystalline solids indicating their reaction with CO<sub>2</sub> and the formation of carbamate salts. The integrity of the salts is established by single crystal X-ray diffraction studies. The structural features of the carbamate salts and the mechanistic way of CO<sub>2</sub> capture will be discussed

Keywords: primary amines, single crystal X-ray diffraction, carbamate salts

## **Adenine-functionalized Spongy Graphene for Green and High-Performance Supercapacitors**

**Dalia M. El-Gendy, Nabil A. Abdel Ghany, E. E. Foad El-Sherbini  
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A simple method is demonstrated to prepare spongy adenine-functionalized graphene (SFG) as interconnected, porous 3-dimensional (3D) network crinkly sheets. Such 3D network structure provides better contact at the electrode/electrolyte interface and facilitates the charge transfer kinetics. The fabricated SFG was characterized by X-ray diffraction (XRD), FTIR, scanning electron microscopy (FESEM), Raman spectroscopy, thermogravimetric analysis (TGA), UV-vis absorption spectroscopy, and transmission electron microscopy (TEM). The synthesized materials have been evaluated as supercapacitor materials in 0.5M H<sub>2</sub>SO<sub>4</sub> using cyclic voltammetry (CV) at different potential scan rates, and galvanostatic charge/discharge tests at different current densities. The SFG electrodes showed a maximum specific capacitance of 333 F/g at scan rate of 1 mV/s and exhibited excellent cycling retention of 102% after 1000 cycles at 200 mV/s. The energy density was 64.42 Wh/kg with a power density of 599.8 W/kg at 1.0 A/g. Those figures of merit are much higher than those reported for graphene-based materials tested under similar conditions. The observed high performance can be related to the synergistic effects of the spongy structure and the adenine functionalization.

Keywords: supercapacitor; spongy; graphene; Adenine; energy density.

## Catalytic Pyrolysis of Plastic Waste with Natural Zeolite

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The chemical recycling (pyrolysis) of plastic wastes is one of the promising recycling process to utilized the disposed polymers by converting them into hydrocarbons liquid oil and other value-added products. In the present study various types of plastic wastes including polyethylene (PE), polystyrene (PS), polypropylene (PP) and polyethylene terephthalate (PET) were decomposed individually and there mixture in a small pilot scale pyrolysis reactor at the temperature of 450 °C with 75 min retention time. The aim of this study was to determine the effect of natural zeolite on catalytic pyrolysis of different plastic waste types. All types of plastic wastes were decomposed to liquid oil containing significant contents of unsaturated hydrocarbons from thermal and catalytic pyrolysis. In thermal pyrolysis, all plastic types were converted into liquid oil except PE and PET due to their complex branched structure. However their mixing with PS and PP resulted in production of liquid oil in different percentages due to the release of free radicals from PS plastic. Overall, thermal pyrolysis yielded low quality liquid oil with presence of solid residues, high acidity, and impurities like sulphur, chlorine and nitrogen along with high parasitic energy demands. To improve the quality of produced liquid oil and the cracking of C-C bonds of main polymers structure natural zeolite was used with the ratio of 10%. Natural zeolite was collected from Harrat Shama located in the north south of Jeddah, Saudi Arabia. To improve the catalytic activity of natural zeolite its thermal (550 °C for 3 hrs) and chemical activation (HNO<sub>3</sub>) was carried out. The strong cracking properties of catalysts produce short carbon chain compounds; reduce the aromatic contents and increase the quantity of desirable compounds in liquid oil and thus overall increases quality of produced liquid oil. The GC-MS analysis of liquid oil reveals the presence of saturated and unsaturated hydrocarbons compounds with the carbon chain ranging from C5 to C30. In addition FT-IR analysis of liquid oil also shows the presence of several aromatic compounds which was in agreement to GC-MS results. The major compounds produced from thermal and catalytic pyrolysis of plastic wastes were styrene, benzene, propylbenzene, ethylbenzene, toluene, methylstyrene, naphthalene, azulene, Phenanthrene, phenol and among other as well. The HHV of produced liquid oil from various types of plastic wastes ranges between 40-43 MJ/kj. Thus pyrolytic liquid oil has potential to be used as alternative source of energy. However it requires post-treatments, including upgrading and blending with conventional diesel to be used as transport fuel. The produced char has also potential to be used as an energy source or in several environmental applications such as removal of heavy metals from wastewater.

Keywords: Plastic waste; Pyrolysis; Natural zeolite; Polystyrene (PS); Polyethylene (PE); Polypropylene (PP); Liquid oil, Value-added products

## **Boron-Modified Silicon Oxycarbide/Graphene Composite Paper Electrode for Electrochemical Energy Storage**

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Heteroatom modification of polymer-derived ceramics is one of the sustainable means of improving their electrochemical energy storage properties as electrode materials. In this study, thin-film composites comprising of boron-modified silicon oxycarbides (SiOCB) ceramic supported on reduced graphene oxide (rGO) sheets were synthesized via vacuum filtration followed by pyrolysis in a flowing argon gas. This configuration ensures a uniform dispersion of the ceramic on rGO sheets and stabilization against re-aggregation due to boron nitride nanotubes (BNNTs) that forms a continuous network connecting the ceramic particles. In electrochemical energy storage application, boron is believed to improve the electronic conductivity and chemical stability of SiOC by modifying its nano-domain structures. Thin films of rGO-supported SiOC modified with different percentages of BNNTs were synthesized, characterized and tested as sodium-ion battery (Na-IB) and supercapacitor electrodes. SiOC containing 0.5 wt.% boron (SiOCB-0.5 wt.%) displayed optimum electrochemical properties among the synthesized boron-modified SiOC. As observed in this study, superior capacity of SiOCB-0.5 wt.% as an electrode material for Na-IB and supercapacitor suggests the existence of an optimum doping level of boron required to enhance desirable properties of SiOC composites.

Keywords: Polymer-derived ceramics, Electrochemical Energy Storage

## **Sulfur Polymers for Stable Lithium–Sulfur Batteries**

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The current and future need for better battery performance is indisputable, and the Lithium–Sulfur (Li–S) system is one of the most promising systems for next-generation, commercial batteries. In particular, Li–S addresses the need for long-lasting and high capacity batteries, which is a missing link to the widespread adoption of renewable energy. However, several challenges remain that prevent the use of Li–S batteries. One of the biggest challenges facing the Li–S system is its long-term instability. This research presents a new class of sulfur polymers that exhibits highly stable cycling. A combination of chemical design, cycling, and ex-situ studies, including Raman spectroscopy, solid-state NMR, and XPS, informed an iterative process to optimize the performance the sulfur polymers.

