Computational Electronic Structure Methods for Atomic, Molecular and Solid-State Systems

A short course organized by IIT Bhubaneswar

through the GIAN Scheme under MHRD, Government of India

Overview

In recent times there has been a rapid growth in chemical, material and biological sciences. Consequently, there has been a lot of great discoveries and novel observations in these areas. Now there is a huge interest in explaining these findings from a fundamental theoretical framework — at the level of basic molecular interactions. Needless to say, understanding these at a fundamental level is the key to developing newer and better technologies, materials and medicines.

The tools necessary to investigate these interactions, commonly termed as Electronic Structure Methods, are being polished to the perfection for last 5-6 decades. However, there has been a huge 'communication gap' between the developers and the potential users of these tools. This is because the methods had to evolve with time in order to deal with the emerging complex phenomena that they should describe at the expense of apparent loss of simplicity.

This course attempts to bridge the gap by helping the participants learn the background theory as well as providing them with hands-on training on the latest and greatest tools from the computational electronic structure theory repertoire.

Modules	• **Module-I: Background: July 08 --10 (Sunday) [3 days]** **(**Basic linear algebra, basic quantum mechanics). • **Module-II: Methods: July 11--12, 14--15 [4 days; July 13 off]** (Hartree-Fock, Configuration Interaction, Coupled Cluster, MCSCF, MRCI, DFT) • **Module-III: Applications: July 16--18 (Friday) [3 days]** (Geometry optimization, thermochemistry, applications in scattering theory and dynamics) **Registration starts on: May 16, 2016** **Last day for registation: June 30, 2016**
You Should Attend If…	You are a student, a researcher, a scientist or an engineer insterested to learn about the underlying principles behind modern quantum chemistry tools, their relative merits/applicability, as well as how to apply them to • explain the structure and reactivity of chemical and biological systems • explore chemical/biological reaction pathways • design new materials/ drugs and investigate their efficacy **Number of participants for the course will be limited to fifty.**
Fees	• **Students (B.Sc./B.Tech./M.Sc./M.Tech./Ph.D.):** Rs. 2,000. • **Paricipants from academic/technical/R&D institutions:** Rs. 5,000. • **Paricipants from industry:** Rs. 7,000. • **Participants from abroad:** US$ 200. The above fee includes all instructional materials, computer use for tutorials and assignments, and 24-hour free internet facility. The participants will be provided with accommodation on payment basis.

The Faculty

Prof. Danny L. Yeager is a full professor at Texas A&M University, College Station, TX, USA. He is one of the pioneers of quadratically-convergent multi-configurational self-consistent field theory, a very accurate and computationally tractable electronic structure method. Later he developed multiconfigurational spin-tensor electron propagator, a Green's function based method to compute ionization potential and electron affinities from a multiconfigurational reference state for highly correlated systems. He also developed multi-reference based framework to investigate transient electron-atom/molecule scattering resonances. He is the author of more than 100 research articles in reputed international journals. He has also been an excellent teacher at Texas A&M where he has taught several courses including quantum chemistry (introductory and advanced level), statistical mechanics and physical chemistry courses over a period of about four decades.

(http://www.chem.tamu.edu/rgroup/yeager/)

Dr. Kousik Samanta is an assistant professor at Indian Institute of Technology Bhubaneswar. His research involves development of theoretical tools to investigate bound and temporarily-bound states, non-adiabatic effects and dynamics. He teaches quantum chemistry (introductory and advanced level), and computational methods and applications courses at IIT Bhubaneswar.

(http://www.iitbbs.ac.in/profile.php/kousik/).

Government of India

Important Dates

Registration Deadline: June 30, 2016

Classes start: July 08, 2016
Classes end : July 18, 2016

Venue

Indian Institute of Technology Bhubaneswar
Bhubaneswar, Odisha 751007, India
www.iitbbs.ac.in

Course Coordinator

Dr. Kousik Samanta
Phone: +91-674-254-6088 (Office)
+91-707-709-4766 (Mobile)
E-mail: kousik@iitbbs.ac.in

School of Basic Sciences
Indian Institute of Technology Bhubaneswar
Bhubaneswar, Odisha 751007, India

.....

Register online at:
http://www.gian.iitkgp.ac.in/GREGN

(Registration deadline: June 30, 2016)