Density Functional Theory and Molecular Dynamics Workshop

7th – 8th April 2022
Masinde Muliro University of Science and Technology
School of Natural Sciences, Kakamega, Kenya

The workshop aims at introducing and enhancing understanding of *ab initio* calculations and molecular dynamics simulation to researchers in natural sciences and engineering disciplines.

Description:

Electronic structure methods have become mature enough to be used by scientists not trained in the development of the methods themselves. This is a shift away from traditional practice, in which the know-how and the right to use the code was acquired through a long internship. Nowadays, most codes are distributed with very light licensing restrictions. While this ease of access is in principle a good thing, it carries the risk of uncritical or poor use of the codes by untrained people. Thus, there is an increasing demand for training in the sensible use of these methods, with the goal that the prospective user understands the physical and main technical approximations behind a method. The electronic structure codes such as Quantum Espresso, Siesta and LAMMPS have become quite popular and are increasingly being used by researchers in geosciences, biology and engineering. This workshop aims at introducing these codes to researchers in physical, biological and engineering disciplines and increase proficiency of the existing intermediate users.

Topics:

- Basics of density-functional theory, molecular dynamics simulation and geometry relaxation;
- Generation and use of *pseudo-potentials*;
- Construction of basis sets of strictly localized numerical atomic orbitals;
- Localization for linear scaling both in the computation of the matrix elements and in the resolution of the Hamiltonian;
- Influence of the real-space grid and parallelization;
- Molecular dynamics and relaxations;
- Phonons and vibrational structures;
- LDA+U;
- Wannierization;
- Post-processing and visualization tools;

Facilitators:

Francis GAITHO, Masinde Muliro University of Science and Technology
George MANYALI, Kaimosi Friends University College
James SIFUNA, Catholic University of Eastern Africa

Organizers:

Victor ODARI, Masinde Muliro University of Science and Technology
Boniface NDINYA, Masinde Muliro University of Science and Technology
Celline AWINO, Masinde Muliro University of Science and Technology
Maxwell MAGETO, Masinde Muliro University of Science and Technology
George LAWI, Masinde Muliro University of Science and Technology
Gershom MUTUA, Masinde Muliro University of Science and Technology

How to register:

Go to:
https://mrsk.or.ke/news-and-calls/
Enquiries:
vodari@mmust.ac.ke
All participants are encouraged to come with Linux installed laptops

Grants:

This workshop is supported by MMUST URF Grant No: MMU/URF/2022-1-026. There is no registration fee.

Deadline:

3rd April 2022

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