Keywords: Batteries, Lithium–Sulfur, polymers

## **Narrow Band Gap Copolymer of BODIPY and Benzodithiophene for Organic Photovoltaics**

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D-A copolymers of weak donors and strong acceptors are widely used class of materials for organic photovoltaics. The HOMO of the copolymer is dictated primarily by the HOMO of the donor part and the LUMO of the copolymer by the LUMO of the acceptor part. The HOMO energy level of the polymer is deep due to the weak donor moiety ensuring ambient stability of the material. Stronger charge transfer and narrow band gap is attained due to the strong acceptor subunit. Apart from ambient stability and narrow band gap, good absorptivity is also essential for polymers for photovoltaic applications. Incorporation of organic dye in the polymer backbone ensures high absorptivity of the polymer. In this work a copolymer of BODIPY and Benzodithiophene (BDT) has been studied. The BODIPY is a well-studied class of organic dyes which works as a strong acceptor. BDT is the donor subunit which is rendered a weak donor by substitution with an octyne chain. The extensively conjugated structure allows good pi-pi stacking among the polymer chains which is essential for the intermolecular charge transfer. Substitution with alkyl chains helps in making the polymer soluble in organic solvents. Density functional theory calculations have also been performed to calculate the energy of the frontier molecular orbitals and thus the band gap. UV-vis absorption spectra shows a panchromatic absorption by the polymer. Cyclic voltammetry results show the HOMO to be lower than -5.2 eV and hence ambient stability of the polymer. Thermogravimetric analysis suggests good thermal stability of the polymer.

Keywords: Polymer, solar cells, BODIPY



# **Effectiveness of Bioelectricity Generation from Urine and Its Treatment by Microbial Fuel Cell Using Graphite Electrodes**

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Increasing demand for sustainable energy and treatment of wastewater are emerging problem of the era. Microbial fuel cell is a technique uses wastewater for bioenergy production and simultaneous wastewater treatment. MFC is a promising and emerging technique for sustainable bioelectricity generation and wastewater treatment, different kinds of wastewater could be used in this technique. The effect and potential of urine as a substrate for electricity generation and treatment of urine in MFC has been focused using graphite rod as electrodes, in dual chamber with a high working volume of 1250 mL. The maximum voltage generated was 350 mV 88 days out of 154 days, with a maximum power density of 20.8 mW/m<sup>2</sup>. It showed a 69.9% reduction in COD, 47.8% Nitrogen and 40% Phosphate. This demonstrates that Urine is potential substrate and MFC is promising treatment technique for urine treatment and electricity generation.

Keywords: Urine treatment, MFC, Electricity

## **Design and Synthesis of New Thieno[3,4-c]pyrrole-4,6-dione based D-A Type Low Band Gap Conjugated Polymers Having Different $\pi$ -Conjugated Spacers for Organic Photovoltaics**

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In the last three decades, bulk-heterojunction (BHJ) based polymer solar cells (PSCs) have attracted great interest as a promising clean and renewable energy source, because of its unique advantages such as low cost, light weight, potential of being fabricated by a roll-to-roll process and large-area devices. In general, PSCs are composed of conjugated polymer as a p-type semiconductor and fullerene derivative as an n-type semiconductor inserted between an ITO positive electrode and a low work function metal negative electrode. Here the light absorber polymer material should exhibit broad absorption spectra with a high molar absorption coefficient to obtain a high  $J_{sc}$ , suitable energy level matching with the fullerene acceptor to offer a high  $V_{oc}$ , sufficient solubility to have solution process ability and suitable compatibility with the n-type material to form a nanoscale-bicontinuous interpenetrating network and high hole mobility for efficient charge transport. Therefore, design and synthesis of new low band gap polymer material have been proved to be an effective way to obtain high performance solar cells. Herein, new D–A structured conjugated polymers containing electron-rich benzo[1,2-b:4,5-b']-dithiophene (BDT) unit with alkylthiophene side chains and electron-deficient 5-(2-octyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (TPD) unit are designed and synthesized. To tune the optical and electrochemical properties, polymer main chains are extended by introducing spacers such as thiophene and thieno[3,2-b]thiophene units. By the introduction of thienothiophene from thiophene unit absorption maxima is red shifted from 460 to 502 nm. Energy levels of the polymer, HOMO and LUMO are calculated using cyclic voltammetry. Bulk heterojunction solar cells are fabricated using synthesized polymers with a configuration of ITO/PEDOT:PSS/polymer:PCBM/Al and the best power conversion efficiency of 1.92%, with a short circuit current density of  $10.5 \text{ mA cm}^{-1}$ , an open-circuit voltage of 0.46 V and a fill factor of 39% is achieved for thienothiophene based polymer.

**Keywords:** D-A type conjugated polymers, optical properties, electrochemical properties, polymer solar cell

## **Modeling the Open Circuit Voltage of Heterojunction Solar Cells**

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A bulk -heterojunction organic solar cells are thought as new material active layer. The open circuit voltage  $V_{oc}$  is one of the fundamentals quantity which affect the performance of the solar cells. The solar cell has been designed so that the electrodes make ohmic contact with the blend. The bulk -heterojunction organic solar cells provides that the electrodes make ohmic contact with the active layer and the difference between the electron affinity of the acceptors and donors be 0.5 eV. On using MDMO:PPV Poly[2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene] as donor , and PCBM as acceptors .The measurements gave an open-circuit voltage of about 0.7 V and efficiency of 2.8% . The offset of  $(LUMO)_A - (LUMO)_D$  is 1.1 eV which is greater than the energy needed for exciton dissociation and the electron transfer from donor to acceptor. About 0.6 eV would be dissipated as heat. The efficiency would reach a value of 5.2% if the LUMO of acceptor increase by 0.6 eV

Keywords: open circuit voltage  $V_{oc}$   $(LUMO)_A$  ,  $(LUMO)_D$  ,A bulk -heterojunction , organic solar cells

## **Ecofriendly Synthesis and Spectral Characterization of Silver Nanoparticles from Dill (*Anethum Graveolens*) Leaf Extract**

