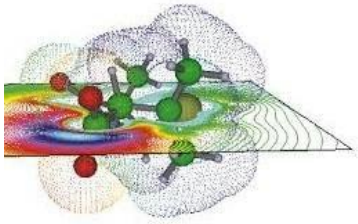

Savitribai Phule Pune University

National Workshop on
Electronic Structure Methods: Density Functional Theoretic Perspectives (NWESM-2016)

March 01-03, 2016

Organized By

Department of Chemistry
Savitribai Phule Pune University,
Pune-411007.

ABOUT THE UNIVERSITY

Pune is the educational hub of Maharashtra with number of educational and technical institutes imparting the knowledge to thousands of students for many years. This gives an extra aura to the city along with its historical background and importance. The city has many historical places to visit which gives the idea of its place in the history of Maharashtra and India. The city has drawn the attention of IT companies for last several years and now days it has become leading IT hub in India. The Savitribai Phule Pune University (formerly University of Pune) is one of the premier universities in India ranked 3rd in the country in the recent survey. It was established on 10th February, 1949 and is situated in 411 acre of area in north-western part of Pune city. With 46 academic departments on the campus, about 307 recognized research institutes and 612 affiliated colleges come under its jurisdiction. It is popularly known as 'Oxford of the East'. Students from all over India and other countries join university for their studies. The university has hostel facility, health centre, the competitive examination centre, and many other facilities. Many renowned centers like IUCAA, NCRA-TIFR, C-DAC and NCCS are also situated in the university campus. The climate during March is pleasant.

ABOUT THE DEPARTMENT

The Department of Chemistry is one of the earliest departments in the University established in April 1950. The department offers programs leading to M.Sc., M.Phil and Ph.D. degrees. Department of Chemistry is rated as one of the best in the country for its teaching and research activities and UGC has recognized it as Centre for advance Studies (CAS). The department has close collaboration with the National Chemical Laboratory (NCL), Pune and BARC Mumbai, for teaching and research activities. The department is also supported under the DST-PURSE and DST-FIST programs. Various other government funding agencies viz. CSIR, DST, DAE, INSA, ISRO, DRDO, C-DAC have also given funds for execution of research projects.

SCOPE OF WORKSHOP

This National Workshop on "Electronic Structure Methods: Density Functional Theoretic Perspectives (NWESM-2016)" will highlight importance of theoretical and computational chemistry methodologies through a series of invited lectures and tutorials/practical sessions by eminent scholars/faculty/scientists from research institutes/Indian Universities covering theory as well as applications of modern density functional theory.

THEME OF THE WORKSHOP

The National Workshop on "Electronic Structure Methods:Density Functional Theoretic Perspectives (NWESM-2016)" from March 01-03, 2016 is being organized by Department of Chemistry, Savitribai Phule Pune University. Density Functional theory (DFT) originated with the pioneering works of Hohenberg and Kohn (1964) endowed the status of basic variable to electron density (3-dimensional entity compared to 3N dimensional wavefunction). Development of Kohn Sham SCF theory has enabled one to compute structural, spectral and energetic unraveling interactions in molecular systems upto nearly 100 or more atoms to a varying degree of accuracy through local density-, generalized gradient-, and meta generalized gradient approximations. Modern density functional theory has emerged as an important interdisciplinary discipline encompassing diversified areas. A variety of software programs such as GAUSSIAN09, TURBOMOLE, VASP etc. incorporating modern density functional theory have become available to date. Nonetheless the underlying theoretical methods have not been dealt with in details in most of the academic of PG or pre-Ph. D. courses curricula. The present workshop will precisely focus on these aspects to unravel of molecular interactions using computer modeling as a tool. Computational Chemistry finds applications in diverse areas such as catalysis, nanotechnology, chemical and biosciences. The Workshop will emphasize on theoretical perspectives of DFT methods and encompass

- *Introductory Hartree Fock Theory and correlated Methods*
- *Hohenberg Kohn Theorem, exchange correlation*
- *Kohn Sham SCF method*
- *Modern functionals in dispersion corrected DFT*
- *Time Dependent Density Functional Theory*
- *Applications of DFT*

SELECTION CRITERIA

Interested research students/faculty members at the colleges or Indian Universities/Academic institutes should send their application in the prescribed format to the Convener, NWESM-2016, Department of Chemistry, Savitribai Phule Pune University, Pune-411007, in the form of a hard copy or by e-mail to *stcg@chem.unipune.ac.in* on or before February 29, 2016. The participants need to be actively engaged in teaching or research related to computer modeling or electronic structure calculations or using these methods to support their findings. A background of 'Elementary Quantum Chemistry' and 'Chemical Bonding' is desirable for attending the workshop.

Registration Fee:

- Faculty : Rs. 1,000/-
- Participants from Industry : Rs. 1,500/-
- Research Scholars : Rs. 500/-

Deadline of Registration: February 29, 2016

The number of participants is limited to 30.

Selection for attending the workshop would be solely at the discretion of NWESM-2016 Local Organizing Committee. The registration fee includes Workshop kit, lunch and dinner. Because of limited funds the outstation participants are requested to make their own arrangements for accommodation.

Acceptance of Participation**:** Will be communicated by February 29, 2016

CORRESPONDENCE ADDRESS

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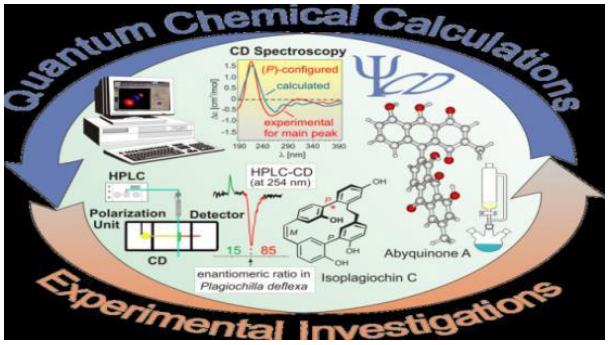

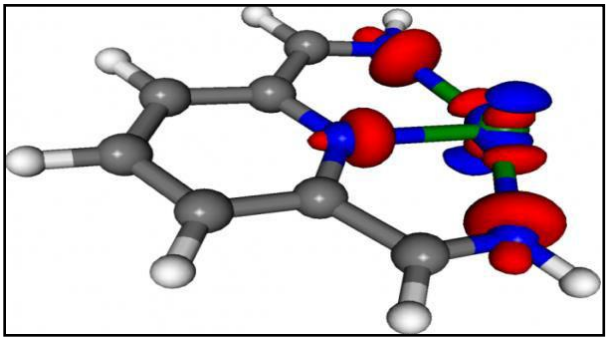

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Hon'ble Vice-Chancellor,
Savitribai Phule Pune University

Patron

Dr. V. B. Gaikwad,
Director, BCUD,
Savitribai Phule Pune University

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REGISTRATION FORM

National Workshop on

Electronic Structure Methods: Density Functional Theoretic Perspectives

(NWESM-2016)

Organized By
Department of Chemistry
Savitribai Phule Pune University, Pune-411007
March 01-03, 2016

Delegate Name: (Professor/Dr./Mr./Ms)

_____

Address: _____

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Tel No: _____ Mobile No: _____

E-mail: _____

Gender: (M / F**): _____**

Registration fee: (Faculty / Industry / Research scholar)

Dated: _____ Amount (Rs.): _____

Signature: _____

Contact Email: *stcg@chem.unipune.ac.in*