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The effect niobium doping on the major spinel LiMn2O4 surfaces: DFT study

Lithium manganese oxide (LiMn2O4) is one of the promising cathode materials for lithium-ion batteries (LIBs), however, it suffers from capacity fading mainly due to surface manganese (Mn2+) ion dissolution during Charge/discharge processes. Although many studies focused on reducing Mn-dissolution, surface modification has proven to be an ideal method of reducing Mn2+ ion dissolution in secondary Li-ion batteries. In this study, the density functional theory calculations were carried out to study investigate the effect of Nb doping on major LiMn2O4 spinel surfaces. The facet with the lowest surface energy was the (001) slab, which compares well with the reported literature. Upon surface Nb doping, the calculated surface free energies are lower as compared to the surface energies of pure pristine surfaces, indicating that the surfaces stabilize. However, the (001) surface remained the most stable facet, with a similar trend of increasing energies and decreasing stability, i.e. (001) < (011) < (111). The morphology of the pure pristine surfaces showed a dominance of the (001) plane, which was enhanced upon Nb doping. The partial density of states shows no effect of Nb on the Fermi, hence we observed the same trend of surface stability before and after Nb doping. Due to the stronger binding energy of Nb-O as compared to Mn-O, doping with Nb can suppress the Mn dissolution during cycling and hence improve the electrochemical performance.

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