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Recent advances in nanotechnology have enabled us to produce pure silver, as nanoparticles, which are more efficient than macro silver ions. Silver has long been recognized as having inhibitory effect on microbes present in medical and industrial process. Silver nanoparticles are attractive because they are non-toxic to the human body as nano scale and have broad spectrum antibacterial actions. Plant contains abundant natural compounds such as alkaloids, flavonoids, saponins, steroids, tannins and other nutritional compounds. In this present study green synthesis of silver nanoparticles from aqueous silver nitrate through a simple and eco-friendly route using extract of dill (*anethum graveolens*) as reductant. *Anethum Graveolens* extract was selected as it is of high antioxidants which act as reducing and capping agents and it does not require any sample preparation so, it is cost-effective. The color change from yellow to dark brown confirmed the formation of nanoparticles. The bioreduced silver nanoparticles were characterized by UV-Vis spectrophotometer, transmission electron microscope (TEM), X-Ray diffraction (XRD), thermal gravimetric analysis (TGA) and fourier transform infra-red (FTIR) spectroscopy. The aim for the synthesis of silver nanoparticles by ecofriendly method is to apply an anti-cancer to measure the viability for breast, colon and liver tumor cells. Also apply an antibacterial and anti-fungi.

Keywords: silver nanoparticles, Dill, *Anethum Graveolens*, green synthesis, silver nitrate

## **Graphene Oxide/Zinc Oxide Composites as Photoanodes for Dye-Sensitized Solar Cells**

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Graphene-based materials, already brings brand new opportunities, and it may further improve the Dye-Sensitized Solar Cells (DSSC) photoanode, reduce the DSSC cost, and set a new record of energy conversion efficiency in solar energy applications. The properties of graphene-based materials are highly dependent on the sizes, thickness, and surface conditions, thus the controllable synthesis of graphene materials with tunable morphology and adjustable properties is highly desirable but still challenging. In the present work, graphene oxide (GO)/zinc oxide (ZnO) nanocomposites (GZn) with different ZnO morphologies were prepared using a simple hydrothermal method and its application as a photoanode for DSSC was investigated. The ZnO morphologies such as nanodisk, nanorods, spindles and nanoflowers were obtained by adjusting the pH of the solution. The synthesized composites were characterized by scanning electron microscope (SEM) and X-ray powder diffraction (XRD) which indicated that the ZnO nanoparticles are adorn on the surfaces and the interlayers of the graphene oxide sheets. The spectrophotometric study showed that the synthesized GZn nanocomposites has significant visible light absorption. The DSSC performance using the synthesized photoanodes was investigated in 0.6 M sodium sulfate electrolyte. The results of this study showed that the morphology of the ZnO nanoparticle has a crucial effect in the efficiency of the DSSC; the highest value of a power conversion efficiency of 5.10% for nanoflowers like morphology was obtained, due to high surface area. The current voltage (I-V) and capacitance voltage (C-V) characteristics of the synthesized films were investigated.

Keywords: Nanocomposite, Graphene, Solar Cells, Zinc Oxide

## **Core/shell Quantum Dots Importance for Multiple Excitation Generation Solar Cells**

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Semiconductor Quantum dots are area of rigorous research since last few years. Its narrative properties attract the researches for fundamental science and technical applications. QDs have specific attention for solar cell implementation owing to their capability to enhance efficiency by the generation of multi excitation from a single photon. The rivalry between MEG and other hot electron-cooling processes are accountable for the performance of MEG in colloidal Quantum dots. Core/shell QDs with Type-II band alignment provides additional degrees of freedom for Core/shell QDs in arbitrate both the optical dipoles and the Coulomb interface between charges for the assistance of MEG efficiency.

Keywords: Absorption, core/shell, multi excitation generation (MEG), quantum dot solar cells Configuration interaction (CI).

## **Synthesis and Properties of Bi-based Hybrid Double Perovskites for Photovoltaic Applications**

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The discovery of lead-free hybrid double perovskites  $(MA)_2BIBiX_6$  (BI = K, Tl, Ag and X = Cl, Br), provides a viable approach in the search for stable and environmentally benign photovoltaic materials as alternatives to the lead-containing systems such as  $MAPbX_3$  (X = Cl, Br, I). The first hybrid double perovskite,  $(MA)_2KBiCl_6$ , synthesized via solvent evaporation and hydrothermal methods, has a relatively big bandgap  $\sim 3.04$  eV. In order to reduce the bandgaps for photovoltaic applications, replacing K and Cl by Pearson softer ions such as Tl, Ag and Br, I has been attempted. And another two hybrid double perovskites,  $(MA)_2TlBiBr_6$  and  $(MA)_2AgBiBr_6$  have been obtained. The former compound, isoelectronic with  $MAPbBr_3$ , shows a direct bandgap of 2.16 eV, and the latter has an indirect bandgap of 2.0 eV. The properties of these materials have been investigated by resonant ultrasound spectroscopy, single crystal X-ray diffraction, nanoindentation, UV vis spectroscopy combined with density functional theory calculations.

Keywords: Lead-free perovskite, hybrid double perovskite

## **Deciphering the Mechanism of Phase Separation in Organic Photovoltaics**

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Organic-photovoltaics (OPVs) commonly referred to as organic solar cells provide a cost-efficient means of harnessing solar energy. However, optimum OPV performance depends on a thorough understanding of the complex process-structure-property relationship of organic semiconductor (active layer of OPV). The morphology of organic semiconductor influences electronic properties of the solar cell. One of the essential steps of device fabrication involves spin coating the blend onto a substrate. Solvent evaporation during spin coating leads to phase separation within the polymer blend, resulting in electron-acceptor (n-type) and electron-donor (p-type) organic semiconductors. These semiconductors then disperse randomly within the active layer to form bulk heterojunctions (BHJ's). The initiation of phase separation is expected around 10 seconds from the start of spin coating as per the literature for other blends. The typical length scale of the phases in morphology for P3HT:PCBM system is ~10 nm. There are two possible driving forces for phase separation i.e., spinodal decomposition and nucleation and growth. If the morphology shows a spatially correlated pattern, corresponding to both P3HT and PCBM phases during the start of phase separation with length scale around 10 nm (as has been found by our analytical calculations), then it can be suggested that the blend undergoes spinodal decomposition. On the other hand, if only one phase can be observed, it would imply that the phase separation is crystallization induced by that phase. This work is aimed at determining the driving force for the evolution of this morphology, since then the phase separation can be modeled and optimum morphology can be determined in contrast to the trial and error approach employed now. Experimental studies have been carried out on P3HT:PCBM blend by observing the embryonic temporal evolution of morphology. A set-up was devised to freeze the morphology during spin-coating, morphology was frozen by exploiting the chemistry of the organic blend by choosing a suitable solvent to delay the kinetics of solvent evaporation. The mechanism of phase separation has been probed using phase-contrast AFM imaging.

