TIFR Centre for Interdisciplinary Sciences
21, Brundavan Colony, Narsingi, Hyderabad 500 075

Seminar

Computational Design of Materials: A Multi-scale Approach

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This talk will focus on applying multiple length scale modeling to understand fundamental material properties and design of new materials with improved properties. In the first half of the talk, a methodology to study non-equilibrium processes, called "The Phonostat" will be presented. This method will be employed to understand the anomalous energy dissipation in carbon nanotubes within the framework of molecular dynamics (MD) simulations. The pathways of energy flow in carbon nanotubes are identified using this method, which will help in improving the quality factor (Q) for sensing applications. The second part of the talk will shed light on the role of grain boundaries (GBs) in energy conversion processes. Here, some results from the density functional theory (DFT) and a device model based on finite element method (FEM) will be discussed. It will be shown that a judicious choice and arrangement of GBs is necessary to improve the efficiency (η) of already best performing crystalline silicon solar cells.

Wednesday, Mar 8th 2017

4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS