Seminar

Speaker: Dr. Malay Kumar Rana

Affiliation: University of Michigan, USA

Title of the Talk:

Solvation behavior of nanoscopic hydrophobic solutes in polar liquids & Carbon capture

Abstract:

Hydrophobic interactions are ubiquitous and play a critical role across diverse scientific fields. However, the interfacial phenomena between hydrophobic solutes and polar liquids are sometime difficult to study by experiment alone. By computational simulation techniques, we have established a clear picture for the behavior of different hydrogen bonded and simple polar liquids in the vicinity of various nanoscopic hydrophobic solutes and in their confined narrow dimensional regions. Studies have been performed for graphene-/graphite-like plates, fullerene, carbon nanotubes etc. embedded in water, ammonia or simple dipolar fluids. Wetting/dewetting of the hydrophobic surfaces or filling/emptying of the confined nanopores and dynamics of the solvents perturbed by the solutes are the main discussions of the talk.

The increased accumulation of CO2 gas in atmosphere has led to the global climate change. This is implicated to the heavy burning of fossil fuel in the power plants. To capture CO2 from flue gas emitted from power plants, viable materials are in search. This talk will also focus on the microporous crystalline materials such as zeolite imidazolate frameworks (ZIF) and metal organic frameworks (MOF) for carbon or CO2 capture applications. We provide insights into the promising materials on the basis of computational calculations. As computational tools, we have applied ab initio simulation techniques based on the density functional theory (DFT), classical molecular dynamics, grand canonical monte carlo etc. in our studies.

Date & Time: 12.11.2013 at 4.00 P.M.

Venue: Boson

Organised by: CBMS Dept.

All are cordially invited to attend the Talk.

Tea/Coffee will be served before the Talk.