12th Conference of African Materials Research Society

Introduction to Computational Materials Science

Facilitators

- Omololu Akin-Ojo · University of Ibadan
- Lorenzo Bastonero · University of Bremen
- Cierra Chandler · Pennsylvania State University
- Ismaila Dabo · Carnegie Mellon University
- Nelson Dzade · Pennsylvania State University
- Henry Eva · Pennsylvania State University
- Jessica Wen · Carnegie Mellon University

Day 1: Saturday, December 14

Electronic Structure

- Software Installation (8:30 am - 9:00 am)
- Fundamentals: Schrödinger Equation (9:00 am - 9:30 am)
- Overview of Density-Functional Theory: Single-Particle Equations (9:30 am - 10:30 am)
- Hands-on: Convergence of Self-Consistent-Field Calculations (10:45 am - 1:00 pm)

Molecular Geometry

- Fundamentals: Interatomic Forces (2:00 pm - 3:00 pm)
- Overview of Geometry Optimization Methods (3:00 pm - 3:30 pm)
- Hands-on: Molecular Geometries (3:45 pm - 5:00 pm)

Day 2: Sunday, December 15

Crystal Geometry

- Fundamentals: Mechanical Stress (9:30 am - 10:30 am)
- Hands-on: Crystal Geometries (10:30 am - 12:30 pm)

Vibrational Spectroscopy

- Fundamentals: Vibrational Modes (1:30 pm - 2:30 pm)
- Hands-on: Infrared Spectra (2:45 pm - 4:30 pm)

Practical Challenges

- Frequently Encountered Problems (4:30 pm - 5:00 pm)
- Q&A and Helpful Resources (4:30 pm - 5:00 pm)