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Computer simulated study of the structural and electronic properties of β-MnO2 nanoclusters as cathode materials in rechargeable lithium-ion batteries

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Significant attention has recently been focused on transition metal-oxides due to their allotropic polymorphs having distinct structural and electronic properties. Pyrolusite (β-MnO2), the most stable polymorph of MnO2, is one of the most promising cathode materials necessary for the creation of improved rechargeable battery systems such as lithium-ion batteries.
In this study, MnO2 nanoclusters were produced using an evolutionary algorithm and first principle methods. Interatomic potentials were used in conjunction with the Buckingham potential and the 12-6 Lennard-Jones potential to generate subsets of stable nanoclusters. A combination of global search techniques and density functional theory (DFT) methodologies were used to refine the energy ordering of the generated nanoclusters and determine their global minima.
The selected interatomic potentials predicted the β-MnO2 bulk structure to within 0.43 % of experimental data. The Ni-doped n3-01 nanocluster on the cation position with the higher coordination was the most stable, most compact and had the highest operational voltage profile of 3.038 V showing nickel to be the preferred dopant in this study. The generated x-ray diffraction patterns for the stable nanoclusters revealed the most dominant and stable peaks with their respective intensities' indicative of the stable rutile phase. Furthermore, the effect of temperature changes on nanocluster stability was studied. The nanoclusters showed a preference toward circular compact bonding patterns at higher temperatures. There are improvements in the stability and electrical conductivity in the nanoclusters as compared to bulk β-MnO2. The DOS revealed that the nanoclusters are metallic at the Fermi level with small band-gap energies. Due to its advantageous electrical conducting qualities and the fact that co-doped nanoclusters had the smallest band-gap energies, Co-doping also demonstrated some potential. The charge density differences of the Ni-doped n3-01 nanocluster displayed a high prevalence of covalent bonding as opposed to ionic bonding observed with Fe- and Co-doping further showing nickel to be the preferred dopant.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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