Transition metal oxide as possible electrode materials for Li-ion batteries: A DFT Analysis

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To solve the problems of climate change and pave the way towards a more sustainable future, research is being done to find out new materials to be used in electrodes of high energy density batteries in different types of electronic equipment. Great efforts are underway to make new materials that can fulfill the requirements of the conditions for new batteries. The layered transition metals oxides are a new kind of material that are under consideration as new electrode materials for rechargeable Lithium-ion batteries. The layered transition metal oxides have garnered attention as a result of their lower production cost and relatively higher energy density that is associated with these materials. The old batteries get heated easily, which restricts their charging speed, and they are dangerous as they can explode due to their lower capacity range in the electronic vehicles arising safety concerns. There is a need to develop improved materials to provide affordable and heavy-duty batteries to employ in smart vehicles and gadgets.

Keywords: DFT, Graphene, Transition metal oxide, Li ion batteries

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