TIFR Centre for Interdisciplinary Sciences
21 Brundavan Colony, Narsingi, Hyderabad 500075

Seminar

Towards bottom-up design of materials: Molecular simulation studies of processes relevant to the environment

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Energy storage, water purification, CO_2 sequestration, and green chemistry are some of the key challenges in the purview of sustainable environment. Our research efforts focus on studying some important materials and processes relevant to these fields at the molecular level using molecular modeling and computer simulations. We are motivated by the philosophy that detailed molecular level insights into material behavior enables bottom up design of materials with desired properties. Our current research focuses on two areas related to water desalination and purification:

(i) Gas hydrates: natural reserves of methane gas hydrates can be potential source of energy and means for CO_2 sequestration and water desalination. We study the nucleation, growth and stability of these hydrates under different environments and conditions. Since studying nucleation events in simulations is computationally challenging we have developed novel platforms to enable such calculations. Our results provide an understanding of how the hydrate nucleation can be controlled by changing solution conditions.

(ii) Dendrimers: Dendritic polymers are novel materials that have potential use in environmental remediation such as oil-spill cleanup. In addition, dendrimers have been investigated to generate regenerable antifouling water purification membranes. We have used large-scale simulations to elucidate the association of aromatic contaminants with dendrimers. Our results can provide guidelines to engineer dendrimers for various applications. In my talk, I will highlight the key results from the studies described above and discuss the broader implications of our methods and research.

Tuesday, Jun 2nd 2015

11:30 AM (Tea/Coffee at 11:15 AM)

Seminar Hall, TCIS