**Keywords:** Organic Photovoltaics, Morphology, Phase separation, Crystallisation, Spinodal decomposition



## ***In situ* Diffraction Studies of Metal-Organic Framework Formation**

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Metal-organic frameworks (MOFs) have emerged as a family of materials with the potential to revolutionise areas such as carbon capture, fuel gas storage, and catalysis. MOFs comprise well-defined metal-containing nodes bridged by organic ligands, combining the advantages of crystalline framework materials with the versatility of organic chemistry. However, a major hurdle to attaining designer MOFs is our poor understanding of MOF formation from a solution of reagents. Making in situ measurements during MOF formation is hence critical but also very challenging, as MOFs are usually prepared at high temperatures and pressures in bulky reaction vessels. In situ X-ray diffraction (XRD) is one of the few techniques capable of interrogating such vessels in real time, and so provides insight into the fundamental chemical processes that govern MOF formation.

To date, most in situ XRD studies of MOF formation have used energy dispersive XRD, which gives reaction kinetics but provides poor structural information. Alternatively, capillary setups provide better structural data, but provide very different reaction conditions to lab-scale preparations. We show that using improved technology at modern synchrotrons, it is possible to obtain high-quality structural information from in situ XRD measurements on reactions under realistic conditions. We present several examples from our work on beamline I12 at Diamond (UK).

A common assumption is that a MOF nucleates and crystallizes uniformly without undergoing further structural changes as it grows. Many topical MOF properties arise from the inclusion of heterogeneity such as in defective MOFs or solid-solution systems that contain mixtures of functionalised ligands or metals. Whether these components are included randomly or with a degree of order is hence an important question. We present evidence that it is possible to extract this level of structural detail from Rietveld refinement of in situ XRD data.[1]

The more complex case in which intermediates form also occurs frequently during MOF formation. This is a result of the large number of MOF polymorphs lying on a relatively flat energetic landscape. This has implications for the deployment of MOFs on large scales, where purity, energy cost (time & temperature), and yield must be optimized. We demonstrate the characterisation of multi-phase behaviour using in situ XRD, including a new model for the quantification of conversion kinetics, and the identification of previously unknown intermediate

phases.[2] We also show how in situ studies can be combined with modelling to obtain the absolute energetics of MOF phase space.[3]

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Keywords: in situ, powder X-ray diffraction, metal-organic framework, MOF

## **Industrial Waste Fly Ash Cenosphere Based Lightweight Microwave Absorber**

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Thermal power plant's solid waste fly ash cenospheres (FAC) of average size 50  $\mu\text{m}$  (typically hollow microspheres) were cleaned by acid-base treatment. The  $\text{MnO}_2$  nanoparticles were coated over FAC by simple one step chemical method and characterized. The uniform coating thickness was found to be  $\sim 800$  nm over FAC. The 10 wt% of  $\text{MnO}_2$ -FAC loaded polyvinylbutyral (PVB)- $\text{MnO}_2$ -FAC composites were prepared by solution processing and characterized by various techniques. The dielectrics and microwave absorption property of as prepared composites were investigated in the X-band (8.2-12.4 GHz) and Ku-band (12.4-18 GHz). The most effective reflection loss (RL) of PVB- $\text{MnO}_2$ -FAC composite (thickness 2 mm) was observed to be -9 dB and -20 dB in the X-band and Ku-band respectively. However, the microwave absorption property of this composite can be tuned by controlling thickness. High dielectric loss and synergetic effect of PVB matrix and  $\text{MnO}_2$ -FAC was found to be responsible for obtained low RL value. The enhancement of EM attenuation constant ( $\alpha$ ) of PVB- $\text{MnO}_2$ -FAC composite with frequency also indicates high EM attenuation and microwave absorption property. Further, microwave absorption property of the as prepared composite can be improved by introducing little amount of PEDOT:PSS in the PVB matrix. This composite film can be considered as a novel high microwave absorbing inexpensive coating material for radar, microwave engineering, communications, robotics as well as unmanned vehicles.

Keywords: Fly ash cenosphere, Polymer composite, microwave absorption, dielectrics

## **Evaluation of Mechanical and Microstructural Properties of Alkali Activated Slag Concrete Reinforced with Polystyrene Shredding and Accelerator**

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The Ordinary Portland Cement (OPC) is a major constituent of concrete, which is being used extensively since last half century. The production of cement is impacting not only environment alone, but depleting natural materials. During the past three decades, the scholars have carried out studies to explore the supplementary cementitious materials such as Ground granulated Blast furnace slag [1], silica fumes, metakaolin [2] or fly ash [3].

The alkali activated slag concrete is another innovation which has constituents of cementitious materials like Ground Granule Blast Furnace Slag [4], Fly Ash, Silica Fumes or Metakaolin. Alkaline activators like Sodium Silicate and Sodium Hydroxide is utilized. In view of evaluating properties of alkali activated slag concrete blended with polystyrene shredding and accelerator, research study is being carried out. This research study is proposed to evaluate the effect of polystyrene and accelerating admixture on mechanical and micro structural properties of Alkali Activated Slag concrete. The mechanical properties included the compressive strength, splitting tensile strength, flexural strength and permeability. The tests conducted in the laboratory for evaluating mechanical properties are: Compressive Strength, Flexural Strength, Split Tensile and Permeability Test. The outcome of this research will be useful for developing concrete, which will avoid brittle and instantaneous failures in concrete.

