MECS – Cluster of Excellence
MATERIALS FOR ENERGY CONVERSION AND STORAGE

TECHNISCHE UNIVERSITÄT WIEN · universität wien · ISTA Institute of Science and Technology Austria · universität innsbruck

Seminar

Henrik Grönbeck

Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

Wednesday, 29th November 2023, 14:00 s.t.
TU Wien, Institut für Materialchemie, E165
1060 Wien, Lehargasse 4
Building BC, 2nd Floor, Seminar Room Lehar 2

Site-communication in hydrogenation reactions over dilute alloy nanoparticle

Single atom alloy catalysts offer possibilities to obtain turn-over frequencies and selectivities unattainable by its mono-metallic counterparts. Examples are selective hydrogenation of acetylene to ethylene over Pd embedded in Cu [1] and direct formation of H_2O_2 from O_2 and H_2 over Pd embedded in Au hosts [2]. We use first principles based kinetic Monte Carlo simulations [3] to investigate the catalytic performance of Pd embedded in nanoparticles of Cu and Au. The simulations reveal an efficient site-separation where Pd monomers act as active centers for H_2 dissociation, whereas the hydrogenation steps proceed over under-coordinated Cu- and Au-sites. The simulations show that tuning the nanoparticle composition and reaction conditions can enhance the selectivity towards the desired product.

References

[1] M. Jørgensen and H. Grönbeck, J. Am. Chem. Soc. 141, 8541 (2019).
[2] R. Svensson and H. Grönbeck, J. Am. Chem. Soc. 145, 11579 (2023).
[3] M. Jørgensen and H. Grönbeck, J. Chem. Phys. 149, 114101 (2018).

All interested colleagues are welcome to this seminar lecture
(45 min. presentation followed by discussion).

Günther Rupprechter
Director of Research

André Vogel
Coordinator