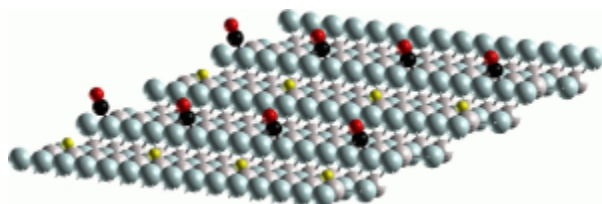


Heterogeneous catalysis

Methanol Steam Reforming on Pd/Zn/ZnO Catalysts



The aim of the project is to understand, at a microscopic level, reactions involved in methanol steam reforming on bimetallic Pd/Zn catalysts. The study is based on density functional calculations of the electronic and geometric structure of Pd/Zn materials (Pd and Cu are used as reference) and adsorption complexes, as well as their reactions on surfaces of these materials.

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The Surface Composition of the Catalyst During Methanol Steam Reforming: A Thermodynamic Analysis Based on Quantum Mechanical Modeling, *ChemPhysChem* **7**, 1802-1812 (2006). DOI: [10.1002/cphc.200600262](https://doi.org/10.1002/cphc.200600262)

[2] Z.-X. Chen, K. H. Lim, K. M. Neyman, N. Rösch:

The Effect Steps on the Decomposition of CH₃O at PdZn Alloy Surfaces, *J. Phys. Chem. B* **109**, 4568-4574 (2005). DOI: [10.1021/jp044843e](https://doi.org/10.1021/jp044843e)

[3] Z.-X. Chen, K. H. Lim, K. M. Neyman, N. Rösch:

Density Functional Study of Methoxide Decomposition on PdZn(100), *Phys. Chem. Chem. Phys.* **6**, 4499-4504 (2004). DOI: [10.1039/b407688e](https://doi.org/10.1039/b407688e)

Theoretical Studies of Acrolein Hydrogenation on Silver Catalysts

The project seeks to clarify, at a microscopic level, an unusually high selectivity of silver catalysts during acrolein hydrogenation, which is employed to produce technologically important unsaturated alcohols. For this purpose, periodic DFT slab models have been employed, in order to study acrolein adsorption and its reactions on model silver substrates.

[4] K. H. Lim, Z.-X. Chen, K. M. Neyman, N. Rösch:

Adsorption of Acrolein on Single-Crystal Surfaces of Silver: Density Functional Studies, *Chem. Phys. Lett.* **420**, 60-64 (2006). DOI: [10.1016/j.cplett.2005.12.018](https://doi.org/10.1016/j.cplett.2005.12.018)

Adsorption of Gold and Silver Particles on Silica and Alumina

This project aims at better understanding of the structural, bonding and electronic properties of small sub-nanoscale Au species, supported on technologically important oxide substrates such as silica and alumina. For silver on silica, also the interaction with molecular oxygen has been inspected. O₂ dissociation at supported silver clusters seems to be feasible, but is associated with relatively high barriers. For a proper modeling of isolated adsorbed metal particles, cluster models embedded in an elastic polarizable environment have been applied.

[5] A. Del Vitto, G. Pacchioni, K. H. Lim, N. Rösch, J.-M. Antonietti, M. Michalski, U. Heiz, J. Jones:

Gold Atoms and Dimers on Amorphous SiO₂: Calculation of Optical Properties and Cavity Ringdown Spectroscopy Measurements, *J. Phys. Chem. B* **109**, 19876-19884 (2005). DOI: [10.1021/jp054794l](https://doi.org/10.1021/jp054794l)

[6] V.A. Nasluzov, T. V. Shulimovich, E.A. Ivanova-Shor, A.M. Shor, N. Rösch:

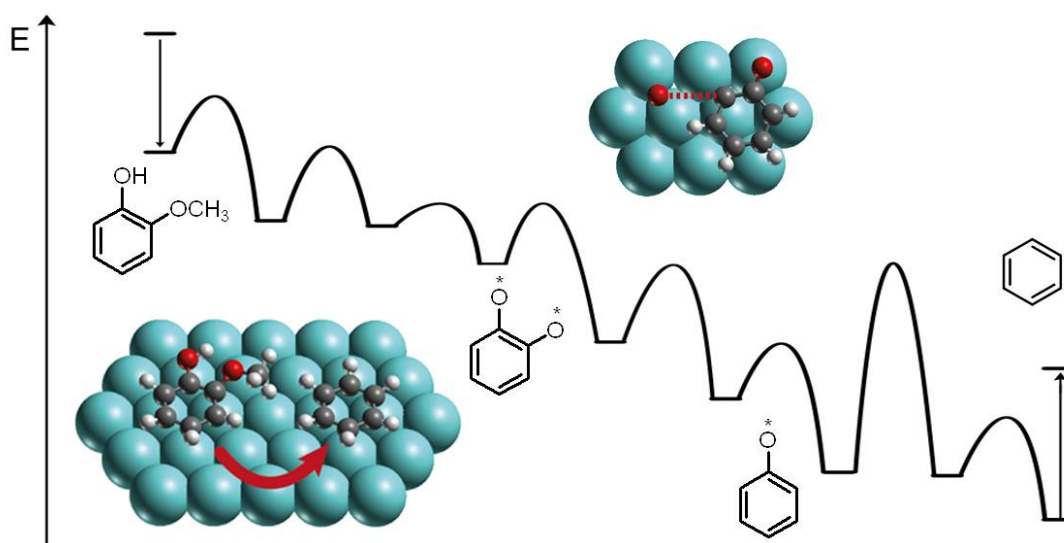
Small Gold Species at Hydroxylated Alumina Surfaces. A Computational Study Using Embedded-Cluster Models of -Al₂O₃(0001), *Chem. Phys. Lett.* **494**, 243-248 (2010). DOI: [10.1016/j.cplett.2010.06.004](https://doi.org/10.1016/j.cplett.2010.06.004)

[7] A. M. Shor, E. A. Ivanova-Shor, S. S. Laletina, V. A. Nasluzov, N. Rösch: Small Silver Clusters at Paramagnetic Defects of Silica Surfaces. A Density Functional Embedded-Cluster Study, *Surf. Sci.* **604**, 1705-1712 (2010). DOI: [10.1016/j.susc.2010.06.019](https://doi.org/10.1016/j.susc.2010.06.019)

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Biomass Conversion

The efficient usage of biogenic materials for the production of energy and of value added chemical is likely to be a key technology for the upcoming post-fossil-fuel era. An important issue for the development of the corresponding technologies is the catalytic conversion of biomass derived feedstocks. We investigated the conversion of various model molecules by the transition metal catalyst Pt and Ru. These studies cover the reaction of ethanol and propanol to model the chemistry of sugar derived materials. The conversion of aromatic feedstocks, as derived from lignin, has also been explored using the model molecule guaiacol.



Deoxygenation of guaiacol on Ru(0001)

Heterogeneous catalysis is also modeled at the Catalysis Modelling Group in Singapore

[9] D. Basaran, A. Genest, N. Rösch: Comment on "Towards understanding the bifunctional hydrodeoxygenation and aqueous phase reforming of glycerol", *J. Catal.* **287**, 210-213 (2012). DOI: [10.1016/j.jcat.2011.12.010](https://doi.org/10.1016/j.jcat.2011.12.010)

[10] D. Basaran, A. Genest, J. A. Lercher, N. Rösch: Formation of CO₂ and Ethane from Propionyl over Platinum: A Density Functional Theory Study, *ACS Catal.* **3**, 1730-1738 (2013). DOI: [10.1021/cs400204p](https://doi.org/10.1021/cs400204p)

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