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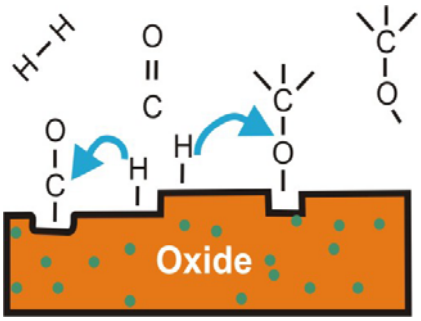

SFB 558
„Metall-Substrat-Wechselwirkungen in der heterogenen Katalyse“

Einladung
zum Vortrag von

Dr. Jörg Behler
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Neural Network Potentials for Chemical Reactions: From Dynamics at Surfaces to Phase Transitions in Solids

Abstract: Potentials obtained from first principles allow to study many chemical processes with high accuracy. Often, however, these potentials are computationally very costly to evaluate and thus cannot be applied to extended dynamical studies of large systems. In recent years neural networks (NN) have become a promising new tool to represent potential energy surfaces (PES) obtained from first principles. While they can reproduce the underlying PES very accurately, they are very efficient to evaluate and thus allow to extend length and time scales of theoretical simulations.
Two applications of neural network potentials are given: First, NNs are used to study the role of nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. For this purpose, the PESs involved in the gas-surface dynamics are represented by NNs. In the second example, a new high-dimensional NN potential for the description of condensed systems is combined with metadynamics simulations to investigate pressure-induced phase transitions in solids. It is shown that for silicon, which has a particularly complex phase diagram, the full sequence of crystal structures can be reconstructed in agreement with experiment.

Termin:	**11.12.2007**
Zeit:	**11:15 Uhr**
Ort:	**HNC 5/99**

Gäste sind herzlich willkommen.