DFT study for alkaline HER enhancement with single heteroatom doping on metal hosts

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Hydrogen evolution reaction (HER), a half-reaction in electrolysis, is a process of generating molecular hydrogen from water and is a key technology for storing renewable energy. Alkaline media expands the scope of electrocatalysis by overcoming instability problem, but causes slower HER kinetics compared to acidic media. Hence, developing catalysts with high activity and reasonable price is an essential requirement for the renewable energy industry.

Doping a non-precious metal with a heteroatom can tune the surface properties to optimize the binding energy of reaction intermediates and enhance intrinsic catalytic activity. In this study, various 3d transition metals (Fe, Co, Ni, Cu, Ti) were added to the host metals (Ru, Ni) as a single atom form to improve alkaline HER activity. Density functional theory (DFT) calculations were performed to investigate the surface electronic structure change by heteroatom doping and its effect on alkaline HER activity. We revealed that OH binding energy is an important factor in the activity, while H binding energy has been in debate as its descriptor. Our results shed light on the rational design principle of alkaline HER catalysts.