An atomic-scale view of single-atom catalysis

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It is now clear that the local coordaintion of a „Single-Atom„ strongly affects its catalystic properties. In this talk, I will discuss examples from our recent work utilizing Fe_3O_4, Fe_2O_3, and TiO_2 model supports, where the structure is precisely known and the local geometry can be determined [1]. Using a combination of atomcally resolved imaging, spectroscopy, and theoretical computations, I will show how the adsorption behavior of reactants can be understood by analogy to coordination complexes utilized in homogeneous catalysis [2]. Finally, I will utilize time-lapse STM movies to show how metal adatoms can be both stabilized and destabilized by adsorption of reactants and other molecules in a reactive environment [3] .

References

[1] R. Bliem et al., Subsurface cation vacancy stabilization of the magnetite (001) surface. *Science* **346**, 1215-1218 (2014)

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

[3] Z. Jakub et al., Local Structure and Coordination Define Adsorption in a Model Ir_1/Fe_3O_4 Single-Atom Catalyst. *Angew. Chem. Int. Ed.* **58**, 13961-13968 (2019).

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