

Atomic Thermodynamics and Microkinetics of Reduction Mechanism of CMDO as an Electrolyte Additive for Facilitating Solid Electrolyte Interphase of Lithium Ion Battery

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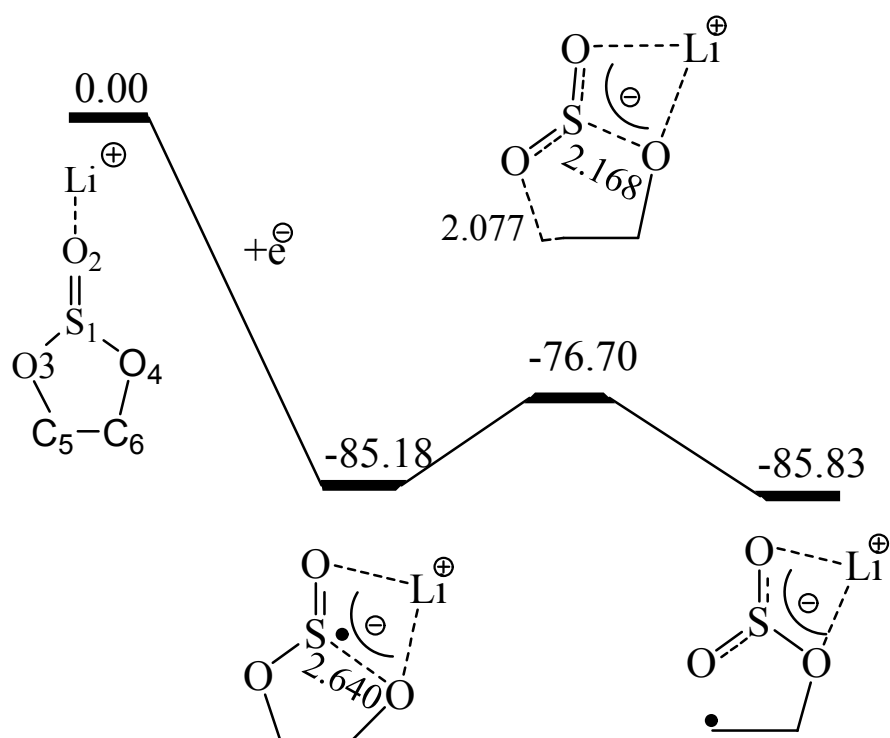


Figure S1. Gibbs free energy profile of $\text{Li}^+(\text{ES})$ with SMD-B3PW91/6311++G(d,p)

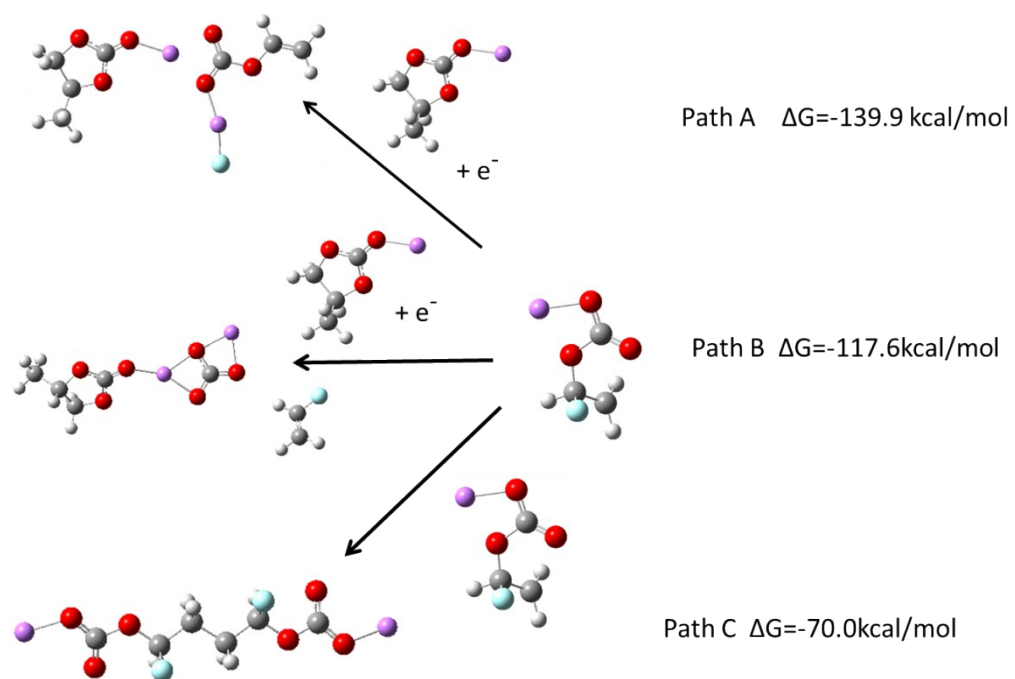


Figure S2. Termination reaction of the opening radical of reduced $\text{Li}^+(\text{FC})$