제일원리 전산모사를 통한 리튬 이온 전지의 $LiMn_2O_4$ 전극-전해질 계면 반응 분석
First-principles Study on the Formation of Solid-Electrolyte Interphase on the $LiMn_2O_4$ Cathode in Li-Ion Batteries

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초 록 : Development of advanced Li-ion battery cells with high durability is critical for safe operation, especially in applications to electric vehicles and portable electronic devices. Understanding fundamental mechanism on the formation of a solid-electrolyte interphase (SEI) layer, which plays a substantial role in the electrochemical stability of the Li-ion battery, in a cathode was rarely reported unlike in an anode. Using first-principles density functional theory (DFT) calculations and ab-initio molecular dynamic (AIMD) simulations we demonstrate atomic-level process on the generation of the SEI layer at the interface of a carbonate-based electrolyte and a spinel $LiMn_2O_4$ cathode. To accomplish the object we calculate the energy band alignment between the work function of the cathode and frontier orbitals of the electrolyte. We figure out that a proton abstraction from the carbonate-based electrolyte is a critical step for the initiation of an SEI layer formation. Our results can provide a design concept for stable Li-ion batteries by optimizing electrolytes to form proper SEI layers.