

Supplemental Information to “Reduction Mechanisms of Additives on Si anodes of Li-ion
Batteries,” by J. M. Martinez de la Hoz and P. B. Balbuena

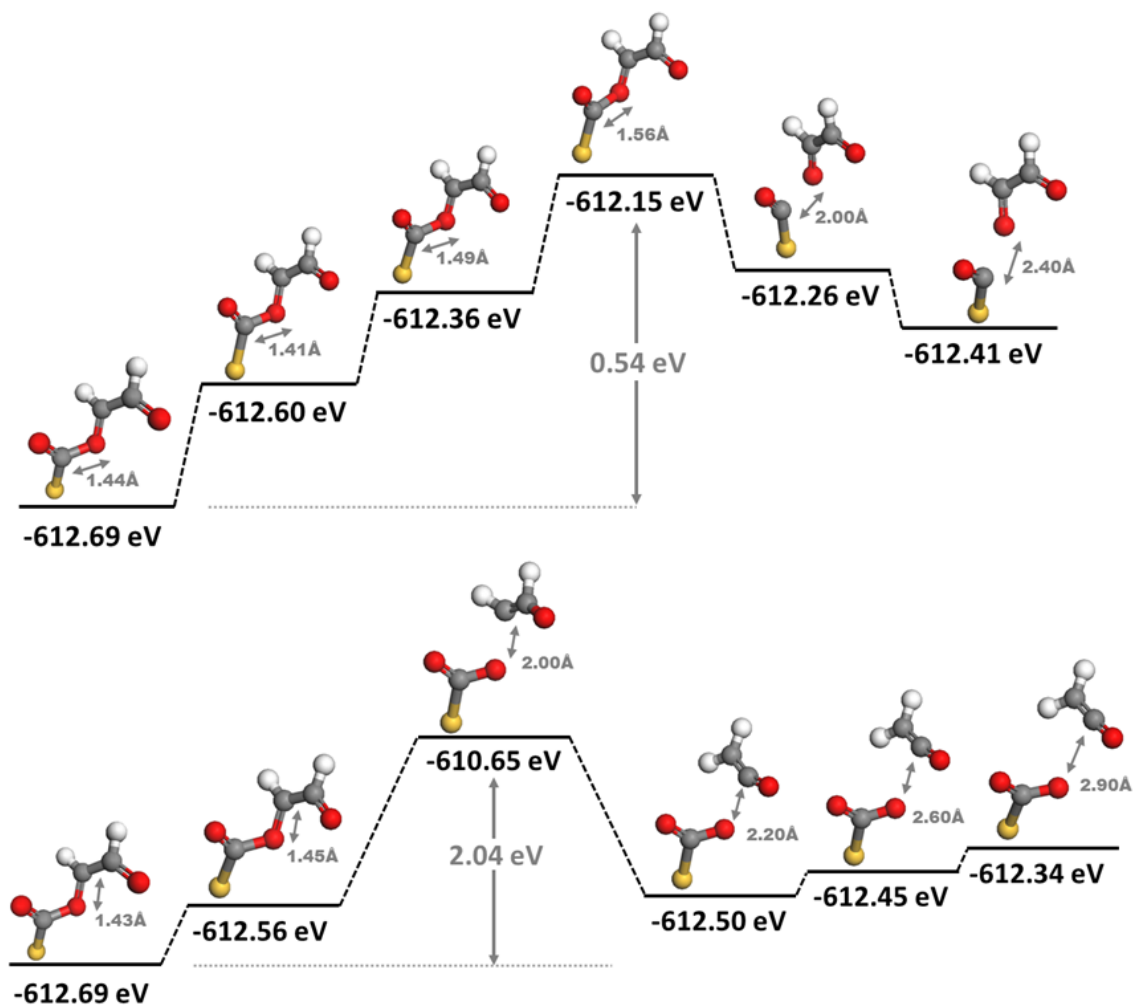


Fig. S1 Optimized configurations and energies along the reaction coordinates for the formation of CO (top) and CO₂ (bottom) from OC₂H₂OCO₂²⁻_(ads). These calculations were performed using the NEB method with a single OC₂H₂OCO₂²⁻ species (gas-phase) on LiSi(101)-H.