TECHNISCHE UNIVERSITÄT CHEMNITZ

Institut für Physik

Physikalisches Kolloquium

Mittwoch, 10.05.2023, um 11:15 Uhr

Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude,
Raum C10.013

Prof. Dr. Gareth S. Parkinson

TU Wien

GAEDE-PREISTRÄGER 2018

Atomic-Scale Studies of Model Single-Atom Catalysts

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) or weaken it (as for Ni_1-CO), but CO-induced structural distortions reduce adsorption energies from those expected based on electronic structure alone [3]. 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

[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).
[4] M. Meier et al., CO oxidation by Pt_2/Fe_3O_4: Metastable dimer and support configurations facilitate lattice oxygen extraction. Science Advances 8, eabn4580 (2022)

Acknowledgments
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Alle Zuhörer sind ab 11:00 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt:
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