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Evolutionary algorithm simulation study of Manganese dioxide nanoclusters

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Abstract content
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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 house hold appliances. Manganese dioxide is one of the promising materials that are studied as potential cathode materials for rechargeable lithium-ion batteries. Pyrolusite is chosen for this study as it is the most stable polymorph of manganese dioxide. This study aims to show that pyrolusite when refined nano-structurally can be used to improve the current state of the cathode when used in secondary/rechargeable batteries. Evolutionary algorithm techniques and energy minimisation methodologies are used to generate Manganese dioxide nanoclusters. A combination of global search techniques and density functional theory methods are employed to determine the stabilities of Manganese dioxide nanoclusters across the energy land-scape. We investigate the energetics, structural and thermodynamic properties of manganese dioxide nan-oclusters. Structural stabilities of the nanoclusters correlate with those for isostructural Silica and Titanuim dioxide clusters from previous studies. Compact ring structures are the most stable for the nanoclusters from n=1 to n=6 atoms. The most stable nanoclusters are made of a cubic diamond consisting of two manganese and two oxygen atoms. The stable structures tend to migrate to a more circular compact configuration after optimisation. X-Ray Diffraction patterns for the nanoclusters indicated the (0 1 -1) peak as the most dominant and stable with its intensity always in the range between 100 and 110. Temperature changes on nanocluster stability was also studied. Total energies are given through 200K to 1600K temperature range to determine the temperature at which the nanoclusters converge and stabilise. Increase in temperature results in increase of bonding distances between the atoms. The higher the temperature the less stable the nanoclusters become.

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