The d-band center is not enough: Efforts toward better descriptor for surface reactivity and bonding

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The d-band center has become a popular language in the community of heterogeneous catalysis, including electrocatalysis. In some particular cases, the d-band center of transition-metal surface seems to be a good reactivity index, but it can hardly be a satisfactory one when a wide range of transition metals are involved (Figure 1), not to mention its disability in comparing different adsorbates on the same surface.

In our recent research on new discription for chemical bond, we use a complex number, termed the chemical amplitude \((R = ae^{i\theta})\), to characterize a reactant (be it an atom or a surface); and the bond energy is deduced to be the absolute square of the interfered chemical amplitudes of two involved reactants. This model turns out to work very well for both covalent bonds in molecules and adsorption bonds on transition metal surfaces. As an example, we show in Figure 2 the result of Cl adsorption on 25 transition metals, the model-predicted bond energy matches the DFT-calculated adsorption energy with satisfied accuracy.

Detailed information about the theoretical model and relevant calculations will be presented in the meeting.

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Figure 1. The d-band center is not able to describe the surface reactivity for a wide range of transition metals.

Figure 2. The chemical-amplitude model proposed in this work can predict the adsorption energy in an accuracy within the error of DFT calculations.