

Abstract Submitted
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Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111) H. ZHANG, Sichuan University, China, A. SOON, The University of Sydney, Australia, B. DELLEY, Paul-Scherrer-Institut, Switzerland, C. STAMPFL, The University of Sydney, Australia — Iridium-based catalysts are widely used in several important chemical reactions. Despite this, very little is known about the surface structure of the catalyst and the atomic and molecular processes involved. As a first step towards a microscopic understanding, we use density-functional theory, coupled with *ab initio* atomistic thermodynamics [1], to investigate chemisorption of oxygen on Ir(111), and the stability of surface oxides. We find for on-surface adsorption, oxygen prefers the fcc-hollow site for all coverages considered, where with increasing coverage, the adsorption energy decreases substantially. Subsurface adsorption is found to be highly unfavourable. The most favourable surface-oxide-like structure has a tri-layer-like (O-Ir-O) configuration, which however, the (p, T) phase diagram predicts is only metastable. For practically all conditions, except ultra-high vacuum, the bulk oxide is thermodynamically the most stable, and the only other stable phase predicted is the on-surface (2x2)-O structure for coverage 0.25 ML [2]. These studies point to the possible importance of oxidized iridium for heterogeneous oxidation reactions. [1] C. Stampfl, Catal. Today 105, 17 (2005). [2] H. Zhang, A. Soon, B. Delley and C. Stampfl, submitted to Phys. Rev. B.

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