

**Solvent Reduction and SEI Layer Formation:
Theory and Experiments**

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Quantum chemical calculations have been performed to investigate the reduction and decomposition mechanisms of ion-solvent-cosolvent systems of several degrees of complexity. We focus on the reduction of ethylene carbonate as well as on the role of vinyl carbonate as additive.[1] New insights are obtained about the possible paths for solvent reduction and decomposition, and the relation of these findings to experimental results is analyzed in detail. We discuss the impact of this novel approach to achieve a theoretical-guided electrolyte design.

References [1] Y. Wang, S. Nakamura, M. Ue, and P. B. Balbuena, Theoretical studies to understand surface chemistry of carbon anodes for lithium ion batteries: Reduction mechanisms of ethylene carbonate and the role of vinyl carbonate as additive, *J. Am. Chem. Soc.*, submitted.