Abstract Submitted
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Comparison Between Crystalline and Amorphous Surfaces of Transition Metal Oxide Water Oxidation Catalysts: a Theoretical Perspective[1] JONATHAN H. SKONE, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — Amorphous films of transition-metal oxide water oxidation catalysts (WOCs) often show an enhanced catalytic activity compared to their crystalline counterparts [1-4]. In particular, in the case of cobalt-oxide based WOCs the observed similarity in their electrochemical properties and catalytic activity, under oxidative conditions, has been correlated with the formation of similar amorphous surface morphologies, suggesting the presence of a common, catalytically active amorphous structural motif [3,4]. We present ab initio calculations of cobalt oxide based material surfaces and we compare the electronic properties of crystalline and amorphous surfaces, with the aim of identifying differences related to their different catalytic activity.

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