Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Screened Hybrid Exact Exchange Schemes to Adsorption Energies on Perovskite Oxides ELTON SANTOS, Department of Chemical Engineering, Stanford University, Stanford, California 94305, USA, ALEKSANDRA VOJVODIC, SLAC National Accelerator Laboratory, Menlo Park, CA, 94305, JENS K. NORSKOV, Department of Chemical Engineering, Stanford University, Stanford, California 94305, USA — The bond formation between an oxide surface and oxygen, which is one of the important intermediates for oxygen evolution reaction, is investigated using hybrid functionals. We show that there exists a linear correlation between the adsorption energies of oxygen on LaMO3 (M=Sc-Cu) oxides at hybrid calculations to those computed using semilocal density functionals through the magnetic properties of the bulk phase. The energetics of the spin-polarized surfaces follow the same trend as corresponding bulk systems, which can be treated at a much lower computational cost. The difference in adsorption energy due to magnetism is linearly correlated to the magnetization energy of bulk, i.e., the energy difference between the spin-polarized and the non spin-polarized solutions. This suggests that one could estimate the correction to the semilocal density functional adsorption energies directly from the hybrid bulk magnetization energy.

Elton Santos
Stanford University

Date submitted: 17 Oct 2014 Electronic form version 1.4