Computational investigation into cobalt-doped NiSe$_2$ and its catalysis of the oxygen evolution reaction

Electrocatalytic water splitting represents an environmentally friendly method to chemically store energy as H$_2$ to later be released in hydrogen fuel cells. Widespread production of H$_2$ from H$_2$O is hampered by the slow kinetics of the oxygen evolution reaction and the high cost of state-of-the-art catalysts for this reaction. Nickel compounds are attractive alternatives due to their catalytic activity and relatively low cost. Doping these nickel compounds, particularly nickel oxides, with cobalt has been shown to improve the material’s catalytic activity. While much research has been done on nickel oxides and hydroxides, very little is known about their selenide counterparts despite having desirable properties such as higher conductivity and known structures for a wide range of stoichiometries. Here, we shall discuss the effects of cobalt levels and surficial symmetry on the stability of NiSe$_2$. We shall also show how the dopant levels and distribution affect the energetics of the oxygen evolution reaction on various low Miller index surfaces.