Quantitative assessment of catalytic site activity via nc-AFM

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Active site, the smallest spot where catalytic process happens, is the fundamental concept in heterogeneous catalysis. Identifying activity of hundreds of sites in real systems is a prerequisite for understanding the structure-activity relationship and further designment of catalyst. Parameters describing the catalytic activity of sites, named descriptions, are useful concept in theory but hard to measure in practical, especially at atomic level. Our research proposed a novel method to visualize and quantify the activity of surface sites at atomic scale via non-contact Atomic Force Microscopy (AFM). The method is based on oxygen-terminated tip and "Scaling relation". Interaction force or energy between oxygen-terminated tip and catalytic site was supposed to have positive correlation with oxygen adsorption energy, which is a renowned descriptor in theoretical chemistry. Several kinds of single atoms catalyst (SAC), dispersed on Cu(110)-2×1-O, were fabricated as a platform to test activity assessment method. The order of interaction force for SACs follows Mn>Fe>Co≈Cu, so the predicted order of oxygen adsorption energy should be the same. To examine such prediction, decomposition of oxygen molecule reaction and DFT calculation were done on SACs, and the initial temperature at which decomposition happens and calculated oxygen adsorption energy do confirm the prediction and the activity assessment method.

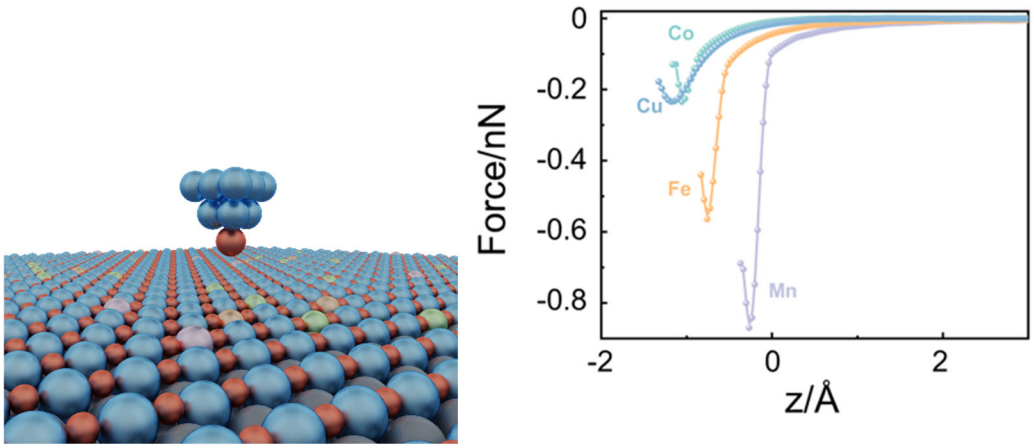

Figure 1. Schematic of activity assessment method and example force spectra.

Reference

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[2] J. Berwanger, et al. Phys. Rev. Lett. **2020**, 124 (9).

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