



# THE CATHOLIC UNIVERSITY OF EASTERN AFRICA (CUEA)

A.M.E.C.E.A

Consecrate them in the Truth

DATE

8th - 10th

July

2024

## Faculty of Science

### The East-African School on Density Functional Theory & its Applications

The goal of the school is to introduce **cutting edge methodologies in Natural Sciences and Engineering**. This encompasses ab initio techniques, Molecular dynamics and Machine learning. On the other hand, it will also enhance understanding of such methodologies for the intermediate and experienced researchers.

### Description:

The behavior of any material can be simulated in a computer by resorting to the hypothesis that it is made of atoms whose electrons follow the equations of quantum mechanics. The numerical calculations to solve those equations require, in principle, only a few fundamental physical constants as input, so this methodology is called first-principles or ab initio. First-principles calculations are a powerful tool to help the understanding of experiments, learn about materials in conditions that are very expensive or impossible to replicate in the lab, and design new materials that might not yet have been found or synthesized.

The advent of **Density Functional Theory (DFT)** to solve the quantum many-body problem paved the way for the practical applications of such first-principles methods in a variety of disciplines, such as **Physics, Chemistry, Material Sciences, Geology, or Engineering** to name just a few.

Here, we propose a three-day tutorial to teach the basics of DFT, molecular dynamics simulation and geometry relaxation, which are common to most DFT-based codes. The theory sessions will be followed by practical hands-on sessions based on the SIESTA-code.

More recent aspects, such as artificial intelligence or machine learning techniques to predict molecular properties and accelerate materials discovery will be presented. Together, these methodologies promise excellent outcomes in Natural Sciences and Engineering.

### Topics to be Covered:

- Density Functional Theory (DFT)
- Molecular Dynamics
- Artificial Intelligence (AI) in Electronic Structure Methods
- Interdisciplinary Collaboration

### Speakers:

1. Javier JUNQUERA -UNICAN
2. George AMOLO - TU-K

### Directors of the School:

1. Mary WAINAINA - CUEA
2. George AMOLO - TU-K
3. Javier JUNQUERA- UNICAN

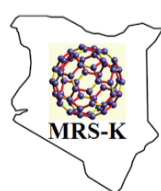
### Organizers:

1. James SIFUNA - CUEA
2. Victor ODARI - MMUST
3. Michael ATAMBO - TU-K
4. Leah NYANGASI - CUEA
5. Carolyne SONGA - CUEA
6. Stephen CHEGE - TU-K

### Sponsors of the School:

This school has been supported by the sponsors below. There is **NO registration fee**. We will provide **Travel and accommodation support** to the selected participants.

UC | Universidad de Cantabria



National Commission for Science, Technology and Innovation

kenet  
Kenya Education Network

In case of any queries,  
please contact: [dft@cuea.edu](mailto:dft@cuea.edu)

**Deadline: 30<sup>th</sup> April, 2024**

**Female** researchers are encouraged to apply.

[Click Here to Register](#)

A basic knowledge in Linux will be an advantage

[www.cuea.edu](http://www.cuea.edu)