Universality in Surface Mixing Rule of Adsorption Strength for Small Adsorbates on Binary Transition Metal Alloys

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Understanding the adsorption phenomena of small adsorbates that involve in a surface reaction on transition metals is important because their adsorption strength can be descriptors for predicting the catalytic activity. Although density functional theory (DFT) is a fast method to calculate the adsorption energy, tremendous computational efforts are still required to explore it on a wide range of binary transition metal alloys. Using DFT calculations, here we suggest "surface mixing rule" to predict the adsorption energies of H, O, S, CO and OH on binary transition metal alloys, based on the linear interpolation of adsorption energies on each pure surface. We also demonstrate that the 1st layer d-band center of binary transition metal alloys can be predicted from the weighted average of 1st layer d-band center of each pure metal. This can be thought of as an origin of theoretical framework for the surface mixing rule of adsorption energy. Our results provide a useful tool for rapidly estimating the adsorption energies, and furthermore, the catalytic activities on multi-component metal alloy surfaces.