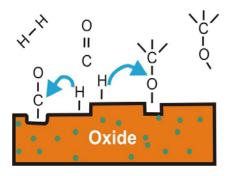
## **Ruhr-Universität Bochum**



SFB 558 "Metall-Substrat-Wechselwirkungen in der heterogenen Katalyse"

Einladung zum Vortrag von

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## "The Energy of Metal Atoms on Surfaces: Relationship to Reactivity"

<u>Abstract</u>: The energetics of adsorbed species provide key insight into surface reactions of importance in catalysis, microelectronics fabrication and nanotechnology. Novel calorimetric methods for measuring adsorption energies will be described, and some systematic measurements of energies will be discussed. The adsorption energy of late transition metals atoms is very large on early transition metals, moderate on late transition metals and small on the oxide surfaces typically used as catalyst supports. Their adsorption energy on metal nanoparticles decreases strongly with particle size below ~7 nm. Tiny (~2 nm diameter) metal particles are ~100 kJ/mol less stable (per metal atom) than predicted by the Gibbs-Thompson relation assuming constant surface energy. We argue that this difference is the dominant reason for the failure of all previous mechanistically-accurate kinetic models for nanoparticle sintering, and propose a modified model that fits well sintering kinetics with physically reasonable parameters for the first time.

The energetics of late transition metal adatoms correlate with the strength with which they bind simple ligands like CO and O: the more weakly the metal is adsorbed on a surface, the more strongly it binds the ligand. This allows the reactivity and catalytic activity of the same metal element to be tuned rather dramatically by controlling either the chemical nature or particle size of the material upon which it is anchored.

These energetics also correlate with the metal atom's sticking probability as well as the morphology of the thin film that evolves when metal adsorption is continued: surfaces with low metal adsorption energies have low sticking probabilities and give 3D metal islands whose number density increases with adsorption energy; moderate adsorption give 2D islands and layer-by-layer growth, and very strong adsorption gives a 2D wetting layer followed by 3D particles. Supported by NSF and DOE-BES Chemical Sciences.

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