CSIR-NCL Integrated Skill Initiative

Skill Development Course in

Density Functional Theory

Course Code: SDP-NCL18

Duration: 2nd to 20th July, 2018, 3 Weeks

Number of Participants: 20-30

Eligibility: M. Sc., M. Pharm., B. E., B. Tech., M. E., M. Tech.

Course Fees:

- Students: Rs.10,000/-
- Faculties: Rs. 25,000/-
- Industry Participants: Rs. 50,000/-

(Fee includes breakfast, tea and lunch)

Accommodation (Three weeks + 2 days):

- Students: Rs. 500/-
- Faculty/Professionals: Rs. 1000/-

Participants can make payment either by DD or Online Transfer. For details see SDP website

About the course: Density functional theory (DFT) is a state-of-the-art computational method for bringing out correlation between the structure and properties within systems ranging from molecules to surfaces to bulk. It is the most widely used methodology in chemistry and materials science for understanding processes, mechanisms and response properties. Employing DFT, one can understand why one chemical reaction happens and another does not, and thus is exteremely useful in predicting the properties of newly developed molecules and materials. This course will provide all the necessary know-how, starting from an elementary level, of the fundamental concepts of DFT, as well as how one can apply it for solving problems in physics and chemistry. In the course, both atom centered and plane wave based methods will be covered.

A candidate who has taken up this course will have: (i) an overall broad perspective of different methodologies in quantum chemistry and their applicability, (ii) an ability to perceive applications of quantum chemical codes to his/her research areas, (ii) an ability to apply the codes so as to extract the properties and fingerprint it with his/her experimental data, (iv) and finally with her/his own bit of homework can eventually gain expertise on the applications of quantum mechanics (QM) to realistic systems.

Course Content: **(a) Theory** Concepts of QM; Hartree Fock and DFT; pros and cons of DFT; theoretical understanding on the application of DFT to various problems ranging from molecules and surfaces to bulk, geometry relaxation algorithms; concepts of simulations.

(b) Practical Hands on training: Linux OS; Usage of graphics software's such as Molden, xCrysden etc.; an understanding of Z matrices and inputting molecular structure data for calculations such as geometry optimizations as well as transition state optimization calculations; reactions on surfaces; computing spectra (IR, UV, Raman, NMR etc.) for various molecules and comparing them with experimental ones; simulating the behavior of clusters/surfaces /bulk.

How to Apply

Application form is available at

http://www.ncl-india.org/files/SDP/Default.aspx

Mailing Address

Coordinator,

CSIR-NCL Skill Development Program, CMC Division, CSIR- National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India.

Email: ncl.sdtc@ncl.res.in

(email applications are accepted)