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Atomic-Scale Mechanisms for Electrolyte Decomposition in Li-ion Battery Cathodes[1] MALLORY FUHST, University of Michigan Department of Applied Physics, DONALD SIEGEL, University of Michigan Department of Mechanical Engineering — Li-ion batteries using high energy density $LiCoO_2$ (LCO) intercalation cathodes are known to generate gaseous species inside the cell, which can lead to venting flammable solvent vapor. It has been hypothesized that reactions at the cathode/electrolyte interface catalyze the production of these gaseous species. To elucidate the underlying reaction mechanism, first principles calculations were used to model interactions between LCO surfaces and Ethylene Carbonate (EC), a commonly used solvent in Li-ion batteries. A Metropolis Monte Carlo algorithm was used to identify likely low energy adsorption configurations for EC on the (10-14) surface of LCO. Several of these geometries were further analyzed with DFT. The thermodynamics and kinetics of EC decomposition were evaluated for plausible reaction pathways and associated various solvent decomposition mechanisms, such as hydrogen abstraction. Preliminary results indicate that hydrogen abstraction may lead to the spontaneous decomposition of EC into CO and other adsorbed species at the surface.

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