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Effect of iron content on the catalytic activity of Fe-MnOx electrodeposited films in water oxidation[1] ELIZABETH SELINGER, KEVIN RYCZKO, University of Ontario Institute of Technology, GREGORY LOPINSKI, National Research Council of Canada, MARCO ARMANDI, BARBARA BONELLI, Politecnico di Torino, ISAAC TAMBLYN, University of Ontario Institute of Technology, National Research Council of Canada — We report on the experimental and computational optimization and characterization of an MnOx structure containing a small amount of Fe, used as a catalyst for the water oxidation reaction (WOR), the key limiting reaction in water splitting. MnOx materials are earth-abundant and known to be efficient for WOR, and the method of cathodically electrodepositing catalysts allows for quick synthesis and a homogeneous coverage of the substrate. We present an increase in WOR activity due to the presence of Fe in this MnOx catalyst structure. First, we explored the optimal range for $Fe(NO_3)_3$ concentration in an $KMnO_4$ solution for electrodeposition and tested for WOR activity. The catalyst structure was then analyzed using FESEM, XPS, and a Kelvin probe. We then developed a computational model of this structure, using density functional theory to obtain adsorption energies, work functions, projected density of states, and Born-Oppenheimer molecular dynamics. In this theoretical framework, we explore how these observables change with respect to concentration of Fe, and compare the theoretical model with experiment.

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