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Keywords: Ground granulated Blast furnace slag, Alkali Activators, Accelerator, Polystyrene, Ordinary Portland Cement

## **Morphological Control in Pechini Gel Synthesis: A Study of Porous Metal Oxides**

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The Pechini method is a facile sol-gel technique for the preparation of metal oxides. In this method, citric acid, ethylene glycol, and metal nitrates are dissolved in water, gelled overnight at raised temperatures, and then combusted to form metal oxides. When combined with colloidal crystal templating (CCT) methodologies, ordered or disordered porosity can be observed in the final metal oxide product at the nanometer scale. With regards to previous experimentation, a quasi-phase consisting of macroporous microspheres was observed in ceria and ceria-magnesia systems. This study, then, concerned the generalization of the production of the macroporous microsphere quasi-phase to other metal oxide systems via stoichiometric control of precursor components. Precursor component ratios were varied to produce a variety of iron(III) oxide and manganese(II,III) oxide samples, and structural confirmation was carried out via scanning electron microscopy. The results of these studies were then used to develop a general method for the synthesis of the macroporous microsphere quasi-phase in metal oxide systems via the Pechini gel technique.

Keywords: Nanomaterials, Porous materials, Sol-gel synthesis, Colloidal crystal tempting

## **The Effect of Fuel to Oxidizer Ratio on the Formation of Nanocrystalline $\text{FeCr}_2\text{O}_4$**

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Nanocrystalline  $\text{FeCr}_2\text{O}_4$  powders were synthesized via solution combustion method. The fuel (glycine) to oxidizer ratio was varied as a factor in the synthesis process. XRD, EDS and FTIR studies have confirmed the formation of single phase nanocrystalline  $\text{FeCr}_2\text{O}_4$  powders. SEM studies have revealed that the fuel to oxidizer ratio had an effect on the morphology and porosity of the synthesized nanocrystalline  $\text{FeCr}_2\text{O}_4$  powders. Structural analyses have shown that glycine to oxidizer ratio affected crystallite size, lattice parameter and lattice strains and distortions. Optical absorption analyses have indicated a red shift (1.37–1.44 eV) for the direct band gap of the synthesized nanocrystalline  $\text{FeCr}_2\text{O}_4$  powders. The variation of the fuel to oxidizer ratio could be used as a factor in synthesizing nanocrystalline  $\text{FeCr}_2\text{O}_4$  with different properties.

Keywords: Spinel nanomaterial; Solution combustion method; fuel to oxidizer ratio.

## **Fabrication and Characterization of Size-Selected Cu Nanoclusters using a Magnetron Sputtering Source**

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Nanoparticles are microscopic entities with a very wide variety of applications in various fields. The small size of nanoparticles make the surface/volume ratio larger, and so the nanoparticles will be more reactive with the environment. Moreover, variation in the size of Nano-clusters leads to changes in their properties. Copper is one of the elements attracted the attention of researchers due to its use in many applications.

In this work, different sizes of copper nano-clusters were prepared by using an ultra-high vacuum magnetron sputtering system and gas condensation. Varying the conditions of the preparation method such as the aggregation length ( $L$ ) and the Argon (Ar) gas flow rate allows controlling the size of the produced copper nanoclusters.

# **Effect of High Energy Mechanical Milling on Hysteresis and Dielectric Properties of $\text{Ca}_x\text{Ba}_{1-x}\text{Zr}_x\text{Ti}_{1-x}\text{O}_3$ ( $x=0.0$ and $0.1$ ) Ferroelectric Materials**

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The ferroelectric material with general formula  $\text{Ca}_x\text{Ba}_{1-x}\text{Zr}_x\text{Ti}_{1-x}\text{O}_3$  ( $x=0.0$  &  $0.1$ ) is synthesized by solid state reaction. The ceramic powders of these prepared samples are milled in a planetary ball mill in air, with tungsten carbide vial and 150 tungsten carbide balls of diameter 10 mm for different hours (12, 18 and 30 hrs). The powder X-ray diffractometry is employed to confirm the single phase tetragonal (P4mm) perovskite structure to all the specimens. Morphology and crystallite size have been studied by means of scanning electron microscopy for the ferroelectric samples. The polarization versus electric field (PE) hysteresis loops of ferroelectric specimens for different milling hours are carried using PE hysteresis loop tracer and the dielectric measurements are recorded in the frequency range 100 Hz – 1 MHz at room temperature using impedance analyzer. The properties of ferroelectric materials depended on the size of crystallites. The high energy ball milling is one of the great techniques to control the particle size of the prepared samples. The PE hysteresis loop recorded at room temperature gives the values of polarization, coercivity and remanence. The shape of PE loop drastically changes after the ball milling process and the PE hysteresis parameters are found to change. The polarization decreases and simultaneously the coercivity and remanence increase with ball milling time up to 18 hours and they are found to decrease for the 30 hour milled samples. The dielectric constant is measured for pristine  $\text{BaTiO}_3$  i.e. 2200 at 100 Hz and 412 at 1 kHz frequency. The value of dielectric constant decreases with ball milling time. Similarly, the dielectric constant for  $\text{Ca}_{0.1}\text{Ba}_{0.9}\text{Zr}_{0.1}\text{Ti}_{0.9}\text{O}_3$  ferroelectric specimen is 1650 at 100 Hz and 442 at 1 kHz frequency. Both the present ferroelectric specimens show universal dielectric response with frequency variation. It is to be noted that for  $\text{Ca}_{0.1}\text{Ba}_{0.9}\text{Zr}_{0.1}\text{Ti}_{0.9}\text{O}_3$ , the dielectric constant initially decreases with ball milling time and thereafter it increases with further milling.

Keywords: Ferroelectric, High Energy Milling, PE Hysteresis loop, dielectrics



## **Antibacterial Activity of Metal Nanoparticles (AgNO<sub>3</sub>, ZnO, CuO) Against Pathogenic Bacteria**

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In this study we are interested in evaluating the antibacterial activity of nano-molecules (AgNO<sub>3</sub>, ZnO and CuO) alone and in combination with antibiotics on two different microorganisms Gram, respectively *P. aeruginosa* (Gram negative) and *S. aureus* (Gram positive), because of their extensive involvement in the phenomena of contamination and infection encountered in the medical field by the agar diffusion method, determination of the minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC). The antibacterial activity of certain antibiotics tested on *S. aureus* strains and *P. aeruginosa* is enhanced with a minimum of (1 mm) and maximum (28 mm) with AgNO<sub>3</sub> in both strains an increase of (2 mm and 4 mm) was observed with the *S. aureus* strain on ZnO, the method of well diffusion and blotting paper reveals that the activity is dose-dependent for both *S. aureus* strains and *P. aeruginosa* with AgNO<sub>3</sub>. The minimum inhibitory concentration was determined using seven concentrations of NPs (AgNO<sub>3</sub>, ZnO and CuO): 512, 128, 64, 32, 16, 8, 0 mg/ml. The MIC values (AgNO<sub>3</sub>) for *S. aureus* and *P. aeruginosa* and 16 µg/ml, respectively, the values of CMB (AgNO<sub>3</sub>) for *S. aureus* and *P. aeruginosa* 16 and 512 µg/ml, respectively. The results up the AgNO<sub>3</sub> have a bactericidal effect on *S. aureus* and bacteriostatic effect on *P. aeruginosa*.

