DFT study for oxygen evolution mechanism on nickel ferrite

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Oxygen evolution reaction (OER) is the progress of generating molecular oxygen from water and is a key technology for storing renewable electricity. OER consists of four proton-couple electron transfer and an ideal catalyst has same energy of each stage, 1.23 eV. Precious metal oxides, such as ruthenium and iridium oxides, show high activities, but their high costs limit universal applications. Hence, developing alternative catalysts is an essential requirement for the renewable energy industry.

The nickel substituted ferrites ($Ni_xFe_{3-x}O_4$) exhibit the promising OER activity in aqueous alkaline electrolytes, and are also based on relatively low-cost metals. In this study, density functional theory (DFT) calculations were performed to investigate the mechanism of OER over (111) surface of nickel ferrite. We examined the effect of Ni:Fe stoichiometry for electrocatalytic activity. Our results shed light on the oxygen evolution mechanism on ferrite-type catalyst and provide descriptors for alternative catalyst screening.