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First-principles determination of LaMnxM1-xO3 surface structures under catalytic conditions XI RONG, ALEXIE KOLPAK, Department of Mechanical Engineering, Massachusetts Institute of Technology, KOLPAK GROUP TEAM — The design of efficient and cost-effective catalysts for the oxygen evolution reaction (OER) is crucial for the development of electrochemical conversion technologies. One of the most important factors determining the activity is the surface/interface structures of catalysts. However, little is known about the atomic and electronic structures and thermodynamic properties of realistic interface reconstructions, which are caused by different environments during fabrication, measurement, and eventual device operation. In this work, we apply first-principles density functional theory computations in combination with kinetic modeling to investigate the environment-dependent chemical and physical properties of perovskite oxide heterostrucutre catalysts, particularly LaMnxM1-xO3. We develop a methodology for accurate identification of constraints on the interface structure phase space and rapid computation of this identification as a function of temperature, pressure, and other chemical environments. Our work could lead to accurate and rapid prediction of surface/interface structures and properties under different environmental conditions, and contribute to the design of new high-activity OER catalysts.

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