Proposal for a Workshop at 2025 CHPC National Meeting.

- This year the workshops run on **Sunday** 30 November only.

Please provide the following information for the proposed short course or tutorial workshop. It is not necessary to fill in everything, complete as much as you can to help us evaluate the proposal.

Title of Workshop: *Materials Modelling Workshop using Density Functional Theory (DFT)*

Lecturer(s): Name, Affiliation, Email Address

1. Prof. Kingsley Onyebuchi Obodo, University of KwaZulu-Natal, obodok@ukzn.a.za

Description: The *Materials Modelling Workshop using Density Functional Theory (DFT)* provides postgraduate students, early-career researchers, and interdisciplinary scientists with a solid foundation in computational materials science. DFT is a powerful quantum mechanical method for predicting the structural, electronic, optical, and magnetic properties of materials, enabling the rational design of novel systems for energy, catalysis, and optoelectronic applications. Through a combination of lectures and hands-on sessions, participants will gain practical experience with leading DFT software tools, learning how to perform structure optimization, electronic structure calculations, and property analysis. The workshop will highlight applications in sustainable energy materials, topological systems, and low-dimensional materials. Participants will also be introduced to emerging approaches that combine DFT with machine learning for accelerated materials discovery and inverse design. By the end of the workshop, attendees will possess both theoretical insight and computational skills to apply DFT (CASTEP in materials studio) techniques effectively in their own research and to contribute to innovation in materials design and development.

Duration: □ ½ day (3h) **Size:** *50-100 Candidates.*

Target Audience: *(who should attend this tutorial)* Postgraduate students (Hons, MSc and PhD), early-career researchers, and interdisciplinary scientists.

Prerequisites: *(what previous knowledge or skills should the attendees have)* Basic knowledge of solid-state chemistry, solid state physics and materials science.

Type of workshop: Mix of lectures and practicals

Special requirements: Bring your laptop and if possible, have access to Materials Studio package on the CHPC.

Timetable: Please provide an outline of full syllabus:

Time	Session Title	Content / Activities	Learning Outcome
13:30	Welcome and Introduction	• Brief overview of the workshop objectives and schedule • Introduction to computational materials modelling and the role of DFT • Software check: Materials Studio/CASTEP environment setup	Participants understand the goals and practical flow of the session.
13:40	Lecture 1: Essentials of Density Functional Theory	• Motivation: Why DFT in materials science? • Basic principles: Hohenberg–Kohn theorems, Kohn–Sham equations • Exchange–correlation functionals (LDA, GGA) • Common applications and limitations	Participants grasp the conceptual foundation of DFT for predicting materials properties.
14:30	Hands-On Session 1: Structure Optimization in CASTEP	• Building or importing a crystal structure in Materials Studio • Setting up geometry optimization in CASTEP • Running the calculation and monitoring convergence • Viewing and interpreting the optimized structure	Participants learn how to perform a full structure optimization using CASTEP.
15:00	Short Break	—	—
15:30	Hands-On Session 2: Electronic Structure and Property Analysis	• Calculating band structure and density of states (DOS) • Visualizing charge density and identifying band gaps • Interpreting key results and linking to material properties	Participants gain practical skills in analyzing and interpreting electronic structure results.
16:30	Lecture 2: Emerging Trends — DFT and Machine Learning	• Overview of data-driven approaches in materials modelling • How machine learning complements DFT for accelerated discovery • Example: Predicting formation energies or	Participants gain awareness of the evolving landscape of computational materials science.

		optimizing materials design	
16:55	Wrap-Up and Q&A	• Recap of key concepts and takeaways • Recommended reading and next-step resources • Feedback and certificate presentation	Participants consolidate learning outcomes and receive guidance for future independent study.