“Single-Atom” Catalysis: An Atomic-Scale View

Speaker: Dr Gareth Parkinson

Institute of Applied Physics, TU Wien, Vienna, Austria

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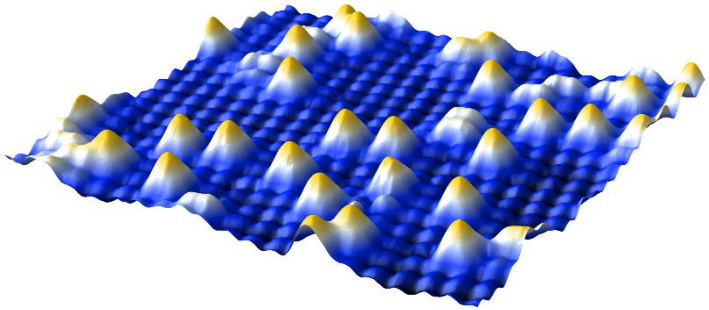
The field of „single-atom” catalysis (SAC) [1] emerged as the ultimate limit of attempts to minimise the amount of prescious metal used in heterogeneous catalysis. The field has grown rapidly and there are many reports of active active catalysts for many important heterogeneous, electrochemical and photoctalystic reactions. Over time, it has become clear that metal adatoms behave very differently to supported nanoparticles [2], primarily because they form chemical bonds with the support and become charged. In this sense, SAC systems resemble the mononuclear coordination complexes used in homogeneous catalysis, and there is growing excitement that SAC could achieve similar levels of selectivity, and even „heterogenize” problematic reactions currently performed in solution. It is important to note, however, that homogeneous catalysts are designed for purpose based on well-understood structure-function relationships. In SAC, the complexity of real systems means that the structure of the active site is difficult to determine, never mind design. In this talk, I will describe how we are using $Fe_3O_4(001)$ as a precisely-defined model support [3; 4] to unravel fundamental mechanisms in SAC. I will show scanning tunneling microscopy (STM, noncontact atomic force microscopy (ncAFM), x-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD) data to show how CO exposure destabilizes Pd adatoms [5], how the local structure of $Ir_1/Fe_3O_4(001)$ and $Rh_1/Fe_3O_4(001)$ single atom catalysts changes based on preparation and adsorption of reactants, and that CO oxidation activity in the $Pt_1/Fe_3O_4(001)$ system results from Pt_2 dimers [6; 7], not single atoms.

References

1. Qiao B et al. (2011). Nat Chem 3:634-641
2. Parkinson GS (2019). Catal Lett 149:1137-1146
3. Bliem R et al.(2014). Science 346:1215-1218
4. Parkinson GS (2016). Surf Sci Rep 71:272-365
5. Parkinson GS et al. (2013). Nat Mater 12:724-728
6. Bliem R et al. (2016). Proc Natl Acad Sci USA 113:8921-8926
7. Bliem R et al. (2015). Angew Chem Int Ed 54:13999-14002



3d representation of an STM image of isolated Au adatoms adsorbed on $Fe_3O_4(001)$ at room temperature