DST – SERB SPONSORED ONLINE WORKSHOP ON

# ELECTRONIC STRUCTURE CALCULATIONS FOR MOLECULES AND MATERIALS

**FROM 17th TO 24th APRIL, 2023**

**Organized by**

**Department of Physics, Bharathiar University**

**Coimbatore – 641 046, Tamil Nadu**

The objective of this workshop is to inculcate knowledge of basic features and recent developments in electronic structure calculations for molecules and materials to young researchers and faculty members working in this area of research.

Electronic structure calculations, based on molecular orbital, density functional theory, molecular mechanics, and dynamics have been widely used to study the properties of molecules and materials, and these areas of research have become increasingly important over the last 30 years because of the developments in theories, methods and increase in computational power. Initially, this research area starts with theories and methods for atoms and simple molecules. Now, the applications are spread across various areas, including material science, atmospheric and biochemical reactions, drug design and development, etc. A quite good number of scientists from our country have actively contributed to the development of various theories and tools of computational quantum chemistry. At present, in line with the world scenario, a large number of researchers of our country are actively working in this area of research.

For this workshop, the following eminent researchers have accepted to be a resource persons and deliver the lectures online; Dr. Pratim Kumar Chattaraj, IIT, Kharagpur, Dr. K. R. S. Chandra Kumar, BARC, Mumbai, Dr. Nisanth N. Nair, IIT, Kanpur, Dr. Arun Venkatanathan, IISER, Pune, Dr. P. Ravindran, CUTN, Thiruvarur, Dr. Ganapathy Vaitheeswaran, UoH, Hyderabad, Dr. R. S. Swathi, IISER, Thiruvananthapuram, Dr. L. Senthilkumar, BU, Coimbatore, Dr. Saurabh K. Singh, IIT, Hyderabad, Dr. L. Sandhiya, CSIR, New Delhi.

In this workshop, theories, and recent developments in wavefunction based Hartree-Fock and post Hartree-Fock methods, density functional theory methods for molecules and materials, classical and ab-initio molecular mechanics and dynamics methods will be trained. In addition, the specific tools and methods used for various applications will be highlighted.

This online workshop is through google meet from 9.30 AM to 5 PM. Only a limited number of participants will be allowed. Interested people must register online, https://forms.gle/3Zz35GPygDSTiq4B7 and a permission letter (template is available on the workshop registration page) issued by the research Supervisor/Head of the department for research scholars, and the Principal of the college/the Director of the institute/the Registrar of the university for faculty members/permanent employees should be sent. The duly filled and signed letter should be sent to the convenor of the workshop by speed post/courier. Registration is open from 15.02.2023 to 31.03.2023. The selected applicants will be informed during the first week of April through email, and a google meet link will be shared to attend the workshop. The participation certificate will be given only to the participants who have attended all the sessions of the workshop. For further details, visit the website: https://b-u.ac.in/288/escmm or the convenor of the workshop may be contacted.


Convenor:

**Dr. K. Senthilkumar**

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