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MULTI-SCALE MODELLING OF P2 AND O2 TYPE MATERIALS FOR UTILIZATION AS CORE-SHELL MATERIALS

The increasing demand for energy and the threat from global warming make electrical energy storage a worldwide policy objective. As such, sodium-ion batteries are currently evolving as a viable substitute for lithium-ion batteries due to the abundant availability and reasonable cost of sodium. Sodium transition metal oxides (NaMO2) with a P2 structure exhibit good Na+ ion conductivity and manganese-based compounds provide a high working potential vs. Na+/Na, and high capacity. Hence, the materials are promising sodium-ion battery cathode materials. However, the layered nature of these materials means that they are prone to structural rearrangements at high voltage or low Na contents, phase transformations and Na+ ion/vacancy ordering transitions, resulting in capacity fade and poor reversibility. In this work, the density functional theory was used to investigate the structural, electronic, and mechanical properties of the P2 and O2 type NaMnO2 and LiMnO2 structures. The electronic band structures illustrated the conductivity of the materials and density of states were used to check the electron contribution at the fermi level. Thus, the electron contribution at the fermi level is due to the p state of oxygen and the d state of Manganese. The structures converged with 6x6x6 k-points and 600eV energy. Moreover, elastic constants and phonons curves compared in details stability of the materials.

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

Yes

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

Hons

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