Departmental Seminar

Speaker: Mr. Snehasis Daschakraborty

Affiliation:

Dept. of Chemistry and Biochemistry, University of Colorado, Boulder, USA

Title of the Talk:

Carr-Parrinello Molecular Dynamics Simulation: How it works?

Abstract:

The Car–Parrinello method, proposed by Roberto Carr and Michele Parinello, is a special type of ab-initio molecular dynamics technique where the molecular dynamics and the density functional theory have been tactfully combined.1-3 This method shows that the coupling between nuclear time evolution and electronic minimization could be treated efficiently via an implicit adiabatic dynamics approach. A fictitious dynamics for the electronic orbitals is invented which, given orbitals initially at the minimum for an initial nuclear configuration, allows them to follow the nuclear motion adiabatically, and thus, be automatically at the approximately minimized configuration at each MD step. In this technique electronic energy is not needed to minimize at each step and therefore the computational cost decreases significantly and various natural processes can be studied efficiently.

In this talk the underlying theory behind this above approach and examples of its various applications will be shown.

References:

1. Carr, R.; Parrinello, M. Phys. Rev. Lett. 1985, 55, 2471–2474.
2. Marx, D.; Hutter, J. Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods; Cambridge University Press: Cambridge, 2009.
3. Tuckerman, M. E. J. Phys.: Condens. Matter 2002, 14, R1297–R1355.

Date & Time: 21.01.2014 at 12.00 Noon

Venue: Fermion

Organised by: CBMS Dept.

All are cordially invited to attend the Talk.