Universality of Mixing Rule of Surface Alloy upon Small-Molecule Adsorption

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In the field of surface chemistry and catalysis, understanding the adsorption phenomena of small molecules that participate in a surface reaction on transition metal surfaces is important because their adsorption energies can be powerful descriptors for predicting the activity. Although first-principle calculations within the framework of density functional theory (DFT) are a fast and economic method to calculate the adsorption energies of small molecules, huge computational expenses are still required to calculate the adsorption energies for a wide range of binary transition metal alloys. We suggest the simple mixing rule of binary alloy surfaces upon small molecule adsorption, solely based on the adsorption energies on pure metal surfaces. The mixing rule, which is a simple approximation depending on the surface composition of host and solute metals, can effectively save both time and cost to estimate the adsorption energies of small molecules on surface alloys. Our results will provide a useful tool for both computationally and experimentally screening the adsorption energies on multi-component metal alloy surfaces.