United Nations Educational, Scientific and Cultural Organization

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

Regional-African School on Electronic Structure Methods and Applications (RASESMA) with ABINIT

27 – 31 January, 2020

University of Rwanda, Kigali, Rwanda

Background and purpose

The determination of many material properties, even before synthesizing the compounds, is possible through first-principle methods. These first-principles approaches rely typically on Density Functional Theory (DFT). 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 DFT and its applications in the prediction of properties of matter. The goal of this regional school is first, to teach researchers DFT and its applications to real life systems and secondly, to train them on how to carry out practical calculations for chemical compounds on the computer. The computation will be carried out using the ABINIT software program with experts present to guide in the optimal ways to use the codes for studying materials and their properties. At the end of the school, participants will have a deeper understanding of DFT and its applications (and limitations) and will be able to determine the properties of existing and novel materials and compounds of their choice.

Topics covered

* Introduction to (ground state) Density Functional Theory
* Planewaves and Pseudopotentials
* Band structure calculations
* Determination of electronic, thermodynamic, and mechanical properties of matter
* Introduction to determination of response functions and excited state calculations
* Hands on applications with the ABINIT software program (http://www.abinit.org/)

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) **in the East and Central African regions** are encouraged to apply. Women candidates are strongly urged to apply. Participants will be selected 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: **workshop20200127@eaifr.org and fill the form here:** https://forms.gle/qUz4XR8hXuCm1Jam9

Deadline for application: November 17, 2019

For further information contact: info@eaifr.org or workshop20200127@eaifr.org