Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Surface-Specific Hubbard U calculations for α-Fe_2O_3 (0001) Surfaces[1] XU HUANG, SAI KUMAR RAMADUGU, SARA MASON, Univ of Iowa — The (0001) surface of α-Fe_2O_3 exists in different terminations that exhibit chemically distinct Fe atoms. The widely studied terminations for this plane are: -O3Fe, -O3Fe2, the ferryl termination (-Fe=O), -Fe2O3, and -Fe3O3. Using GGA+U on the above surface terminations, it has been shown that the most stable terminations in the high oxygen chemical potential were -O3Fe and -Fe=O whereas in the standard GGA the most stable terminations were shown to be -Fe2O3 and -Fe3O3. Experimental studies have shown that the results from standard GGA are in better agreement with the experimental phase diagram. It is known that reducing the dimensionality of bulk hematite to form surfaces results in Fe surface sites that are not chemically equivalent to bulk Fe, and this is proposed to be problematic for DFT+U approaches that apply the same U value throughout to all Fe atoms in the slab. In the current work we show that the surface-specific derived Hubbard U values from the response matrix method affects the energetics, electronic structure, and relative stabilities of α-Fe_2O_3 (0001) surface structure.

[1]NSF CHE 1254127

Sara Mason
Univ of Iowa

Date submitted: 15 Nov 2013 Electronic form version 1.4