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Unifying Concepts in Catalysis

Vortragsankündigung

- im Rahmen des UniCat-Kolloquiums -

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Es spricht: **Prof. Dr. Geert-Jan Kroes,** Leiden Institute of Chemistry, Theoretical Chemistry, Universiteit Leiden, Holland

Zeit: **Mittwoch, 01. Juli 2009** 17:15 Uhr

Ort: **TU Berlin**
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Straße des 17. Juni 115,
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Raum C 243

Thema: **First principles theory for a prototype chemical reaction in Surface Science.**

Abstract: Improving the accuracy of methods for computing the interaction of molecules with metal surfaces is critical to progress in describing chemical reactions on surfaces and heterogeneous catalysis. Dynamics methods allow tests of molecule-surface interaction potentials through comparison with experiments on molecule-surface scattering, provided that a dynamical model is used that is both computationally tractable and accurate for such experiments. Calculations using a static surface, electronically adiabatic model are tractable and accurately reproduce data on the reaction probability as a function of energy and rovibrational state for the dissociation of H_2 (D_2) on Cu(111), and for rotationally inelastic scattering of H_2 from Cu(111). However, modeling the influence of phonons is necessary for an accurate description of vibrational excitation, and of the orientational dependence of reaction.

Organisator: Prof. Dr. Peter Saalfrank (Uni Potsdam)

Gäste sind herzlich willkommen!

Prof. Dr. Matthias Drieß
Sprecher des Exzellenz-Clusters UniCat