MAR17-2016-007585

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Rational design of nontoxic electrolytes for metal-ion batteries

PURU JENA, Virginia Commonwealth University

Most of the electrolytes used in current Li-ion batteries contain halogens, which are both toxic and corrosive. In an effort to search for halogen-free electrolytes, we studied the electronic structure of these complexes using density functional theory and found that the negative ions of all the current electrolytes are superhalogens, i.e., the vertical electron detachment energies of these moieties are larger than that of any halogen atom. Realizing that several superhalogens that do not contain even a single halogen atom exist, we studied their potential as effective electrolytes by calculating not only the energy needed to remove a Li^+ ion but also their affinity towards H_2O. Several halogen-free electrolytes are identified among which $Li(CB_{11}H_{12})$ was shown to have the greatest potential. Replacing H in $Li(CB_{11}H_{12})$ with CN or SCN moieties further improves the electrolyte performance. Validation of our prediction by recent experiments as well as a new family of super-ion inspired solid electrolytes based on anti-perovskite structures will also be discussed. More information can be found from S. Giri, S. Behera, and P. Jena, Angew. Chem. Int. Ed. **53**, 13916 (2014) and H. Zhao, J. Zhou, and P. Jena, Angew. Chem. Int. Ed. (*VIP*) **55**, 3704 (2016).