



Department of Physics Himachal Pradesh University, Shimla

(UGC SAP and DST FIST Funded Department)

SEMINAR CUM WORKSHOP ON FIRST PRINCIPLE AND OTHER SIMULATION METHODS IN CONDENSED MATTER PHYSICS (March 22-29, 2010)

(Organised Under UGC Special Assistance Programme)

In the last two decades Physics, Condensed Matter Physics and other Physical and Applied Sciences have seen the usage of simulation methods in to understand matter and materials, which broadly speaking use Classical Molecular Dynamics, *Ab-initio* Molecular Dynamics using Density Functional Theory and Monte Carlo Methods. Using these methods very interesting large scale simulations have been done to study crystalline materials, liquids, nano-structures, and quantum transport in nano systems.

In this field a number of open source initiatives have been taken which have proved very effective in broadening the scope of understanding the properties of real materials including their structural properties, electronic properties and transport properties involving large number of researchers around the world. Some of the open source codes available include SIESTA (*Spanish Initiative in Electronics Simulations Using Thousands of Atoms*) based on linear scaling Density Functional Theory (DFT) and LAMMPS (*Large Scale Atomic Molecular Massively Parallel Simulator*) of Sandia Laboratory U.S. In the current workshop, of 8 days duration (From 22nd to 29th March 2010, it is proposed to cover the following topics :

- ◆ Introduction to simulations in condensed matter physics.
- ◆ Basics of first principle calculations and DFT.
- ◆ Abinitio calculations using different basis functions.
- ◆ Basics of pseudo potential and abinitio pseudopotential generation and testing.
- ◆ Total energy calculation using SIESTA.
- ◆ Overview of molecular dynamics simulation using LAMMPS.
- ◆ Issues related with installation of SIESTA and LAMMPS on serial mode and on parallel machines will also be discussed.
- ◆ Hands on through case studies.
- ◆ Lectures in frontier areas of Theoretical and Experimental Condensed Matter Physics.

Young research scholars and young faculty members in the universities, institutes and colleges are encouraged to participate. The number of participants will be restricted between 35 and 40. Participants having experience of working in Linux environment and having basic knowledge of FORTRAN or C will be given preference.

It is proposed to have invited lectures from experts drawn from various leading research institutes/ Indian Institutes of Technology and Universities. The tentative dates proposed are: 22nd March 2010 to 29th March 2010. The participants will be charged registration fee and accommodation charges. Effort is being made to get funding from agencies like DST, CSIR, BRNS, New Delhi and financial support from Himachal Pradesh University.

Application Form can be downloaded from HP University Web Site (www.hpuniv.nic.in).

Registration Fee: Rs. 1500/- (This includes, seminar cum workshop material, working lunch and tea during working sessions). Accommodation charges will be separate as per actual in University Faculty House or Local Guest Houses. Registration should be sent by Crossed Demand Draft in favour of **Coordinator, SAP, Physics Department, Himachal Pradesh University Shimla.**

IMPORTANT DATES

Last Date for Registration: 28th February, 2010

Intimation regarding selection for participation: 3rd March 2010. List of selected participants will be displayed on HP University web site: www.hpuniv.nic.in

ORGANIZING COMMITTEE

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CONVENER

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ORGANIZING SECRETARY

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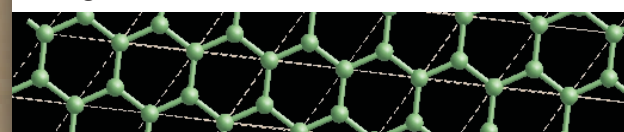
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For more details please visit following website:
<http://www.hpuniv.nic.in>