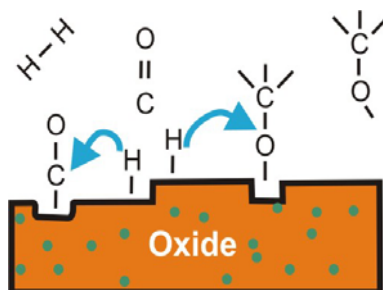


Ruhr-Universität Bochum



SFB 558

„Metall-Substrat-Wechselwirkungen in der heterogenen Katalyse“

**Einladung
zum Vortrag von**

**Dr. Andreas Heyden
Department of Chemistry, University of Minnesota**

Thema:

“Adaptive partitioning in multilevel / multiscale simulations and the N₂O decomposition over iron zeolite catalysts”

In many applications of multilevel/multiscale simulation methods, an active zone must be modeled by a high-level electronic structure method, while a larger environmental zone can be safely modeled by an analytic potential energy function. In some cases though, the active zone must be redefined as a function of simulation time.

Examples include a reactive moiety diffusing through a liquid or solid, or a dislocation propagating through a material. In this seminar, I will present a procedure for efficiently determining smooth potential energy functions in multilevel simulations of systems in which atoms or groups of atoms move between high-level and low-level zones. Molecular dynamics (MD) simulations in the microcanonical ensemble show that our method conserves both total energy and momentum, while previously available methods fail to conserve total energy or momentum or both. Applications of this newly developed method for proton diffusion through water and extensions of our method to adaptive resolution simulations for the efficient study of dense liquids with hybrid atomistic-mesoscale MD simulations will also be discussed.

Finally, I will present recent results of the influence of H₂O and NO on the activity and reaction mechanism of the N₂O decomposition over iron zeolite catalysts. Iron zeolites are active catalysts for the stoichiometric decomposition of N₂O to N₂ and O₂ and are therefore, potentially useful for the abatement of N₂O emissions from industrial waste streams, such as those occurring in nitric acid and adipic acid plants. Using quantum mechanical calculations together with chemical reactor simulations, we have been able to explain many seemingly contradicting experimental findings.

Sondertermin: Montag 26.02.2007

Zeit: 11.15 h

Ort: HNC 5/99

Gäste sind herzlich willkommen.