Structural Models of CF$_x$ for Cathode of Battery and Reduction of Ethylene Carbonate for Formation of Solid-Electrolyte Interface: DFT vs. ReaxFF

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Recent advances in CF battery chemistry have demonstrated improved performance at high discharge rates. To determine the atomistic origin of these improved properties we have predicted the structures (Fig. 1) and properties (interlayer distance, C-F bond distance) of C$_x$F for various F concentrations (from $x=1$ to $x=16$) using a combination of density functional theory (DFT) and reactive force field (ReaxFF).

Also, in rechargeable Li-ion battery, it is commonly known that an organic electrolyte such as ethylene carbonate (EC) is decomposed during the first lithium intercalation into graphite to form a solid electrolyte interface (SEI) film on the graphite anode surface, and it is the SEI film that largely determines the performance of graphite as anode in the rechargeable battery. Thus we investigate reductive decomposition mechanisms of EC using DFT calculations. The reduction of EC is thermodynamically forbidden, however the presence of Li cation considerably stabilizes the EC reduction intermediates such as Li$_2$CO$_3$ and (CH$_2$OCO$_2$Li)$_2$ which is in good agreement with published experimental data.