

East African School on Density Functional Theory and Applications using the Siesta code



11th – 15th October 2021

Technical University of Kenya

School of Physics and Earth Sciences, Nairobi, Kenya

The school aims at introducing ab initio calculations and molecular dynamics simulation to researchers and postgraduate students of different disciplines, using the SIESTA code.

Description:

Electronic structure codes 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. There is thus 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 Siesta code has become quite popular and is increasingly being used by researchers in geosciences, biology, and engineering. Siesta's efficiency stems from the use of strictly localized basis sets and from the implementation of linear-scaling algorithms that can be applied to suitable systems. It's accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of plane-wave methods. This school aims at introducing the Siesta code to researchers in East Africa. Basic practice, a grounding on the capabilities of the method and the approximations used shall be emphasized.

Topics:

- Basics of density-functional theory, molecular dynamics simulation and geometry relaxation;
- Generation and use of pseudopotentials;
- 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;
- Post-processing and visualization tools;

Directors:

George AMOLO, Technical University of Kenya, Kenya.

Javier JUNQUERA, Universidad de Cantabria, Spain.

Nicola SERIANI, The Abdus Salam International Centre for Theoretical Physics (ICTP), Italy.

Omololu AKIN-OJO, ICTP-EAIFR, Rwanda.

Local Organizers:

Dickson ANDALA, Multimedia University of Kenya

Michael ATAMBO, The Technical University of Kenya

Victor ODARI, Masinde Muliro University of Science and Technology

James SIFUNA, The Catholic University of Eastern Africa

How to register:

Go to:
<https://mrsk.or.ke/news-and-calls/>
Enquiries:
siesta2021@tukenya.ac.ke

Grants:

Internet support will be given to selected local participants. There is no registration fee.

Deadline:

24th September 2021



The Abdus Salam
International Centre
for Theoretical Physics

