IC-EEE 2015
International Conference on Energy Harvesting, Storage and Conversion

Organized by
Department of Physics
Cochin University of Science and Technology

February 4-7, 2015
Cochin, India
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<th>Time</th>
<th>Session 3a</th>
<th>Session 3b</th>
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<td>02.00 PM - 02.45 PM</td>
<td>Plenary Talk 1—Prof. Mukundan Thekkinkat (University of Bayreuth, Germany) Title: Self-assembly Tools to Control Nanostructures in Organic/Hybrid Photovoltaics</td>
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<td>Session 3a</td>
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<td>Venue: Kings Court</td>
<td>Venue: Executive Club</td>
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<td>Chair: Prof. John T.S. Irvine (University of St. Andrews, Scotland, UK)</td>
<td>Chair: Prof. Godfrey Louts (Dept. Physics, CUSAT)</td>
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<tr>
<td>2.50 PM - 3.20 PM</td>
<td>IT5: Prof. Prabhakar Misra (Howard University, USA) Title: Characterization Of Nanomaterials Relevant To Energy Storage and Gas Sensing Applications Using Raman Spectroscopy &amp; Molecular Dynamics Simulations</td>
<td>IT6: Dr. Manoj Namboothiri (IISER, Thiruvananthapuram, India) Title: Plasmon Enhanced Power Conversion Efficiency in Inverted Bulk Heterojunction Organic Solar Cell Synthesized in Air</td>
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<td>3.30 PM - 4.00 PM</td>
<td>IT7: Dr. Murukeshan Vadakke Matham (NTU, Singapore) Title: Layered and patterned nanoscale structures for improved absorption in next generation thin film Si solar cells</td>
<td>IT8: Prof. Sathikumar (Toyo University, Japan) Title: Application of nanoformulations as theragnostics materials against cancer</td>
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<td>Tea/Coffee Break and Poster Session 04.00 – 06.00</td>
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7.00 PM – 9.00 PM
Cultural Programme Followed by Dinner at CUSAT CAMPUS
Characterization of Nanomaterials Relevant to Energy Storage and Gas Sensing Applications Using Raman Spectroscopy & Molecular Dynamics Simulations

Prabhakar Misra, Daniel Casimir, Raul Garcia-Sanchez

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United States
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Single-walled carbon nanotubes (SWCNTs) are hollow cylindrical tubes of sp2-hybridized carbon atoms having diameters on the order of nanometers and lengths ranging from microns to centimeters. The thermal expansion property of carbon nanotubes is important for the development of future semiconductor technologies, e.g. in super-capacitors and bio-chemical sensors, and for hydrogen storage applications. In addition, metal oxide nanomaterials used in gas sensors can provide insight into the changes in structure and properties that result from the chemisorption of oxygen in the lattice and the way energy is stored in nanomaterials.

We have examined the characteristics of graphitic and metal oxide nanomaterials using Resonant Raman Spectroscopy at 514, 532 and 780 nm laser excitations using a ThermoFisher DXR Smart Raman spectrometer and a Renishaw inVia Raman Microscope. Computational atomistic analysis of the associated phonon thermodynamics has been performed with the goal of determining the effect that temperature has on the vibrational frequencies of the nanomaterials. The Raman spectra of SWCNTs under thermal loading via two methods, namely laser heating and an external heat cell, were used to demonstrate the bond softening and resultant red-shifting of the various Raman features of SWCNTs. In many future applications of graphitic nanomaterials, the electronic devices may have to endure high temperatures during manufacturing and/or operation, whereby the induced strain and thermal expansion characteristics may serve as significant quality /reliability control factors. Understanding gas-sensing through Raman spectroscopy will help advance the development of sensitive toxic sensors by potentially providing a correlation between the Raman signature and the conductivity changes related to gas sensing in metal oxides.