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Combined Theoretical and Experimental Model of an Oxide-Supported Heterogeneous Catalyst: WO_x/α-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 α-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.

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