Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density Functional Theory on the Studies of Lithium Battery Materials[1] BO WANG, SIJIE LUO, Department of Chemistry, University of Minnesota, DONALD TRUHLAR, Department of Chemistry and Supercomputing Institute, University of Minnesota — Computational studies on the electrode materials in lithium batteries provide crucial information on the structure change and charge flow during the charging and discharging processes. Among various theoretical methods, Kohn-Sham theory provides the best compromise between the accuracy and the computational cost. In the present study, we tested several new density functionals on the lithium-containing materials. M06-L and N12, which have already shown good performance in a variety of databases, outperform the widely used PBE functional to reproduce the experimental structures and averaged intercalation potentials. Especially, M06-L functional gives similar performance as Heyd-Scuseria-Ernzerhof hybrid functional, but with less computational cost. Partial atomic charges provide a very convenient way to describe the charge distribution within molecules and crystals, and they are useful as an analysis tool that reflects charge flow during charging and discharging processes. In the present study, we validated CM5 charge model on a set of small molecules and derived CM5 partial atomic charges of a set of lithium compounds to understand the charge flow during electrochemical processes. Moreover, we applied the new tools to explore some new promising lithium-containing compounds.

[1]This work is supported by DOE

Bo Wang
Department of Chemistry, University of Minnesota

Date submitted: 15 Nov 2013 Electronic form version 1.4