Winter School on Electronic Structure and Molecular Dynamic Simulations using Open Source Softwares: From Theory to Practice

Sept. 27 - Oct. 4, 2020

Introduction

The winter school aims to introduce graduate students and young researchers to the basic concepts of computational simulations, with an emphasis on density-functional theory-based methods and classical molecular dynamics simulations. Density functional theory (DFT) is one of the important tools in the area of materials research to understand the properties of materials, complement the experimental results, and design new materials. Molecular dynamics (MD) simulation is used to study the conformational space and properties of large molecules such as biomolecules and materials like carbon nanotubes and polymers. The school will provide hands-on sessions with tutorials in DFT and MD to the participants and HPC facilities for a month to familiarize and train themselves with the concepts taught in the school.

Topics Covered

The school is divided into two parts - electronic structure calculations and classical molecular dynamics simulations. In the first 4 days, the following topics in electronic structure theory will be covered
(Day-1 to Day-4):

1. Basics of ground-state DFT and Kohn-Sham equations

2. Pseudopotentials

3. Structural optimization

4. Spin polarization including non-collinear magnetism

The second part of the school covers the following topics from MD simulations (Day-5 to Day-7):

1. Basics of MD simulations & demonstration with Gromacs

2. Docking studies with Auto dock vina

3. Topology creation with AmberTools

Apart from the above schedule, a brief training on Linux OS and bash scripting will be provided on Day-0.

Resource Persons

Dr. Prasenjit Ghosh
IISER Pune

Prof. Miroslava Nedyalkova
Sofia University, Bulgaria

Dr. Rajendra Adhikari
Kathmandu University, Nepal

Dr. K. C. Bhamu
Gramin Mahila P. G. College, Rajasthan

Dr. Hridya V. M.
IISER Pune

Dr. R. S. Swathi
IISER Thiruvananthapuram

Dr. Anmol Kumar
University of Maryland, Baltimore, USA

Dr. Reman Kumar Singh
IIT Bombay

Dr. Ayush Agrawal
Raman Research Institute, Bengaluru

*** LIST TO BE UPDATED**

Dr. Praveen C. S.
Cochin University of Science and Technology, Cochin

Dr. Subrahmanyam Sappati
Raman Research Institute, Bengaluru

Dr. Wilbe D Sasikala
Govt. Medical college, Thiruvananthapuram

Dr. Pramod P. S.
Govt. Medical college, Thiruvananthapuram

Registration

This winter school will be open for Ph. D. students, Post-docs, and faculty members. The maximum number of participants is restricted to 50 and those interested are required to register online. After a participant is selected for the winter school an email will be sent to the participant with the mode of payment and payment link.

Registration Details

Designation	Early Bird	After Deadline
Research Scholar	₹ 1800	₹ 2000
Post Doctorate	₹ 2200	₹ 2500
Faculty	₹ 3500	₹ 4000

I. All registration fees include 18% GST
ii. Early Bird Registration Deadline: 12th September 2020
iii. Final Registration Deadline: 21st September 2020

Jointly Organized By
Parvatibai Chowgule College of Arts and Science (Autonomous), Goa - India
& Supercomputer Center, Kathmandu University, Nepal

Technical Partners

NREN SUBISU

SCAN TO REGISTER

Dr. Ashish M. Desai (Convenor): amd006@chowgules.ac.in, 9869356356; Dr. Rajendra P. Adhikari (Convenor): rajendra.adhikari@ku.edu.np;
Dr. Praveen C.S. (Co-Convenor): mnr.praveen@gmail.com

Register At : https://tinyurl.com/y2qptbzy