Insights on Hydrogen Evolution Reaction in Transition Metal Doped Monolayer Tcs2 from Density Functional Theory Calculations

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Abstract

The catalytic activity for hydrogen evolution reaction (HER) in monolayer TcS2 has been investigated using van der Waals corrected density functional theory. Also, the influence of transition metal dopants (Fe, Co, Ni, Pd and Pt) and their respective sulphur vacancy complexes on HER were evaluated. Using the adsorption free energy of H as a descriptor for the catalytic activity of HER, cation substitutional doping was found unsuitable for stable H adsorption on monolayer TcS2. This configuration leads to poor catalytic activity of the monolayer towards HER. However, vacancy complexes involving Ni, Pd and Pt showed improved catalytic activity towards HER. All the transition metal vacancy complex were found to exist as stable bound complexes.

Keywords: Hydrogen evolution, 2D monolayer, Transition metal dopin

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