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Generation of β-MnO2 nanoclusters using global search techniques

A combination of global search techniques and density functional theory (DFT) methods were employed to determine the structural stabilities of β-MnO2 nanoclusters across the energy landscape. Nanostructuring offers the ability to improve material properties by adjusting the size to explore their novel collective optical, mechanical, magnetic and electronic properties. Several nanostructured MnO2, including nanocrystals of different shapes have been synthesised for potential applications in catalysis, rechargeable batteries and supercapacitors. However, structural features that exist at the nanoscale are difficult to characterise experimentally, and therefore, atomistic computer simulations offer a unique window of exploration into nanomaterials, particularly the synthesis of nanoclusters. The Interatomic Potential (IP) calculations where performed with the Knowledge-Led Master Code (KLMC) using the GULP code to generate nanoclusters (n=2–50 atomic numbers). DFT calculations were performed using Accelrys Materials Studio with the CHPC on the Lengau cluster with 64 cores running in parallel using Intel MPI in order to converge successfully and accommodate the large amount of produced data in a timely manner. The nanoclusters were validated using the DFT planewave method and ranked in order of stability according to their ground state energy. Comparisons are made between the different potentials used and techniques employed. The prevalence of compact ring structures consisting of a cubic structure with manganese and two dangling oxygen atoms dominates the make-up of the most stable structures and their structural and mechanical properties have been investigated and reported.

Presenter Biography

I am a second year PhD student based at the University of Limpopo, Materials Modeling Centre. My study is focused on investigating the structural make up of pyrolusite in order to improve its properties for potential applications as a cathode material for rechargeable batteries. I have collaborated with researchers from the University College London and I have presented my work in London, Liverpool (UK) and Berlin (Germany) where i also attended workshops to improve my knowledge.

Primary author: MASOGA, Wesley (University of Limpopo)

Co-authors: NGOEPE, Phuti (University of Limpopo); MAPHANGA, Regina (CSIR); Prof. CHAUKE, Hasani (University of Limpopo); CATLOW, Richard (Department of Chemistry, University College London)

Presenters: MASOGA, Wesley (University of Limpopo); Dr WOODLEY, Scott (University College London); Dr SOKOL, Alexey (University College London); Dr LAZAUSKAS, Tomas (University College London)

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