# Chemical Accuracy for Molecule-Surface Interactions: Ab Initio Energies and Entropies

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle Since 1965

Frontiers in Catalysis Science and Engineering

Seminar Series

**Presented by…**


## Prof. Dr. Joachim Sauer

- Institut für Chemie
- Humboldt-Universität
- Berlin, Germany

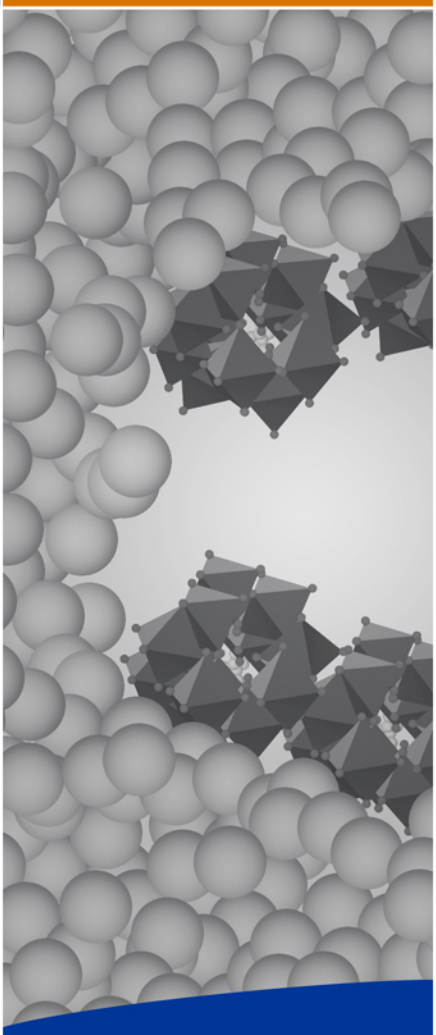

**Abstract**


A hybrid method that combines MP2 on cluster models with DFT+dispersion on periodic models (plus DCCSD(T) corrections) is presented that yields binding energies of molecules on (simple) metal oxide surfaces *ab initio* and with chemical accuracy. Examples are the binding of CO and $CH_4$ on Mg(001), of $H_2$, $CH_4$, CO and $CO_2$ on the internal surfaces of metal organic frameworks (MOF), as well as the adsorption of hydrocarbons in zeolites. Entropies of adsorption can also be calculated with chemical accuracy from vibrational partition functions calculated by DFT+dispersion, when anharmonicities are included. This is shown for adsorption of $CH_4$ on MgO(001) and in a zeolite with Bronsted sites (H-chabazite).


http://www.chemie.hu-berlin.de/forschung/quantenchemie/Group

Hosted by: Johannes Lercher

Admin: Brooke Lanigan



Aug. 15, 2014

EMSL Auditorium

1:30 pm