

THEME: Nanotech for Energy and Environment

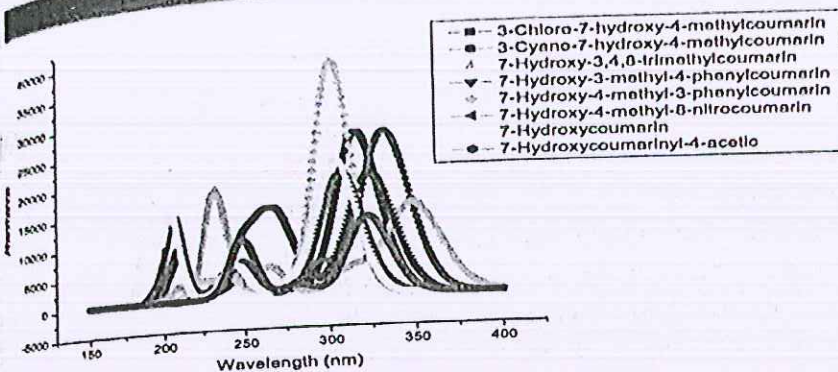
**Coumarin derivatives as Dye sensitized solar cells: A theoretical study using TD-DFT calculations****Mandru V S Prasad<sup>1\*</sup>**, N udaya Sri<sup>2</sup> and B Rajani<sup>3</sup><sup>1</sup>Molecular Spectroscopy Laboratory, Department of Physics, D.N.R.College,Bhimavaram, W.G.Di.-534202, INDIA.<sup>3</sup>Govt. Degree College, Kukalpalli,Hyderabad, Telengana.<sup>\*</sup>Corresponding author. Mobile: (+91) 9440143723; E-mail: prasad2008mandru@gmail.com**Table of contents**

Figure 1. Simulated UV-Visible spectrum of coumarin derivatives using TD-DFT/6-31G(d) level of theory

**ABSTRACT**

Coumarins are used as a component of fluorescence probes based on intramolecular quenching which are employed as reporter of radical reaction in the thin polymer films. Coumarins that contain an electron-releasing group in the 7-position, and a heterocyclic electron-acceptor residue in the 3-position, are recognized as fluorescent dyes for application to synthetic fibers. In this work we have performed comprehensive density functional theory studies of 7-Hydroxy coumarins. Time dependent density functional theory (TD-DFT) calculations have been carried out to study the electronic structure and the optical properties of eight coumarin derivatives. The calculated UV-Vis spectra of 7-Hydroxy coumarins are compared with the experimental spectra of some closely related compounds. Based on the theoretical results of second order hyperpolarizability obtained for these compounds we have found out that the position and width of the first band in the electronic absorption spectra, the absorption threshold and the HOMO-LUMO energy with respect to the conduction band edge are key parameters in order to establish some criteria that allow evaluating the efficiency of coumarin derivatives as sensitizers in Dye Sensitized Solar Cells (DSSC). Those criteria predict the efficiency ordering for the coumarin series in good agreement with the experimental evidence. Presumably, they might be used in the design of new efficient organic based DSSC.

Keywords: Coumarins, DFT, TDDFT, Hyperpolarizability, HOMO-LUMO.



(ISBN: 978-81-924726-4-5)

