Contribution ID: **179** Type: **Invited Talk**

Exploration of future magnetic and cathode materials through computer-based simulations.

Wednesday, 4 December 2024 13:30 (20 minutes)

The field of materials science has seen a significant increase in the use of computational techniques to study the properties and behaviour of different materials at the atomic and molecular level. A key computational method employed in the study of solid-state materials is Density Functional Theory (DFT), which accurately forecasts the electronic structure, mechanical properties, and thermodynamic stability of materials without the necessity for intricate experimental procedures. At the Department of Physics, University of Fort Hare, our focus lies on the simulation of magnetic and cathode materials for potential applications in data storage and rechargeable batteries. Our research utilizes a first-principles approach within the Density Functional Theory (DFT) framework to explore the diverse properties of transition 3d elements and platinum (M-Pt) alloys, as well as M2O4-based (M: Mn and V) cathodes, highlighting their potential for future technological advancements. All calculations are conducted using the CASTEP simulation code integrated into the Materials Studio software and the HPC platform offered by the Centre for High Performance Computing. Our investigations have revealed that alloys like FePt, MnPt and CoPt exhibit excellent properties such as high magnetic moments and magnetocrystalline anisotropies rendering them suitable for magnetic spintronic devices and magnetic data recording applications. Furthermore, polymorphs of CaMn2O4 have been predicted to possess exceptional thermodynamic, mechanical and dynamical stability, good electronic conductivity and intercalation potentials that fall within the prescribed pulse discharge/charge range of 2.7 V to 3.9 V. These properties ensure retention of structural integrity over multiple charge/discharge cycles, good electrochemical performance and reversibility of Ca during charge/discharge process.

Student or Postdoc?

Email address

Co-Authors

CHPC User

CHPC Research Programme

Workshop Duration

Primary author: Dr LETHOLE*, Ndanduleni (University of Fort Hare)

Presenter: Dr LETHOLE*, Ndanduleni (University of Fort Hare)

Session Classification: HPC Applications