First-Principles Study on Thermodynamic Stability of Hybrid Interfacial Structure of LiMn$_2$O$_4$ Cathode and Carbonate Electrolyte in Li-Ion Battery

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Supplementary information

Fig. S1: Determining the vacuum level through the electrostatic potential energy of Li$_x$Mn$_2$O$_4$ surface models
Fig. S2: (a) Choosing the outermost layers of LMO (111) surface model for pDOS calculation; (b) Left panel is pDOS for Mn and O from the outermost layers and right panel is pDOS summing it up without spin consideration.

3 Layers: two O layers and one Mn layer → Total 6 layers for pDOS
Fig. S3: Analyzing work function from the electrostatic potential of proton transferred LMO surface and its model system.

(a) Proton transferred LMO surface
→ Adopted from AIMD simulations
→ Considering symmetry of the system

(b) Potential energy (eV) vs. Position (Å)
Fig. S4: Expanded model systems of LMO surface to investigate effect of surface coverage of proton on the work function in (a) and in (b) calculated work functions of LMO as a function of proton coverage with respect to total adsorption sites.