ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Laboratorium für Physikalische Chemie

Einladung zu einem Kolloquium

Datum/Zeit:	Dienstag, 17. April 2012, 16.45 Uhr
Referent:	Prof. Dr. Joachim Sauer
	Institut für Chemie, Humboldt-Universität, Unter den Linden 6, 10099 Berlin
Thema:	Storage and activation of methane - ab initio approach
Ort:	ETH Zürich, Hönggerberg, Hörsaal HCI J 3

Abstract

A method for the ab initio prediction of adsorption isotherms is presented which relies on a multi Langmuir model and the calculation of equilibrium constants for individual sites by quantum chemistry and molecular statistics [1]. Adsorbate-adsorbate interactions are included using the Bragg-Williams model. For adsorption of methane on the MgO(001) surface it is shown that the quantum chemical multilevel method applied (Hybrid MP2:PBE+D+ ΔCCSD(T)) yields adsorption energies with chemical accuracy (4 kJ/mol) [2]. This method is used for methane storage in metal-organic frameworks (MOF).
The activation of C-H bonds at oxygen radical sites by H abstraction [3,4] and on morphological (corner sites) and electronic defects (F centers) by heterolytic splitting is examined with respect to the oxidative coupling of methane on Li-doped and defective MgO catalysts.

[1] K. Sillar, A. Hofmann, J. Sauer, J. Am. Chem. Soc. 131 (2009) 4143.
[2] S. Tosoni, J. Sauer, Phys. Chem. Chem. Phys. 12 (2010) 14330.
[3] K. Kwapien, M. Sierka, J. Döbler, J. Sauer, ChemCatChem 2 (2010) 819.
[4] S. Feyel, J. Döbler, R. Höckendorf, M.K. Beyer, J. Sauer, H. Schwarz, Angew. Chem., Int. Ed. 47 (2008) 1946.

Der Vortrag wird im Rahmen der Heilbronner-Hückel-Vorlesungen gemeinsam mit der Schweizerischen Chemischen Gesellschaft und der Gesellschaft Deutscher Chemiker organisiert (siehe Chimia).

Gäste sind willkommen
Nach der Veranstaltung laden wir Sie herzlich zu einem Apéro ein.

SCS

Division of
Chemical Research

Heilbronner-Hückel-Lectures 2012

sub auspiciis

Schweizerische Chemische Gesellschaft, Société Suisse de Chimie

Gesellschaft Deutscher Chemiker

Professor Dr. Joachim Sauer

Institut für Chemie, Humboldt-Universität,
Unter den Linden 6, 10099 Berlin, Deutschland

1. Tuesday, 17 April 2012, 16:45 h
   ETH Zurich, Hönggerberg Campus
   Lecture Hall HCI J 3
   "Storage and activation of methane - ab initio approach"

2. Wednesday, 18 April 2012, 16:30 h
   University of Basel
   Department of Chemistry, Physical Chemistry Building
   Klingelbergstrasse 80, Lecture Hall, 2. Stock
   "Zeolites and their catalytic activity - quantum chemical results"

3. Thursday, 19 April 2012, 17:15 h
   Université de Fribourg, Département de Chimie
   Grand Auditoire
   „C-H bond activation by metal oxides in the gas phase and on solid surfaces"

4. Friday, 20 April 2012, 11:15 h
   EPF Lausanne, Institute of Chemical Sciences and Engineering
   Lecture Hall CH G1 495
   "Atomistic understanding of heterogeneous catalysis by oxides – quantum chemistry in concert with experiment"