



**MASINDE MULIRO UNIVERSITY OF SCIENCE AND TECHNOLOGY
SCHOOL OF NATURAL SCIENCES**

DENSITY FUNCTIONAL THEORY AND MOLECULAR DYNAMICS WORKSHOP

PROGRAMME

Thursday, 7th – Friday, 8th April 2022; VENUE: MCU BOARDROOM

DAY 1: Thursday, 7th April, 2022				
TIME	ACTIVITY	TRAINERS	Rapporteurs	SESSION CHAIRMAN
8.00 – 8.30	Arrival and Registration	Wycliffe Isoe & Patience Makungu	Dr. Benard Rapando	Prof. Boniface Ndinya
8.30 – 9:00	Welcome address by 1. Chair Organizing Committee: Dr. Victor Odari 2. Chair Department of Physics: Dr. Maxwell Mageto 3. Dean SONAS: Dr. Joseph Owino 4. Director Research and Postgraduate support: Prof. Peter Bukhala 5. Registrar Academics: Prof. Thomas Sakwa 6. DVC ASA: Prof. Hussein Golicha 7. DVC PRI: Prof. Charles Mutai			
9.00 – 9.20	Computational Modelling and Materials Science and Materials Research Society of Kenya	Prof. Dickson Andala (Multimedia University)		

9.20 – 9.40	DFT in Perspective (Basics of density-functional theory and molecular dynamics)	Dr. George Manyali		
10:00- 10:30	HEALTH BREAK			
10.30 – 11.00	Generation and use of pseudopotentials;	Mr. James Sifuna	Dr. Philip Amuyunzu	Dr. Victor Odari
11.00 – 11.30	Basis sets in DFT	Mr. James Sifuna		
11:30 – 12:00	Influence of the real-space grid and parallelization	Dr. George Manyali		
12:00 – 12:30	HPC environment	Dr. George Manyali		
12.30 - 14:00	LUNCH BREAK			
14.00 – 16:00	Hands-on Session: First runs of simple molecules and solids in Quantum Espresso/Siesta Exercises on pseudopotentials and basis sets	Dr. George Manyali Dr. Francis Gaitho Mr. James Sifuna		
16.00 - 16:15	HEALTH BREAK			
16.15 – 17.30	Hands-on Session: Exercises on the computation of: - Visualization of the charge density: the case of bulk Si - Band structures	Dr. George Manyali Dr. Francis Gaitho Mr. James Sifuna		

	<ul style="list-style-type: none"> - Density of states - Fat bands <p>Exercises on visualization of the charge density.</p> <p>Further exercises on solids</p> <p>Converging the sampling in k-points: the case of metallic Al</p> <p>Converging the sampling in k-points: the case of insulating BaTiO₃</p> <p>Converging the Mesh Cutoff</p>			
Communication from workshop secretariat – Prof. Boniface Ndinya				

DAY 2: Friday, 8th April, 2022				
TIME	ACTIVITY	TRAINERS	Rapporteurs	SESSION CHAIRMAN
8.00 – 8.30	Arrival and Registration	Wycliffe Isoe & Patience Makungu	Dr. Patrick Tonui	Dr. Henry Barasa
8.30 – 9:30	Molecular dynamics and relaxations	Dr. Francis Gaitho		
9.30 – 10.30	Phonons and vibrational structures	Dr. Francis Gaitho		
10:30- 11:00	HEALTH BREAK			

11:00 – 12:00	LDA+U	Mr. James Sifuna	Dr. Celline Awino	Dr. Maxwell Mageto
12:00 – 13:00	Wannierization	Mr. James Sifuna		
13.00 - 14:00	LUNCH BREAK			
14.00 – 16:00	Hands-on Session: Exercises on molecular dynamics and relaxations Exercises on phonons and vibrational structure Phonons at Gamma and Born effective charges for SrTiO ₃ Making a movie with the phonons of Benzene Phonon spectrum of bulk Si	Dr. George Manyali Dr. Francis Gaitho Mr. James Sifuna		
16.00 - 16:15	HEALTH BREAK			
16.15 – 17.30	Exercises on LDA+U Exercises on Wannierization	Dr. George Manyali Dr. Francis Gaitho Mr. James Sifuna		
17:30 – 18:00	Vote of thanks Closing Ceremony and Issue of certificates – Prof. Thomas Sakwa			