Combined Theoretical and Experimental Model of an Oxide-Supported Heterogeneous Catalyst: \( WO_x/\alpha-Fe_2O_3(0001) \) MARTIN MCBRIARTY, ZHENXING FENG, Northwestern University, MICHAEL BEDZYK, Northwestern University, Argonne National Laboratory, DONALD ELLIS, Northwestern University — Spin-polarized density functional theory (DFT) calculations were combined with surface-sensitive experimental techniques to evaluate models of monolayers and sub-monolayers of catalytic \( WO_x \) on the (0001) surface of \( \alpha-Fe_2O_3 \) (hematite). Relaxed structures for various surface configurations were calculated, taking into account the surface lattice position and oxygen coordination of W as well as the presence of hydroxyl groups or adsorbed water. These structures were compared to surface atomic density maps generated by synchrotron x-ray standing wave (XSW) imaging under reducing and oxidizing conditions to deduce the most plausible atomic configurations. Theoretical ionicity of W atoms increased with oxygen coordination; as expected, the formal charges (\( W^{5+} \) and \( W^{6+} \)) inferred from x-ray photoelectron spectroscopy (XPS) were not found. Using charge density maps and local densities of states, surface W-O and W-W interactions were studied and compared to Fe-O interactions in the bulk.

Martin McBriarty
Northwestern University

Date submitted: 19 Nov 2009

Electronic form version 1.4