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A joint theoretical and experimental study of the (Ni,Fe)-oxyhydroxide oxygen evolution catalyst for water splitting[1] ZACHARY K. GOLDSMITH, APARNA K. HARSHAN, Department of Chemistry, University of Illinois at Urbana-Champaign, MARTON VOROS, Argonne Natl Lab, JAMES GERKEN, SHANNON S. STAHL, Department of Chemistry, University of Wisconsin-Madison, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago and Argonne Natl Lab, SHARON HAMMES-SCHIFFER, Department of Chemistry, University of Illinois at Urbana-Champaign — Recent experiments showed that iron doped nickel oxyhydroxides are excellent catalysts for driving the oxygen evolution reaction (OER) of water splitting; however, the role played by iron is still controversial.[1, 2, 3] In a joint theoretical and experimental study, we investigated the optoelectronic properties and oxidation potentials of the (Ni,Fe)-oxyhydroxide layered materials, and we determined oxidation states, band gaps and analyzed the role of iron doping. We found that Fe(IV) is present in catalytically active, doped oxyhydroxides, consistent with the suggestions of recent in operando Mossbauer experiments,[3] and that oxygen atoms bound to the Fe dopants might be the most active sites for OER in oxyhydroxide films. We also showed that hybrid functionals give a more accurate account of the optical properties of these materials than the widely adopted DFT+U level of theory. [1] L. Trotochaud et al., JACS 136, 6744 (2014). [2] D. Friebel et al., JACS 137, 1305 (2015). [3] J. Y. C. Chen et al., JACS 137, 15090 (2015).

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