

**Prediction of Reduction and Oxidation Potentials with
Ab Initio Methods, and an Evaluation of Reduction
Mechanisms for Alkyl Carbonates**

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We present and assess a methodology for using *ab initio* techniques to predict reduction and oxidation potentials of electrolyte components. On a series of standards this method was shown to yield reduction potentials within 0.29 eV, on average, of the experimental values. This methodology has been used to screen additive candidates for the second generation Li⁺ ion cell, by predicting their stability over the desired operating potential range. We will also present our findings for various reduction mechanisms for several cyclic carbonates. These investigations have provided valuable insight into why some cyclic carbonates were effective additives while others were not.