PhD Positions Available Immediately in ERC Funded Research Project:

Evolving "Single-Atom" Catalysis:

Fundamental Insights for Rational Design

Project Description

Rare and expensive metals tend to make the best heterogeneous catalysts, and minimising or replacing these materials is a major research target as we strive to develop an economy based on more environmentally-friendly, energy-efficient technologies. "Single-atom" catalysis (SAC) represents the ultimate in efficiency, and the chemical bonds formed between the metal atom and the support mean these systems strongly resemble the organometallic complexes utilized in homogeneous catalysis. If all active sites were identical, SACs could achieve similar levels of selectivity, and even be used to "heterogenize" difficult reactions currently performed in solution. There is a problem however: homogeneous catalysts are designed based on well-understood structure-function relationships. In SAC, the structure of the active site is unknown, and rational design is currently impossible.

The group in Vienna has pioneered the use of the model supports to understand fundamental mechanisms in SAC. Our work with Fe_3O_4(001) proves that we can *precisely determine* and even *selectively modify* the active site, and unravel the role of structure in catalytic activity. Real progress, however, requires realistic active sites, realistic supports, and realistic environments. In this project, we will determine the sites that robustly anchor metal atoms on five of the most important supports in ultrahigh vacuum (UHV), and test their performance in newly-developed high-pressure and electrochemical cells. The origins of selectivity for PROX, hydrogenation, hydroformylation, methane conversion, and the oxygen reduction reaction (ORR) will be determined, and the best atom/support combinations for each reaction identified. Robust XANES and IRAS spectra will allow us to bridge the complexity gap and recreate the optimal active sites on real SACs and lead the way into a new era in which heterogeneous catalysts are designed for purpose, based on a fundamental understanding of how they work.

Masters degree in Physics or Chemistry required.
Applications by email to:

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