Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First-Principles Study on Thermodynamic Stability of Hybrid Interfacial Structure of $LiMn_2O_4$ Cathode and Carbonate Electrolyte in Li-Ion Battery

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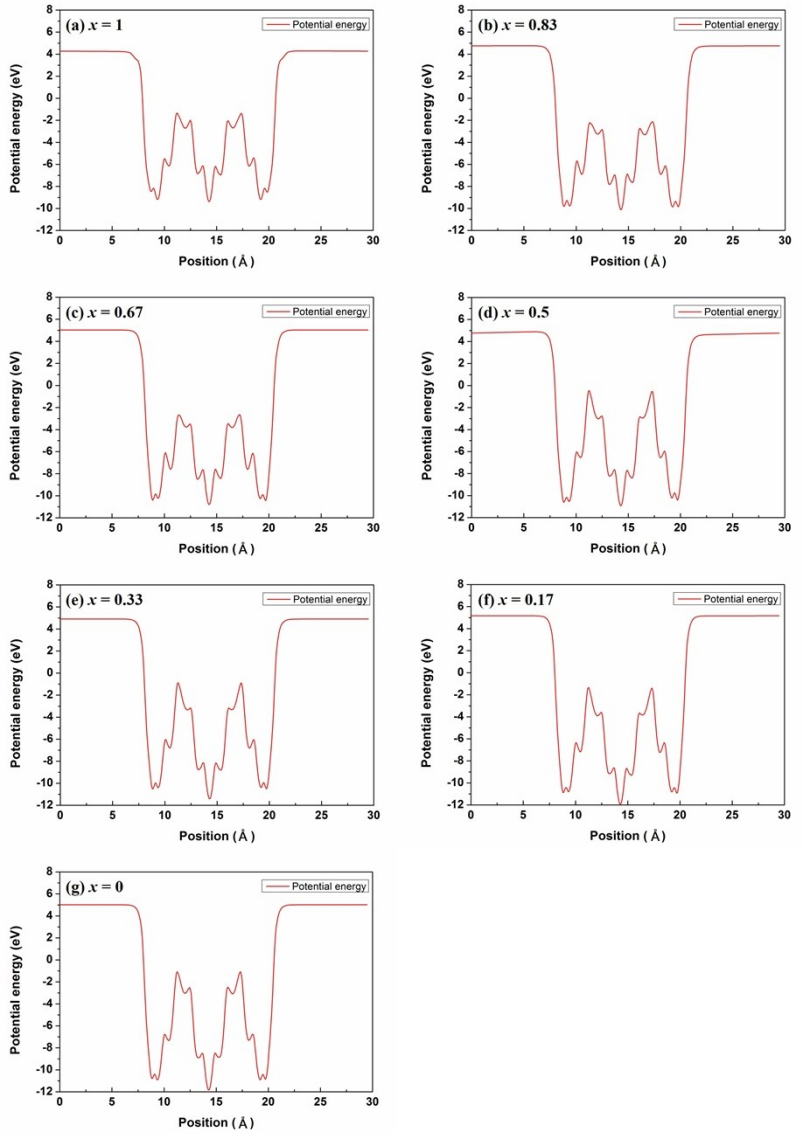
Supplementary information

Fig. S1: Determining the vacuum level through the electrostatic potential energy of $Li_xMn_2O_4$



