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Diffraction Anomalous Fine Structure on 2D Metal Oxides

Two-dimensional metal oxides are attractive model systems for applications in catalysis and electrochemistry due to their high surface areas and tunability of chemical properties by combining elements across the periodic table. Grazing incidence X-ray absorption spectroscopy, although sensitive to the electronic state and coordination environment around absorbing atoms, cannot differentiate the atoms located at different depths from the surface. Standard X-ray diffraction, on the other hand, cannot differentiate between elements with comparable atomic numbers to identify their location and activity within the layers. We present a proof-of-concept diffraction anomalous fine structure (DAFS) measurement on the surface rod of a 3-layer iron oxide film grown on a Ag(100) surface [1]. We extract element and depth specific electronic information in this system by combining DAFS at different regions on the surface rod with simulated spectra from atoms at different layers calculated by ab initio methods [2]. This experiment opens the possibility to study the dynamics of atom and depth specific oxidation states and coordination information of active catalytic sites in an operando experiment.

[1] L. R. Merte *et al.*, **2020**, Structure of two-dimensional Fe_3O_4, *J. Chem. Phys.* 152, 114705
[2] Joly Y *et al.*, **2018**, Simulation of Surface Resonant X ray Diffraction. *J. Chem. Theory Comput.* 14, 973–980

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Studies of atomic and nanostructured surfaces and interfaces

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