Ab Initio Spectroscopy and Screening of Materials for the Li/Air Batteries

B. Kozinsky and R. S. Sanchez-Carrera

Research and Technology Center North America, Robert Bosch LLC, Cambridge, MA 02142, USA.

The Li/air battery has recently received much attention because of its high theoretical energy density. However, there are still many technical problems impeding the development of a practical Li/air battery; even a basic understanding of the molecular reactions governing this electrochemical system remains elusive. We have used first-principles calculations to improve our understanding of the molecular reaction mechanism and to investigate the Raman and NMR spectroscopic signatures of possible Li/air reaction products/by-products. Our simulations of candidate molecules indicate that specific spectroscopic characteristics can be used to determine the structure and composition of the discharge products from measured spectra. The electrochemical stability of the solvent is another challenge, affecting reversibility of the Li/air battery. We identify a set of descriptors of electrochemical stability based on total energy computations. Subsequently we perform systematic screening of a large database of potential candidate solvent molecules, and extract useful design rules and trade-off relationships.

Contact: Boris.Kozinsky@us.bosch.com