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Synthetic screening of electrolytes for Li-Air batteries

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Abstract

There is increasing interest in designing and manufacturing high-performance batteries for a wide variety of applications; however, finding the best electro-chemical system and configuration is a challenging task given all the possibilities. In particular, choosing an electrolyte optimal for a given battery configuration and chemistry is a daunting and crucial task in and of itself. We propose a computational approach to electrolyte screening and selection for a Li-air battery. Li-air batteries are particularly attractive for mobile and transportation applications given their high theoretical volumetric and gravimetric energy densities, which in part is due to using environmental oxygen. Through a combination of techniques, starting with *ab initio* calculations to provide fundamental parameters, to molecular dynamics which, in turn, provides transport coefficients to a full-scale model battery, we can predict battery performance. Predictions using these techniques spanning many spatio-temporal scales are compared with a limited set of cyclic voltammetry experiments for validation before applying the process to a wide range of solvent, salt and other permutations to select the best candidates for intensive development. The concept of computational screening for battery development is not novel, *e.g.* the work the Ceder group, but here we focus on identifying ideal electrolytes for Li-air batteries where the diffusion of dissolved Li ions and molecular oxygen have been identified as power performance metrics.

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