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In Situ **Synchrotron Studies of a Model Catalyst: WO_x/α-Fe_2O_3**
MARTIN MCBRIARTY, ZHENXING FENG, Northwestern University, JOSEPH LIBERA, JEFFREY ELAM, Argonne National Laboratory, DONALD ELLIS, MICHAEL BEDZYK, Northwestern University — Statistically averaging surface-sensitive X-ray techniques are employed to elucidate the surface morphology of a model oxide-supported heterogeneous catalyst, tungsten oxide (WO_x) on hematite (α-Fe_2O_3). Atomically flat α-Fe_2O_3 (0001) single crystals were coated with sub-monolayer WO_x by atomic layer deposition (ALD). *In situ* X-ray standing wave (XSW) imaging with X-ray fluorescence (XRF) was used to determine W position relative to bulk-like cation lattice sites under nominally reducing and oxidizing chemical conditions. X-ray absorption fine structure (XAFS) reveals details of W coordination, bond length, and chemical state on WO_x-coated hematite single crystals and nanopowders. Synchrotron characterization results are compared with morphologies predicted by density functional theory (DFT) calculations for clean WO_x/α-Fe_2O_3 surfaces. Thermodynamics and atomic configurations for H_2O and CO adsorption are also predicted. Excited-state self-consistent field (SCF) calculations are used to model X-ray photoelectron spectroscopy (XPS) results.

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