VORTRAG IM RAHMEN DES SONDERFORSCHUNGSBEREICHS 623
DER UNIVERSITÄT HEIDELBERG
MOLEKULARE KATALYSATOREN: STRUKTUR UND FUNKTIONSDESIGN

Freitag, 06. Dezember 2002, 11.15 Uhr

Hörsaal West, Im Neuenheimer Feld 252

Dr. Horst Weiss

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"First principles exploration of catalytic reactions in solvents and on surfaces with Car-Parrinello Methods"

Abstract:
Density Functional Theory (DFT) calculations are carried out today routinely by researchers to support elucidation of reaction mechanisms. Although the chemical models are rather crude in many cases (vacuum environment, naked and charged catalyst species without additives and cotatalyst, no temperature, no pressure), they offer valuable insights. In some cases, however, one has to check whether these simplifications are appropriate. Through the availability of high speed computers, Car Parrinello methods are now applicable to chemically interesting (complex) systems. They allow to carry out Molecular Dynamics simulations with periodic boxes within the framework of DFT. We are thus able to study chemical reactions with specific solvents under a certain pressure at a certain temperature. Applications dealing with catalytic reactions in water with late transition metals and simulations on heterogeneous Ziegler Natta catalysis will be shown.

Gäste sind herzlich willkommen.

Bei Interesse an einem Gesprächstermin bitte melden im:
Büro des SFB 623 Tel.: 06221-54-8415 Fax: 06221-54-4885

DER SPRECHER
gez. P. Hofmann