



United Nations
Educational, Scientific and
Cultural Organization



ICTP - East African Institute
for Fundamental Research
under the auspices of UNESCO



Mini-African School on Electronic Structure Methods and Applications (MASESMA)

11 November – 15 November, 2019

University of Rwanda, Kigali, Rwanda

Background and purpose

The properties of materials are dictated by the interactions of the electrons and the atoms in the system. Once we know the configuration of atoms in a system, we can, in principle, predict its behavior: whether the material will be an insulator or conductor and how conducting it will be, how hard the material will be, how reactive the compound will be, whether it will superconduct or not, what color it will appear to be, whether it will be magnetic or not, and many other properties. The goal of this mini school is to train researchers in the fundamentals of the behavior of electrons (“electronic structure”) that can be useful in predicting properties of chemical compounds and helpful in discovering new materials. An intense 5-day school will be conducted at the ICTP-EAIFR premises of the University of Rwanda, Kigali in order to introduce participants to Electronic structure theory/method and some applications.

Topics covered

- * Introduction to Quantum Mechanics of many-particle systems
- * Born-Oppenheimer approximation: decoupling electrons and nuclei motion
- * Hartree-Fock Theory and Slater Determinants
- * Configuration Interaction Method
- * Density Functional Theory
- * Basis Functions and Pseudopotentials
- * Recovering electron correlation
- * Excited States
- * Hands on applications with electronic structure codes

Participation Information

University lecturers in solid state physics, quantum chemistry, materials science and related fields, as well as advanced post-graduate students (masters and doctoral levels) are encouraged to apply. Women candidates are strongly encouraged to apply. Selection of participants will be based on their technical background. Priority will be given to applicants who are familiar with quantum mechanics and scientific computing and who will be presenting posters of their current work. There is no registration fee. A limited number of grants are available to support attendance of some selected participants. To apply, send your CV to: workshop20191111@eaifr.org and fill the form here: <https://forms.gle/jjkr5fo6T3KoTxkc9>

Deadline for application: October 20, 2019

For further information contact: info@eaifr.org or workshop20191111@eaifr.org