Keywords: Nanoparticles, AgNO<sub>3</sub>, ZnO, CuO, antibacterial activity, CMI, CMB, *S. aureus*, *P. aeruginosa*.

## **Structural and Vibrational Properties of Bulk and Few-Layer Td-WTe<sub>2</sub>: A Combined Experimental and Theoretical Analysis**

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The recent discovery of non-saturating giant positive magnetoresistance has renewed much interest in Td-WTe<sub>2</sub>. We have investigated structural and vibrational properties of bulk and few-layer Td-WTe<sub>2</sub> experimentally and theoretically. Spin-orbit coupling is found to govern the semi-metallic character of Td-WTe<sub>2</sub> and its structural link with the metallic 1 T form provides an understanding of its structural stability. Electronic band structure remains similar in bulk as well as monolayer Td-WTe<sub>2</sub> in contrast with related transition metal dichalcogenides. Lattice vibrations of Td-WTe<sub>2</sub> have been analyzed by first-principles calculations. Out of the 33 possible zone-center Raman active modes, five distinct Raman bands are observed around 112, 118, 134, 165 and 212 cm<sup>-1</sup> in bulk Td-WTe<sub>2</sub>. Based on symmetry analysis and calculated Raman tensors, we assign the intense bands at 165 cm<sup>-1</sup> and 212 cm<sup>-1</sup> to the A<sub>1</sub>' and A<sub>1</sub>'' modes respectively. Most of the Raman bands stiffen with decreasing thickness and the ratio of the integrated intensities of the A<sub>1</sub>'' to A<sub>1</sub>' bands decreases in the few-layer sample, while all the bands soften in both the bulk and few-layer samples with increasing temperature. Notably, the thickness-dependence of Raman bands is different from that observed in the well-studied 2H-forms of MoS<sub>2</sub> and WS<sub>2</sub> due to low-symmetry, and mixing of in-plane and out-of-plane vibrational modes in Td-WTe<sub>2</sub>.

Keywords: Td-WTe<sub>2</sub>, magnetoresistance, Raman spectroscopy

## ***Ab Initio* Statistical Mechanics of Martensitic Phase Transition in NiTi Shape Memory Alloy (SMA)**

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NiTi exhibits a shape memory effect in which it returns to a predetermined shape when heated. The mechanism of this effect is fundamentally related to martensitic transformation, in which NiTi changes from a high temperature cubic (B2) phase to low temperature monoclinic (B19')[1] phase. The transformation is a displacive first order phase transition including change in the crystal shape[2]. Using cubic B2 phase as a reference structure, we develop an effective Hamiltonian to capture its low-energy structural distortions that are relevant to the martensitic phase transitions, and determine all its parameters from first-principles density functional theory calculations. Our model contains the physics of nonlinear elasticity and coupling between strains and phonons. We present statistical mechanical analysis of the effective Hamiltonian using Monte Carlo simulations and establish the martensitic transformation at 260 K from B2 to B19', in good agreement with experimental transition temperature of 310 K. We uncover the specific coupling and mechanism that govern the B2 to B19' structural phase transitions.

### References:

1. Michal, G. M.; Sinclair, R. The Structure of NiTi martensite. *Acta Cryst.* 1981, B 37, 1803-1807.
2. Lindgard, P. A.; Mouristen, O. G. Theory and Model for Martensitic Transformations. *Phys. Rev. Lett.* 1986, 57, 2458-2461.

Keywords: Shape memory alloys, Martensitic Transformations

## **Temperature Driven Phase Transformation in Desolvated Zeolitic Imidazolate Framework**

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Metal organic frameworks (MOFs) are known to exhibit a variety of crystal structures under pressure, temperature, and gas adsorption. Desolvated zeolitic imidazole frameworks shows temperature dependent phase transition. On cooling to 140 K, its volume contracts by 23%, while its symmetry remains the same. Through first-principles calculations, we attempt to understand the dynamical properties of high and low temperature phases. We find unstable modes in the high temperature phase indicating its instability, which is responsible for its transformation to the low temperature phase. The low temperature phase, with no unstable modes is stable.

Keywords: ZIF-4, Phase transition, DFT, Phonons, Symmetry

## **Oxygen Vacancy Clustering and Electron Localization in Rutile TiO<sub>2</sub>**

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The oxygen-vacancy cluster in TiO<sub>2</sub> and its associated electron localization have been successfully addressed by the hybrid functional method. We find that the oxygen vacancies tend to appear in the linear cluster of VO-Ti-VO in (110) plane of rutile TiO<sub>2</sub>, accompanied by strong electron localization at the 3d state of the Ti ions. Such vacancy clustering and electron localization lead to a profound impact on materials properties, e.g., the appearance of characteristic optical spectra, and the increase in electrical conductivity, offering an accurate interpretation of such experimental results as transport behaviours and optical absorption properties. Additionally, the kinetic analyses have been done on the migration of such vacancy cluster, and its high kinetic stability also suggests the physical reality of such clustering of oxygen vacancy. Our outcomes provide a viable route to understand various physical behaviours, especially transport properties, of the rutile oxides that are inherently prone to oxygen nonstoichiometry, and also demonstrate that material properties can be substantially influenced by the vacancy clusters through the region such as interface or grain boundary where the nonstoichiometry is often enhanced.

Keywords: TiO<sub>2</sub>, oxygen vacancy clustering, electron localization, optical properties

## **Electronic and Optical Properties of Aluminum Nitride Nano-Clusters**

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Aluminum-Nitride (AlN) is a piezoelectric material that has the ability to maintain piezoelectricity up to 1200 °C, AlN is also a promising material for use in surface acoustic wave (SAW) devices, sensor, thin film resonators, metal-oxide semiconductor (MOS) applications and microelectronic devices. In the past decade, various techniques were employed to produce Aluminum Nitride thin films and nanostructures such as, pulsed laser deposition (PLD).

