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Ab-initio study of hydrofluoric acid and ethylene carbonate adsorption on the Nb-doped on the LiMn2O4 surfaces

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Surface cationic doping has been deemed one of the most effective methods of reducing the number of trivalent manganese (Mn³⁺) ions that undergo a disproportionation reaction in lithium manganese oxide-based (LiMn₂O₄) lithium-ion batteries. However, the effect of surface doping on the major LiMn₂O₄ surfaces and their interactions with the electrolyte components is not yet fully understood. In this work, we present the effect of surface Nb doping and the adsorption of electrolyte components (ethylene carbonate and hydrofluoric acid) on the major LiMn₂O₄ (001),(011), and (111) surfaces using the spin-polarized density functional theory-based calculations [DFT+U-D3 (BJ)]. During Nb ⁵⁺ substitution on the top (Nb_{*t*}) and sub-surface layers (Nb_{*s*}), it was found that the stability of the (111) surface plane greatly improves for Nb_{*s*}, causing it to dominate the morphology. This is an interesting, since it has previously been suggested that exposing the (111) surface promotes the formation of a stable solid electrolyte interphase (SEI), which could significantly reduce Mn dissolution. Moreover, both EC and HF greatly preferred binding with the surfaces through the Nb instead of Mn atoms, and the largest adsorption energy was calculated for EC on Nb_{*b*} (Nb-doped on both Nb_{*t*} and Nb_{*s*}) of (001) and HF on Nb_{*t*} (111) surfaces. Furthermore, the EC/HF adsorptions further enhance the stability of the Nb_{*s*} (111) surface plane. However, minimal charge transfer was calculated for both HF and EC interacting with the pure and Nb-doped surfaces.

Keywords: Doping, adsorption, Density functional theory, Li-ion batteries, Surface chemistry

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

Yes

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

PhD.

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