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

Internal Seminar

Investigating Statistical Mechanics problems via Molecular Simulations: Two Case Studies (i)Solids and liquids at interfaces (ii)Thermodynamics of Buettiker-Landauer Brownian Motor

Ronald Benjamin

Heinrich-Heine University, Duesseldorf

Molecular simulations have become an important tool to investigate problems related to Statistical Mechanics. Here, I present two cases where we have used such simulations to obtain useful information about the system under investigation. In the first case, I discuss a Brownian motor driven by a spatially inhomogeneous temperature bath. Using Molecular Dynamics, we validate the Langevin and Fokker-Planck equations as well as show that such a motor cannot reach Carnot efficiency in the quasistatic limit, establishing the failure of over-damped models (Brownian dynamics) in determining the heat flow when temperature is non-uniform. In the other study I present a novel molecular simulation technique to determine the free energy of interfaces between solids and liquids which is an important parameter governing nucleation, crystal growth and wetting behavior of a crystal near a wall. A direct determination of this quantity is not possible in experiments and indirectly the available estimates are unreliable. Our computational scheme yields accurate estimates of this quantity for systems interacting via model potentials such as Hard-Spheres and Lennard Jones.

Friday, Oct 28th 2016

2:00 PM (Tea/Coffee at 1:45 PM)

Seminar Hall, TCIS