



2015 INTERNATIONAL YEAR OF LIGHT
AND LIGHT-BASED TECHNOLOGIES

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**



1.00 PM -2.00 PM Lunch		
Session 3		
Venue : Main Hall		
Chair : Prof. John T.S. Irvine (University of St.Andrews, Scotland, U.K)		
02.00 PM – 02.45 PM	Plenary Talk 1– Prof. Mukundan Thelakkat (University of Bayreuth, Germany) Title : Self-assembly Tools to Control Nanostructures in Organic/Hybrid Photovoltaics	
	Session 3a Venue : Kings Court Chair : Prof. John T.S. Irvine (University of St.Andrews, Scotland, U.K)	Session 3b Venue: Executive Club Chair: Prof. Godfrey Louis (Dept. Physics, CUSAT)
2.50 PM - 3.20 PM	IT5 : Prof. Prabhakar Misra (Howard University, USA) Title : Characterization Of Nanomaterials Relevant To Energy Storage and Gas Sensing Applications Using Raman Spectroscopy & Molecular Dynamics Simulations	IT6 : Dr. Manoj Nampoothiri (IISER, Thiruvananthapuram, India) Title : Plasmon Enhanced Power Conversion Efficiency in Inverted Bulk Heterojunction Organic Solar Cell Synthesized in Air
3.30 PM – 4.00 PM	IT7 : Dr. Murukeshan Vadakke Matham (NTU, Singapore) Title : Layered and patterned nanoscale structures for improved absorption in next generation thin film Si solar cells	IT8 : Prof. Sakthikumar (Toyo University, Japan) Title : Application of nanoformulations as theragnostics materials against cancer
Tea/ Coffee Break and Poster Session 04.00 – 06.00		
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

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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.