# SOUVENIR & ABSTRACTS



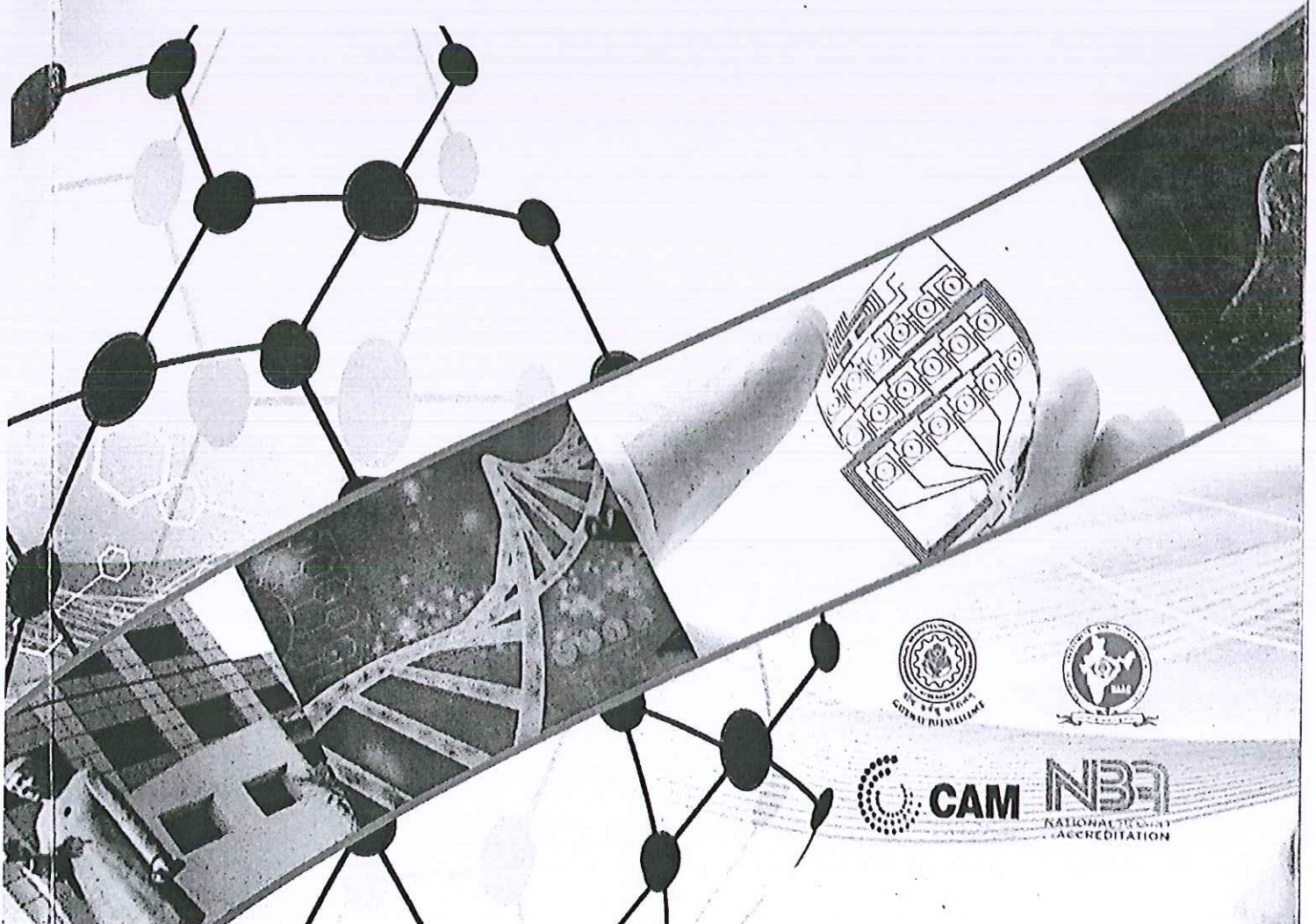
## 2<sup>nd</sup> International Conference on Nano Science & Engineering Applications -2018

4<sup>th</sup> to 6<sup>th</sup> October 2018

Sponsored by TEQIP-III

Organized by

Centre for Nano Science and Technology, Institute of Science and Technology;  
Jawaharlal Nehru Technological University Hyderabad (<http://jntuhist.ac.in/viewdept/14>)  
In Collaboration with Center For Advanced Materials (CAM), Qatar University, Qatar.



**CAM**



**NBA**  
NATIONAL BOARD OF  
ACCREDITATION