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**Effect of electrolytes on the evolution of the solid electrolyte interphase (SEI) in Li-ion batteries: a Molecular Dynamics study** SANG-PIL KIM, VIVEK SHENOY, Brown University, BROWN UNIVERSITY TEAM — Controlling and understanding the atomic level reactions at the interface between electrode and electrolyte is a prerequisite for the improvement of the performance of Li-ion batteries. The solid electrolyte interphase (SEI), which forms on the negative electrode of Li-ion batteries, is known to significantly affect the battery performance leading to irreversible charge loss, exfoliation of graphite anode and affecting the safety. In spite of the large body of work on SEI, a quantitative understanding of the mechanisms of SEI formation is currently not available. In this work, we employ molecular dynamics simulations with reactive force fields to investigate the compositional and structural properties of the SEI. Our simulations capture the mechanisms of SEI formation as Li atoms react with different kinds of electrolytes (ethylene carbonate (EC), dimethyl carbonate (DMC), and their mixtures) and are able to quantitatively predict the properties in terms of the SEI thickness, byproducts, charge loss, and rigidity.

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