IAP Seminar

Tuesday, 23rd Jan. 2024, 16:00 s.t.
TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

Ali Rafsanjani-Abbasi

Institute of Applied Physics
TU Wien

A Comparative Study of Late-Transition Metal Single Atoms on $Fe_2O_3(1\bar{1}02)$

Precious metals supported on oxides exhibit exceptional effectiveness in various chemical reactions, such as hydrogen evolution, water gas shift, photocatalytic processes, and CO-oxidation reactions due to their elevated activity and/or selectivity. Downsizing catalysts to single atoms enhances the efficiency, and so-called “single-atom catalysis” is now an important field of research. Nevertheless, achieving stable single atoms of late-transition metals on oxide supports without compromising catalytic activity raises significant challenges. This seminar centers on surface science techniques to examine the specific binding environment of rhodium, platinum, and iridium adatoms on α-$Fe_2O_3(1\bar{1}02)$-(1×1). Using STM and XPS, I will discuss the stability of single atoms at room temperature, their adsorption sites, and the impact of O_2. Additionally, the sintering behavior of single atoms at elevated temperatures will be traced using XPS and STM.

Panukorn Sombut

Institute of Applied Physics
TU Wien

Computational Studies of the $Fe_3O_4(001)$ Surface as a Model for Single-Atom Catalysts

Single-atom catalysts (SACs) represent a new frontier in heterogeneous catalysis due to their particular local environment, resulting in a unique electronic structure in comparison with traditional supported nanoparticle catalysts. While the hydroformylation reaction between alkenes and syngas (CO and H_2) conventionally involves Rh-based complexes, there is growing evidence suggesting that SACs can selectively catalyze this reaction. In this study, we employed a combination of DFT and surface science techniques, including STM, TPD, and XPS to investigate the interaction of C_2H_4, CO, and H_2 on Rh_1-decorated $Fe_3O_4(001)$. We explore the intricate details of how individual molecules interact with Rh adatom. We show that the local binding environment of the Rh_1 adatom on the support also influences how molecules absorb. By unraveling these molecular interactions, we aim to contribute valuable insights into the understanding of SACs and their potential catalytic performance in hydroformylation.

All interested colleagues are welcome to this seminar lecture(s)
(2 x 20 min. presentations followed by discussion)

Friedrich Aumayr
(LVA Leiter)

Gareth S. Parkinson
(Seminar Chair)