



## The 879<sup>th</sup> and 880<sup>th</sup> IMS colloquiums



### Prof. Biman Bagchi

Indian Institute of Science, India

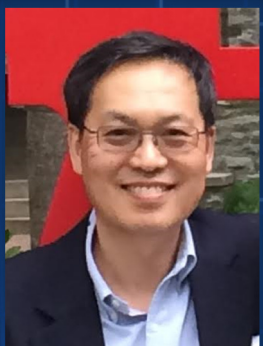
<http://bimanbagchi.com/>

Date&Time: 2015/11/20 (Fri.) 16:00-

Place: IMS Research Building Room 201

### Path from Microscopics to Phenomenological Theories: Examples from Physical Chemistry and Condensed Matter Physics

We shall discuss with several examples drawn from electrochemistry, time dependent statistical mechanics and relaxation phenomena the concepts and methods involved in the transition from molecular approaches to well-known phenomenological expressions.



### Prof. Hyung Kim

Carnegie Mellon University, USA

<http://www.chem.cmu.edu/groups/kim/>

Date&Time: 2015/11/20 (Fri.) 17:00-

Place: IMS Research Building Room 201

### Computer Simulation Study of Carbon-based Supercapacitors with an Ionic Liquid Electrolyte

Electric double layer capacitors (EDLCs), or supercapacitors, are an important energy storage system that offers high power densities and reasonable energy densities. In this talk, we present highlights of our recent molecular dynamics computer simulation study to understand the capacitance behavior of supercapacitors based on carbon materials, in particular, activated microporous carbon and reduced graphene oxide. As an electrolyte, the ionic liquid, 1-ethyl-3-methylimidazolium tetrafluoroborate, is employed. The influence of pore size of the microporous electrodes on the specific capacitance is analyzed by employing carbon nanotube as a model system. Their anomalous capacitance behavior observed experimentally is explained in terms of the solvation effect of ions inside pores ("internal solvation"). In the case of reduced graphene oxide supercapacitors, the influence of the electrode oxidation on the electrolyte structure, cell voltage and capacitance is examined and compared with available experimental results.

Contact: Shinji Saito (Theoretical and Computational Molecular Science)  
Shigeyuki Masaoka & Ryota Iino (IMS colloquium FY2015 committee)