Abstract ID

Comparative analysis of electrochemical properties of $LiMO_2$, $LiMSiO_4$ and $LiMPO_4$ (M=Fe, Co and Mn): A first principles study

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Polyanion based cathode materials are most promising candidates for lithium ion batteries due to low cost, safety, environmental friendliness, etc. [1-5] We performed first principles based DFT calculations to understand the stability, charge transfer mechanism and electrochemical performance of olivine phosphates, silicates and its comparison with the transition metal layered oxides based cathode materials. We have computed the changes in oxidation states using Bader method of topological analysis and charge re-distribution by analysis of partial density of electronic states. For olivine-type $LiFeSiO_4$, our results show the major role of O-2p states instead of 3d-orbitals of transition metal in charge transfer processes during lithiation/delithiation. We also show comparative analysis of the effect of cationic substitution of transition metals by non-transition metals on the stability and electrochemical performance of the cathode materials.

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