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Phase stability of calcium manganese oxide (CaMn2O4) polymorphs cathode materials in calcium ion batteries.

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The demand for energy storage devices with high energy density has increased with the development of renewables occurring. Calcium ion batteries (CIBs) have gained attraction due to their abundance, high energy density, low cost, and low risk. Supercapacitors and Batteries are the currently used energy storage devices with Batteries being the dominant/most used. This study presents computational calculations that were carried out on the structural, thermodynamics, electronic and mechanical properties for CaMn2O4 polymorphs. The computational method used the density functional theory (DFT) that is imbedded in the CASTEP code in Material Studio. Since we were dealing with transition metal oxides, we had to employ the Hubbard U-correction to take care of the highly-correlated electrons in the d-orbital of the Mn atoms. The lattice parameters found were in good agreement with available experimental results validating the approach taken. The heats of formation are both negative which suggest that the structures can be synthesized experimentally. During the analysis of the DOS the considered CaMn2O4 polymorphs showed a relatively poor conductivity and can be classified as semi-conductors. Furthermore, Pbca-CaMn2O4 has lower states around the Fermi level as compared to Pbcm-CaMn2O4, suggesting that the Pbca-CaMn2O4 polymorph is more stable. This is consistent with the calculated heats of formation.

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

Yes

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

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