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Towards Controlling the Structural Evolution and Kinetic Properties of Monolayer (Hydr)oxide-Metal Interfaces ZHENHUA ZENG, JOSEPH KUBAL, JEFF GREELEY, Purdue University — Ultrathin (hydr)oxide films grown on transition metal surfaces have widespread applications in processes related to electrocatalysis, photocatalysis, coating and corrosion inhibition, and heterogeneous catalysis, among others. These hybrid systems with novel properties are often prepared and characterized under very specific conditions, such as ultra-high vacuum. When subsequently used in various applications, however, significant structural evolution, which depends strongly on the reaction conditions in-situ, is expected and has been widely observed. Nevertheless, the atomic-level details of these structural changes are generally unknown, particularly in the case of electrocatalytic environments. In order to identify structure-property relationships and, ultimately, predict new materials with improved performance, the development of such understanding is essential. In the present study, on the basis of detailed density functional theory calculations, and using Ni (hydr)oxide films on Pt(111) and Au(111) electrodes as model systems, we describe a detailed structural analysis of film growth and electrocatalytic analysis of hydrogen evolution at three-phase boundaries under alkaline electrochemical conditions.

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