Single-Atom Catalysts: An Atomic-Scale View

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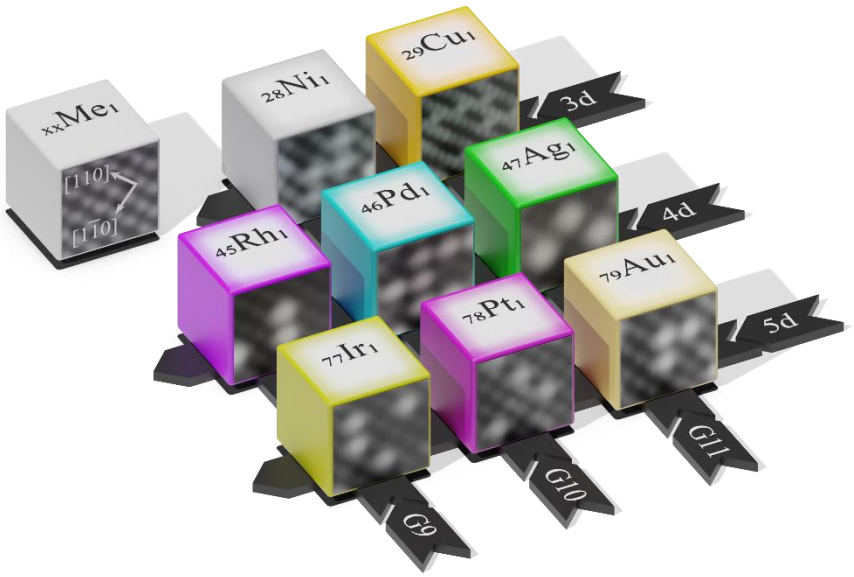
Understanding how the local environment of a "single-atom" catalyst affects stability and reactivity remains a significant challenge. In this talk, I will discuss under what circumstances single metal atoms can be stable on flat, well-ordered metal oxide surfaces, including examples from our work on Fe_3O_4, Fe_2O_3, and TiO_2 single-crystal model supports. Thereafter, I will focus an in-depth study of Cu_1, Ag_1, Au_1, Ni_1, Pd_1, Pt_1, Rh_1, and Ir_1 species on $Fe_3O_4(001)$; a model support where all metals occupy the same 2-fold coordinated adsorption site upon deposition at room temperature[1]. Surface science techniques reveal that CO adsorption strength at single metal sites differs from the respective metal surfaces and supported clusters.[2] Charge transfer into the support modifies the d-states of the metal atom and the strength of the metal-CO bond. These effects could strengthen the bond (as for Ir_1-CO) [3] or weaken it (as for Ni_1-CO), but CO-induced structural distortions reduce adsorption energies from those expected based on electronic structure alone. The extent of the relaxations depends on the local geometry and could be predicted by analogy to coordination chemistry. In extreme cases, CO adsorption leads to sintering, and I will show that metastable $(PtCO)_2$ dimers are active for CO oxidation in the – nominally – $Pt_1/Fe_3O_4(001)$ system.[4]



References

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2. J. Hulva et al., Unraveling CO adsorption on model single-atom catalysts. *Science* 371, 375 (2021)
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