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

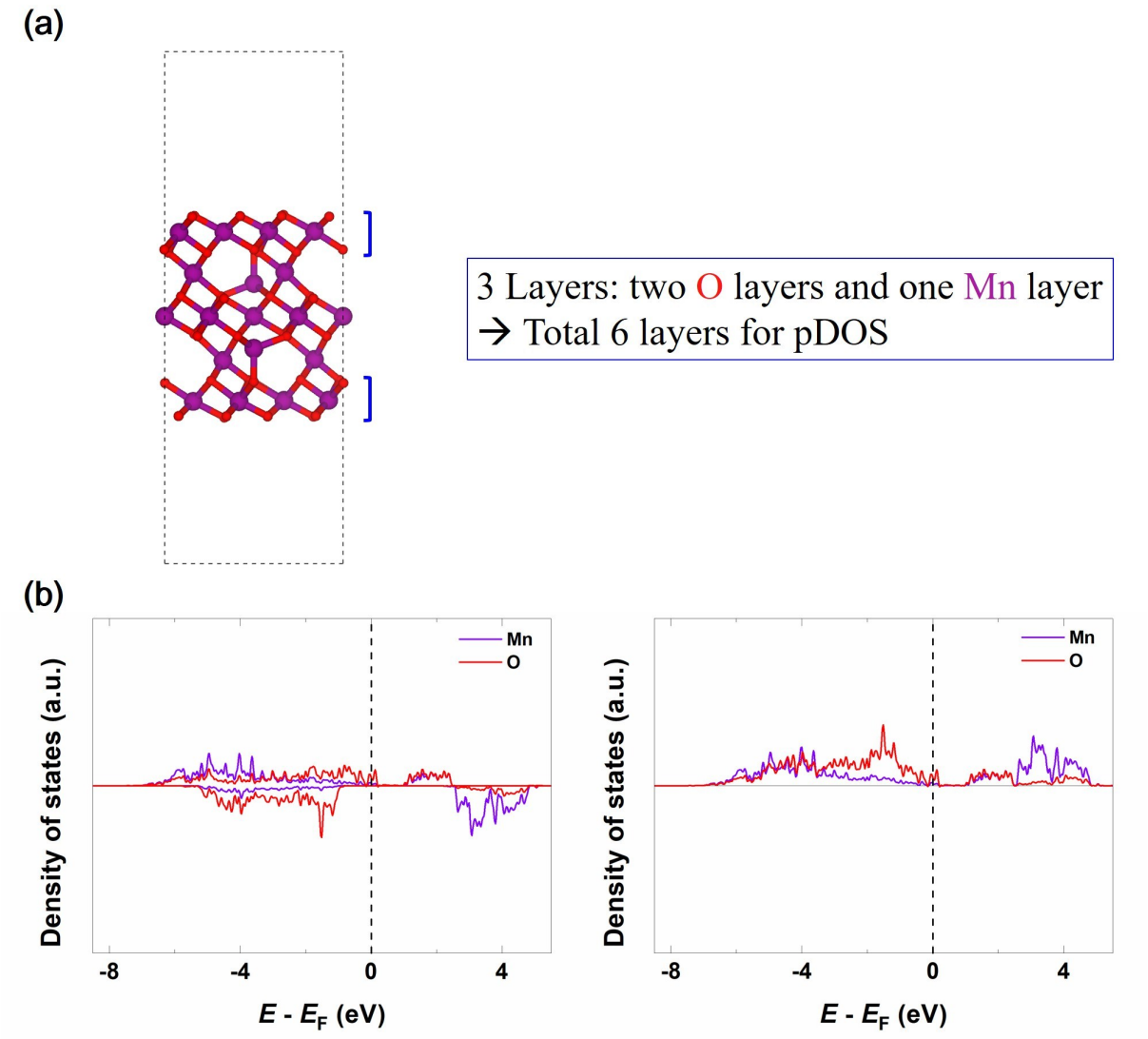


Fig. S3: Analyzing work function from the electrostatic potential of proton transferred LMO surface and its model system

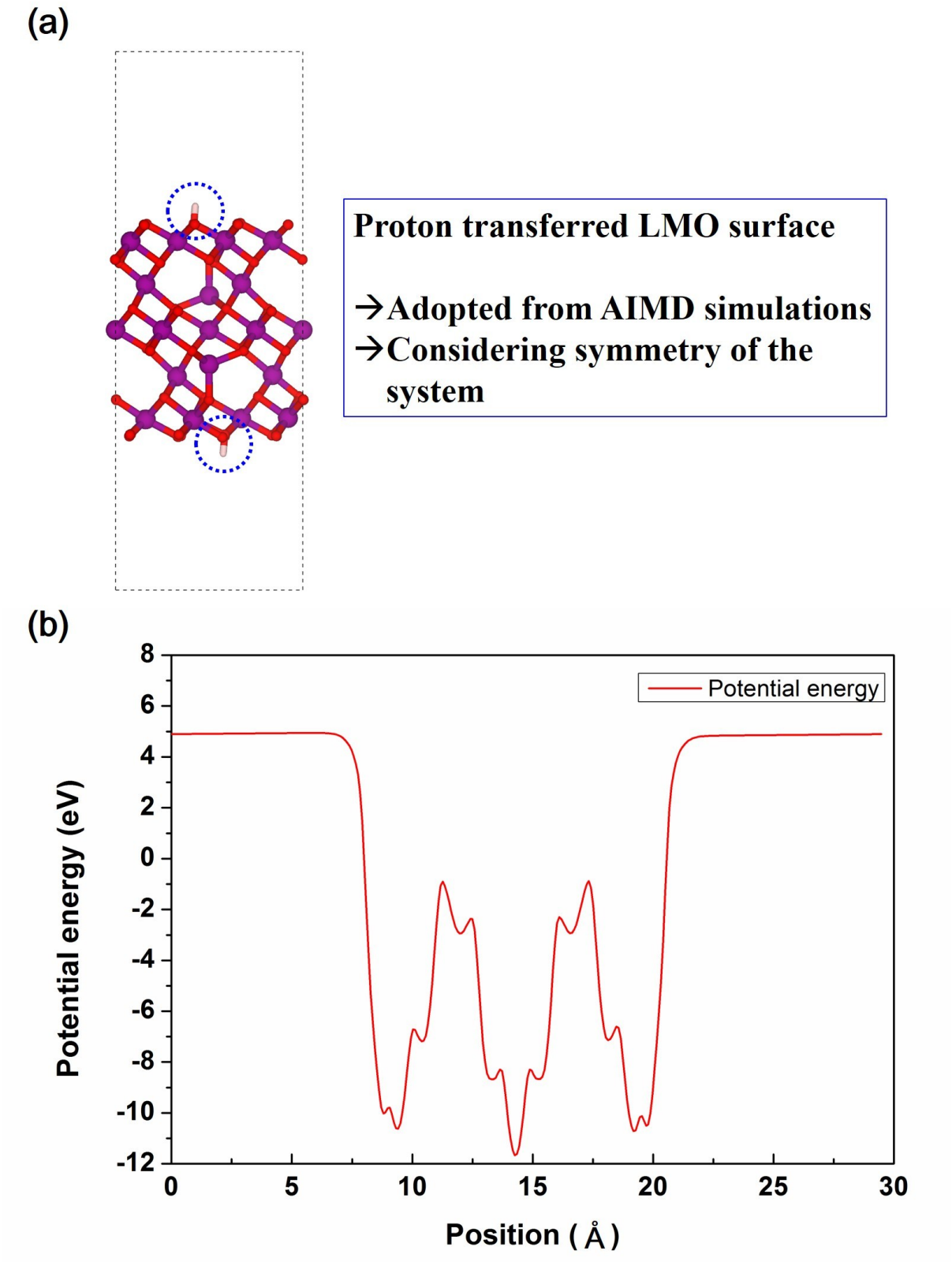


Fig. S4: Expanded model systems of LMO surface to investigate effect of surface coverage of proton on the work function in (a) and in (b) calculated work functions of LMO as a function of proton coverage with respect to total adsorption sites.