

Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2005)

Time: wednesdays 14:15, Location: Seminarraum NC 03/399

13. 04. 2005 **Alan Mark**, Department of Biophysical Chemistry, University of Groningen
Self-organization in biomolecular systems: Simulating the folding and aggregation of peptides, proteins and lipids
(Joint seminar with FOR 436 "Water at Interfaces")
20. 04. 2005 **Wenjian Liu**, Institute of theoretical & computational Chemistry, Peking University
Time dependent relativistic density functional theory and application
- Special date** **Mats Persson**, Department of Applied Physics, Chalmers/Göteborg University of
Tu 26. 04. 2005 Technology
11:15, NC 5/99 *Control and characterization of matter on the atomic scale*
(Joint seminar with SFB 558 "Heterogeneous Catalysis")
- Special date** **Jeppe Olsen**, Theoretical Chemistry, University of Aarhus
Th 28. 04. 2005 *The electronic structure and spectra of quantum dots using quantum chemical*
Time: 17:15 *methods*
04. 05. 2005 **Alexander Hofmann**, Quantenchemie, Humboldt Universität Berlin
Strategies for the localisation of transition states on surfaces: the oxidative dehydrogenation of butane on sulphated zirconia
11. 05. 2005 **Josef Wachtveitl**, Physikalische und Theoretische Chemie, Universität Frankfurt
Ultrafast Peptide Dynamics
25. 05. 2005 **Günter Wächtershäuser**, Patentanwaltskanzlei Wächtershäuser & Hartz, München
Retrodiction of the pioneer organism of life in a volcanic setting
(Joint seminar with FOR 436 "Water at Interfaces")
01. 06. 2005 **Casey (James) Hynes**, Département de Chimie, Ecole normale supérieure
Photochemical funnels: environmental impacts on conical intersections
08. 06. 2005 **Annamaria Fiethen**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum
Elektronische Struktur und Austausch-Kopplung in [2Fe2S] Komplexen
22. 06. 2005 **Timo Fleig**, Institut für Theoretische Chemie und Computerchemie, Heinrich Heine
Universität Düsseldorf
Implementation and application of 4-component multi-reference correlation methods
- Special date** **Michael Moseler**, Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg
Tu 28. 06. 2005 *The oxidation of gasphase and metal-oxide supported palladium clusters*
11:15, NC 5/99 (Joint seminar with SFB 558 "Heterogeneous Catalysis")
29. 06. 2005 **Hauke Trinks**, Arbeitsbereich Messtechnik, Technische Universität
Hamburg-Harburg
Frozen sea water mediating early steps in the origin of life
06. 07. 2005 **Ivano Tavernelli**, Laboratoire de chimie et biochimie computationnelles, École
polytechnique fédérale de Lausanne
Charge and electron transfer dynamics in molecular systems using DFT-QM/MM ab initio techniques

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.