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Calculations of structural and electronic properties of manganese dioxide

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Abstract content
   (Max 300 words)

Manganese dioxide is an important material for electrochemical applications; including serving as a cathode material in Li-ion batteries. It is a non-stiochiometric compound that exists in many crystalline forms, such as alpha;-, β-, γ-, and δ- types. The γ-MnO₂ has a complex structure, composed of intergrowths of pyrolusite and ramsdellite structures, twinned ramsdellite, grain boundaries, dislocations and point defects (vacancies and impurities). Experimental methods were used characterize electrolytic manganese dioxide materials and there has been no efficient method to characterize their structures and thereby no means of relating their atomic scale arrangement with their behaviour in batteries. We investigate structural and electronic properties of pyrolusite and ramsdellite polymorphs of manganese dioxide, using the density functional theory where pseudopotential plane wave methods are invoked. In particular, the equations of states are determined and bulk moduli predicted. The partial density of states and charge deformations of pyrolusite and ramsdellite, provide information on their nature of bonding at different pressures.

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Primary author: Dr MAPHANGA, Rapela (University of Limpopo, Materials Modelling Centre, Private bag x 1106, Sovenga, 0727)

Co-author: Prof. NGOEPE, Phuti (University of Limpopo, Materials Modelling Centre, Private bag x 1106, Sovenga, 0727)

Presenter: Dr MAPHANGA, Rapela (University of Limpopo, Materials Modelling Centre, Private bag x 1106, Sovenga, 0727)

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