In this work, we have undertaken a systematic and an accurate theoretical study of the electronic and optical properties of AlN nanoclusters. All the fundamental properties were studied as a function of temperature and pressure. Since any structural change influences on the electronic and optical properties, a correlation between the two effects is analyzed. The properties of AlN nanoclusters can be engineered to desirable values by altering the size of these clusters, therefore a study of the effect of the size of AlN nanoclusters will be investigated.

Keywords: Band structure, nano-clusters, optical.

## **Structural, Electronic and Thermodynamic Properties of CeO<sub>2</sub> Compound: An *Ab Initio* Study**

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The full potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory is employed to investigate the structural, electronic and thermal properties of CeO<sub>2</sub>. Exchange-correlation effects are treated by the generalized gradient approximation (GGA). Results are provided for the lattice constant, bulk modulus, pressure derivative of bulk modulus, band structure and density of states. Our results are compared and showed good agreement with other theoretical works. Furthermore, the thermodynamical properties are predicted through the quasi-harmonic Debye model, in which the lattice vibrations are taken into account. The variation of relative change in volume, bulk modulus, heat capacities and thermal expansion coefficient with temperature and pressure are successfully achieved.

Keywords: FP-LAPW calculations; Electronic structures; Thermal properties

## **Laser Processing of Nano-Crystalline Copper Sulfide Thin Film Prepared by Spray Pyrolysis**

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Copper sulfide ( $\text{Cu}_2\text{S}$ ) thin films were deposited onto glass substrate by spray pyrolysis technique using aqueous solutions from copper chloride dehydrate ( $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ ) and thiourea ( $\text{SC}(\text{NH}_2)_2$ ) at deposition temperature of  $\sim 370$  °C. The deposited film was observed to be blackish brown in color, well adherent to the substrate, pin-hole free and uniform. The structural, surface morphological, optical and electrical properties of the film were carried out before and after laser processing by means of X-ray diffraction, scanning electron microscopy, EDAX, optical transmittance and reflectance measurement techniques and two point probe technique. XRD analysis showed that the deposited and treated films are closed to copper rich phase (chalcocite,  $\text{Cu}_2\text{S}$ ). Increments in crystallite size from 34.81 nm for as deposited film to 54.71 nm for the treated film were confirmed by both X-ray diffraction and scanning electron microscope. From the optical band gap calculations, we found a red shift in its value after laser processing. The type of conductivity for as prepared and laser treated films showed p-type conductivity. Further, the conductivity of the film showed enhancement after exposed to laser radiation.

Keywords: copper sulfide nano-crystalline, thin films, spray pyrolysis, laser processing, structural properties, optical properties, electrical conductivity



## **Covalent Functionalization of Nanosheets of MoS<sub>2</sub> and MoSe<sub>2</sub> by Substituted Benzenes and other Organic Molecules**

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Covalent functionalization has been effectively employed to attach benzene functionalities to MoS<sub>2</sub> and MoSe<sub>2</sub> nanosheets by the reaction with para-substituted iodobenzenes bearing OCH<sub>3</sub>, H and NO<sub>2</sub> as the substituent, where the electron-donating and electron-withdrawing power of the para-substituent varies significantly. The functionalization is based on the formation of a C-S or C-Se linkage at the expense of the C-I bond on reaction of the iodobenzene with electron-rich 1T-MoS<sub>2</sub> or 1T-MoSe<sub>2</sub>. The degree of functionalization is in the 4%-24% range, the value increasing with the electron-withdrawing power of the para-substituent. Semiconducting 2H-MoS<sub>2</sub> and 2H-MoSe<sub>2</sub> nanosheets can also be functionalized with iodobenzene by carrying out the reaction in the presence of the Pd(0) catalyst. We have also carried out functionalization of 1T-MoS<sub>2</sub> with pyrene, coumarin and porphyrin derivatives. Using first-principles density functional calculations, we show that bonding of the functional groups with 1T phase is stronger than with the 2H phase. This gets reflected in notable changes in the electronic structure of the former upon functionalization; a gap opens up in the electronic spectrum of 1T phase. Functionalization with para-substituted benzenes with R = OCH<sub>3</sub> and H groups leads to a reduction in the work function while with R = NO<sub>2</sub> leads to enhanced work function relative to the pristine monolayer.

Keywords: 2D materials; transition metal dichalcogenides; MoS<sub>2</sub>; MoSe<sub>2</sub>; covalent functionalization

## **P-type Mg Doped CuCrO<sub>2</sub> Transparent Conducting Thin Layers**

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Several materials have been investigated as possible p-type TCO candidates: the delafossites (CuMO<sub>2</sub>) where M stands for metallic ion, the spinel family (ZnX<sub>2</sub>O<sub>4</sub> X= Co, Rh, Ir), (Cu<sub>2</sub>S<sub>2</sub>)(Sr<sub>3</sub>Sc<sub>2</sub>O<sub>5</sub>), NiO and ZnO. However, potential p-type TCOs identified at this point, have conductivities at least one-two orders of magnitude lower than their n-type counterparts. The best conductivity reported up to day is for doped CuCr<sub>1-x</sub>Mg<sub>x</sub>O<sub>2</sub>, but has poor transparency.

In this work undoped and Mg-doped CuCrO<sub>2</sub> thin films were deposited by spray pyrolysis at 400 °C on sapphire and fused silica substrates. The deposited layers were amorphous. The delafossite crystal structure formed after thermal annealing between 600 °C and 960 °C in nitrogen atmosphere. The electrical properties (Seebeck and Hall effect) of undoped and Mg-doped CuCrO<sub>2</sub> thin films on both sapphire and fused silica were studied. The effect of both sapphire and fused silica substrates on transport properties (mobility) of undoped and Mg-doped CuCrO<sub>2</sub> thin films was studied. EPR spectroscopy was used for studying the defects related to Cr<sup>3+</sup> and Cu<sup>2+</sup>.

