In Silico Approach for Modelling New Materials: Methodology & Applications

(January 14-20, 2019)

Material science has played a pre-eminent role in modern scientific and technological developments. The invention of new materials is bringing paradigm shift the way new technologies are emerging. In the last couple of decades with the cost effective and powerful computation platforms the in silico material design has opened up new opportunities to design and tailor materials properties using first principle DFT approach leading to a wonderful synergy between in-situ approach and in-silico approach.

Department of Physics and Astronomical Science (DPAS); Central University of Himachal Pradesh (CUHP), Dharamshala is organizing a national level one week workshop titled ***In Silico Approach for Modeling New Materials: Methodology & Applications*** during *January 14-20, 2019*. The main focus of the workshop is to introduce to the students, young researchers and faculty members the basic theoretical background and tools of density functional theory (DFT) based approaches to compute various material properties following a hands on and minds on methodology to demonstrate their application to materials ranging from Bulk to Low Dimensional Systems.

Some of the key aspects proposed to be covered during workshop will include

- *Quantum mechanics of materials*
- *Theoretical challenges to obtain exact quantum mechanical solution for real materials,*
- *Various approximations, and idea of density functionals*
- *Hohenbers-Kohn-Sham approach to DFT, the challenge of exchange-correlation energies and ad-hoc solution for the same,*
- *Idea of local density approximation (LDA) and generalized gradient approximations (GGA),*
- *Idea and application of pseudopotentials, full-potential methods.*
- *Magnetism in DFT*
- *The application of DFT for computing structural, electronic, magnetic, transport, optical and thermal properties of real bulk and nano-scale materials*
- *Hands-on-sessions. For the practical usage of free-open-source software packages such as (ELK, SIESTA, QUANTUM ESPRESSO, SPRKKR, BOLTZTRAP, GULP etc.).*
- *Classical and Quantum Molecular Dynamics*

The overall goal of above workshop is to give participants a quick but complete exposure of modern materials modelling techniques so as to equip them with additional tools for new innovations in material science.

Last Date for Application: December 10, 2018

Confirmation of Acceptance: December 15, 2018

Last date for Registration: December 20, 2018

Date of Conference: January 14-20, 2019

Registration Fee

Research Scholars: Rs. 3,000/- . *Faculties & Scientists*: Rs. 4,500/- Registration fee shall cover working lunch, refreshments for duration of workshop, conference kit. For paying registration fee, the participants should transfer/deposit the amount to university account as per following details:

Name of the Bank: Canara Bank Dharamshala;
Account name: Central University of Himachal Pradesh;
Account number: **2062101009593**;
IFSC Number: CNRB0002062

The details of transaction should be sent via email to jagdishphysicist@gmail.com on or before last date for registration.

Chief Patron: Prof. (Dr.) Kuldeep Chand Agnihotri,
Honorable Vice Chancellor, CUHP, Dharamshala (HP)

Patron: Prof. H. R. Sharma,
Pro Vice Chancellor, CUHP, Dharamshala (HP)

Chairman: Prof. B. C. Chauhan
Dean (SOPMS) and Head (DPAS), CUHP, Dharamshala (HP)

Co-Chairman: Dr. O.S.K.S. Sastri
Professor, DPAS, CUHP, Dharamshala (HP)

Resource Persons

- Prof. Sushil Auluck (Retd. IIT Roorkee)
- Prof. P. K. Ahluwalia (Retd. HPU Shimla)
- Dr. Jiji Pulikkotil (NPL, New Delhi)
- Dr. Ashok Kumar (CU Punjab)
- Dr. Yogyata Pathania (IISER Mohali)
- Dr. Arun Kumar (SVGC Ghumarwin)
- Dr. Munish Sharma (MAU, Solan)
- Dr. Jagdish Kumar (CUHP)
- Dr. OSKS Sastri (CUHP)

Boarding/Lodging

Depending upon availability of funds, we may provide free shared accommodation to participants in nearest hotels/guest houses. However, if we fall short of funds or anyone wants individual accommodation, the participants have to arrange the same at their own expenses. Organisers may provide necessary information and support for the same.

Total Intake

The maximum number of out stationed participants shall be limited to 30. In case we find large number of requests, the preference will be given to research scholars, young faculty members, who are actively engaged with research in material science. The final decision for selection of a candidate for his/her participation will be of organizing committee.

Application Procedure

The applicants interested to participate in the workshop should fill the Performa given at the end of this brochure and send it latest by 10th December 2018 by email to jagdishphysicist@gmail.com

For any further details contact:

Dr. Jagdish Kumar, Assistant Professor, DPAS, CUHP,
Email: jagdishphysicist@gmail.com;
Mobile: +91-8627871474

Dr. Rajesh Kumar Singh, UGC-Assistant Professor, DPAS, CUHP, Dharamshala (HP) Email: rksbhu@gmail.com;
Mobile: +91-9451134253

Website: www.cuhimachal.ac.in

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About Central University of Himachal Pradesh

The Central University of Himachal Pradesh has been established under Central Universities Act 2009 of Indian Parliament and has been operating near beautiful city Dharamshala in Himachal Pradesh since 2010. The University is funded and regulated by the University Grants Commission (UGC). Currently CUHP has a total of 11 schools of studies in different areas varying from basic sciences, business administration, tourism and travel.

The Department of Physics and Astronomical Science is one of the departments under School of Physical and Material Sciences. Currently department is offering undergraduate courses (B.Sc. Honours in Physics), post graduate (M.Sc.) and PhD programs. Department has highly qualified faculty with expertise in different areas of physics such as Material science, Nuclear and Particle Physics, Astronomical Science, Nanomaterials. The expertise of faculty varies from hard core theoretical physics to cutting edge areas of experimental physics. Department of Physics and Astronomical Science is striving hard to establish state-of-the-art research facilities in different areas of physics leading to quality research and innovation.

About Dharamshala

Dharamshala is an international destination Serene Location, pleasant climatic condition, spiritual atmosphere of the location provides an attractive ambience conducive to academic pursuits. Located in the footsteps of perennially white Dhauladhar range of Himalayas, the city of Dharamshala has many magnificent places to visit. A few to mention are: McLeodGanj, the home place of renowned spiritual leader Dalai Lama, International Cricket Stadium, Norbulingka monastery famous for beautiful ambience and Tibetan culture, famous Naddi village offering mesmerizing view of Dhauladhar. An exhaustive list of tourist destination near Dharamshala can be found at http://www.hill-stations-india.com/dharamsala/.

Performa for Application

Name: _____

Sex: Male/Female (To plan and allot accommodation)

Institution:_____

Current Occupation:_____

Educational Qualification:_____

Contact Information:

Mobile No.:_____

Email:_____

Current Research Interests:_____

Research Experience: (Here mention briefly about research work you have done and for how much time you have been working/have worked in that field)

Motivation for attending this workshop: In not more than 100 words. How you think this workshop will benefit you?

Have you ever worked in Linux: Yes/No (This is just to design contents accordingly)

Have you ever worked on Linux command line: Yes/No

Do you require shared accommodation: Yes/No

Would you like to share a brief oral presentation your research results: if Yes (Mention title of your presentation)