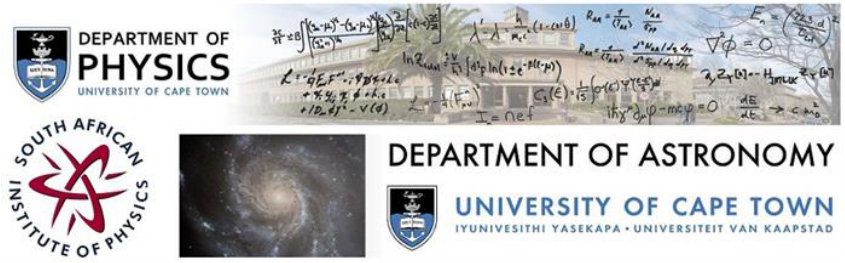

Contribution ID: **325** Type: **Poster Presentation**

Structural prediction of β-MnO2 nanoclusters using global search techniques

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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The increasing demand for high energy density rechargeable batteries has fuelled the interest in the research, development and manufacturing of new battery systems capable of powering high powered machinery as well as rechargeable household appliances. Pyrolusite (β-MnO2) is the most stable and abundant polymorph of manganese dioxide and it is regarded as a potential material for rechargeable lithium-ion batteries. In this study, a combination of evolutionary algorithm techniques and density functional theory methods are employed to determine the stabilities of MnO2 nanoclusters across the energy landscape. We investigate the energetics and structural configurations for (β-MnO2)_{n=1-20} nanoclusters. The most stable nanoclusters are made of a cubic structure consisting of two manganese and two oxygen atoms for various cluster sizes. The stable structures tend to migrate to a more circular compact configuration after geometry optimisation using density functional theory. Calculated x-ray diffraction patterns for the nanoclusters revealed the most dominant and stable peaks with their respective intensities in addition the effect of temperature changes on nanocluster stability was studied. As the temperature is increased from 200K to 1300K, the change in the bond angles and bond distances is measured. An increment of the exterior angles and bonding lengths along with the decrease of the interior angles is observed. The average stable temperature was found to be approximately 300K for (β-MnO2)_{n=1-6} nanoclusters.

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Session Classification: Poster Session (1)

Track Classification: Track A - Division for Physics of Condensed Matter and Materials