Keywords: P-type TCO, Spray pyrolysis, Thin films, Structure and Electrical properties

## **Preparation and Characterization of CeO<sub>2</sub>-based Binary Oxides with Divalent and Trivalent Transition Metal Ions by Microwave Process for CO-PROX Applications**

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Fuel cells are highly attractive green technologies to replace the classical combustion engine for energy generation, yet their limited efficiency due to a variety of operational constraints is yet to be solved for proper market implementation. For example, one of the main impeding issues in the Proton Exchange Membrane fuel cell, is the presence of CO impurity at about 2 vol. % in the hydrogen gas fuel stream, which frequently causes the poisoning of the noble metal catalyst electrode. To improve and maintain the efficiency of the fuel cell, the concentration of the CO impurity must not exceed 10 ppm in the supply gas. Among the various approaches to address this problem, preferential CO oxidation using ceria as heterogeneous catalyst is very promising due to its high selectivity and lower cost of implementation.

Using a fast and simple microwave synthesis methodology, this study aims for advancing the CO-PROX performance of the popular ceria catalyst through a metal-doping approach with divalent and trivalent metal additives (Ce<sub>x</sub>M<sub>1-x</sub>O<sub>2</sub> catalysts, where M: Fe<sup>3+</sup>, Mn<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Zn<sup>2+</sup> and Co<sup>2+</sup> and x:0.80) to improve both the thermal stability and ionic conductivity of the material. A variety of physicochemical characterization techniques were used to get insight information about the microstructure (XRD), morphology (SEM), porosity (BET), thermal stability (TGA), and the acid/base surface properties (TPD-CO<sub>2</sub>, TPD-NH<sub>3</sub>). The catalytic CO oxidation studies were investigated between 200 and 450 °C. XRD results showed that all the catalysts form a fluorite cubic lattice having a crystallite size ranging between 8.8-16.4 nm, and that is strongly affected by the presence of the metal cation additive. The thermal stability of the precursor composite was found to be associated with the second metal-cation added, with Ce-Mn-O losing 60% of its mass at 110 °C, whereas Ce-Fe-O, Ce-Co-O, Ce-Zn-O and Ce-Ni-O catalysts only lost less than 20% at 250 °C. Among these, the Ce-Co-O system experienced the least weight loss at 35% at temperatures above 400 °C. The surface acid/base character was found to be dependent of charge of the transition metal cation additive. The surface acidity was found to play a key role in determining the catalytic CO oxidation activity.

Keywords: microwave;sol-gel;CeO<sub>2</sub>-based oxides;CO oxidation

## **Adsorption of CO<sub>2</sub> on Fe-doped Graphene Nano-Ribbons: Investigation of Transport Properties**

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Density functional theory combined with the non-equilibrium Green's function formalism is used to study the conductance response of Fe-doped graphene nano-ribbons (GNRs) to CO<sub>2</sub> gas adsorption. A single Fe atom is either adsorbed on GNR's surface (aFe-graphene) or it substitutes the carbon atom (sFe-graphene). Metal atom doping reduces the electronic transmission of pristine graphene due to the localization of electronic states near the impurity site. The reduction in the transmission is more pronounced in the case of sFe-graphene. Moreover, the aFe-graphene is found to be less sensitive to the CO<sub>2</sub> molecule attachment as compared to the sFe-graphene system. Due to the chemisorption of CO<sub>2</sub> molecule and breaking of its  $\pi$ -bonds, the charge transfer from the adsorbent surface to the molecule is shown to be responsible for affecting the density of states at Fermi level and consequently the conductivity. This is consolidated and rather confirmed by calculating the IV characteristics from which the gas response sensitivity is estimated. Since the change in the conductivity is one of the main outputs of sensors, our findings will be useful in developing efficient graphene-based solid-state sensors.

**Keywords:** Gas sensing, Chemisorption, Physisorption

## **Synthesis and Characterization of $\text{Mg}_{1-x}\text{Mn}_x\text{CuP}$**

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The idea of thermoelectric materials is to recover waste heat and convert it to electricity. A good thermoelectric material has a high Seebeck coefficient, high electrical conductivity and low thermal conductivity in a temperature range of relevance. Zintl or Zintl-like compounds are good candidates to fulfill this profile. Based on the system  $\text{MCuP}$ , where M is a variable cation, we showed  $\text{MgCuP}$  to exhibit comparatively high figures of merit,  $zT > 0.3$ . An enhancement of these values was obtained by substitution of magnesium through a certain amount of manganese. Therefore, the synthesis and investigation of isostructural  $\text{MnCuP}$  and the solid solution,  $\text{Mg}_{1-x}\text{Mn}_x\text{CuP}$ , became of great interest. The synthesis of  $\text{MnCuP}$  was achieved from  $\text{MnP}$  and  $\text{Cu}$  by using a hightemperature preparation route. Between  $100\text{ }^\circ\text{C}$  and  $500\text{ }^\circ\text{C}$   $zT$  values were determined to rise from 0.002 to 0.06. A phase transition from  $\text{MnCuP}$  at  $700\text{ }^\circ\text{C}$  was observed by differential scanning calorimetry and high-temperature X-ray diffraction. Manganese-rich compounds in the solid solution could not be synthesized, but the synthesis of the magnesium-rich phase was successful up to  $x = 0.2$ . A maximum  $zT$  value of 0.75 was observed for  $x = 0.15$  at  $650\text{ }^\circ\text{C}$ , which makes these phosphides very promising thermoelectric materials.

## **Effect of Supercritical Fluid Extraction on the Adsorption Capacity of Date Pits Powder for Lead Removal**

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In this research, the adsorption capacity of raw Khalas date powder was compared to that of the residue date pit powder left after performing supercritical fluid extraction. Performing supercritical fluid extraction allows us to not only benefit from the collection of extract, in the form of date pit oil, but to also use the powder residue as a possible adsorbent for removal of lead ions from solution. To the best of the authors' knowledge, this is the first research to propose using the residue of the extraction process as a possible adsorbent.

In order to maximize the adsorption capacity of the adsorbents, the effect of factors on adsorption including pH, particle size, adsorbent dose was studied. This is an ongoing investigation. Initial investigations were used as screening experiments in the building of an experimental design with Response Surface Methodology, which is to be carried out in order to find the optimum adsorption conditions for each adsorbent type. Preliminary results show that pH and adsorbent dose have a significant effect on adsorption capacity; meanwhile the effect of particle size has proven to difficult to capture. Furthermore, preliminary experiments indicate that raw date pits and extraction process residue show similar adsorption capacity.

Keywords: Adsorption, Lead Removal, Supercritical Fluid Extraction

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