

## Solid-Electrolyte Interphase in the Spinel Cathode Exposed to Carbonate Electrolyte in Li-Ion Battery Application: An *ab-initio* Study

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**초 록:** Due to key roles for the electrochemical stability and charge capacity the solid-electrolyte interphase (SEI) has been extensively studied in anodes of a Li-ion battery cell. There is, however, few of investigation for cathodes. Using first-principles based calculations we describe atomic-level process of the SEI layer formation at the interface of a carbonate electrolyte and  $\text{LiMn}_2\text{O}_4$  spinel cathode. Furthermore, using beyond the conventional density functional theory (DFT+U) calculations we examine the work function of the cathode and frontier orbitals of the electrolyte. Based on the results we propose that proton transfer at the interface is an essential mechanism initiating the SEI layer formation in the  $\text{LiMn}_2\text{O}_4$ . Our results can guide a design concept for stable and high capacity Li-ion battery cell through screening an optimum electrolyte fine-tuned energy band alignment for a given cathode.