Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

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Theoretical Chemistry Colloquia (SS 2006)

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

Special date 05. 04. 2006 **Time: 10.15**	**Andreia Luisa da Rosa**, Department of Physics, Uppsala University *Ferromagnetism in transition-metal doped wide band gap semiconductors*
12. 04. 2006	**Andreas Köhn**, Physikalische Chemie, Universität Mainz *Treatment of doubly-excited states in coupled-cluster theory*
19. 04. 2006	**Jean-Marie Mouesca**, Département de recherche fondamentale sur la matière condensée, CEA Grenoble *Electronic and magnetic properties of [2Fe-2S] redox systems: Theory and experiments*
Special date **Tu 25.** 04. 2006 11.15, NC 5/99	**Peter Kratzer**, Theoretische Physik, Universität Duisburg-Essen *Chemical reactions and surface diffusion of hydrogen on the Si(001) surface - a test ground for methodologies* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
03. 05. 2006	**Peter Hildebrandt**, Fakultät für Chemie, Technische Universität Berlin *Photoinduced processes in sensory photoreceptors - Insight by resonance Raman spectroscopy* (Joint seminar with FOR 436 "Water at Interfaces")
10. 05. 2006	**Arezoo Dianat**, Theoretische Chemie, Universität Ulm *Hydrogen Dissociation Dynamics on Transition Metal Surfaces*
Special date **Fr 12.** 05. 2006 10.00, HNC 30	***Colloquium in Honor of Professor Staemmler***
17. 05. 2006	**Timo Fleig**, Theoretical and Computational Chemistry, Heinrich-Heine-Universität Düsseldorf *Advances in relativistic 4-component electron correlation methods*
24. 05. 2006	**Ilka Hegemann**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum *Copper atoms interacting with polar zinc oxide surfaces*
Special date 31. 05. 2006 **Time: 11.15**	**Kok Hwa Lim**, Lehrstuhl für Theoretische Chemie, Technische Universität München *DFT studies relevant to methanol steam reforming*
31. 05. 2006	**Alexander Auer**, Department of Chemistry, Technische Universität Chemnitz *Prediction of molecular properties for large systems*
07. 06. 2006	**Giovanni Ciccotti**, Department of Physics, University of Rome "La Sapienza" *Quantum-classical statistical dynamics with trajectories*
14. 06. 2006	**Christian Neiß**, Institut für Nanotechnologie, Forschungszentrum Karlsruhe *Response properties using explicitly correlated coupled cluster theory*
Special date **Tu 20.** 06. 2006 11.15, NC 5/99	**Marek Sierka**, Theoretische Chemie, Humboldt-Universität Berlin *Interplay between theory and experiment in the quest of oxides with reduced dimensionality* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
28. 06. 2006	**Rodolphe Vuilleumier**, Laboratoire de Physique Theorique de Liquides, Universite Pierre et Marie Curie Paris *Vibrational spectroscopy at finite temperature from ab initio Molecular Dynamics simulations* (Joint seminar with FOR 618 "Aggregation")
05. 07. 2006	**Ralf Drautz**, Department of Materials, University of Oxford *Bond-order potentials: bridging the electronic-atomistic modeling hierarchies in materials science* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
Special date **Th 06.** 07. 2006 **Time: 14.15**	**Gerald Brönstrup**, Institut für Festkörperphysik, Universität Jena *Ion tracks in GaAs*
Special date **Mo 10.** 07. 2006 **Time: 14.15**	**Oleg Prezhdo**, Department of Chemistry, University of Washington (Seattle) *Photoexcitation dynamics in quantum dots, carbon nanotubes and molecule-semiconductor interfaces*
Special date 12. 07. 2006 **Time: 10:15**	**Jordi Boronat**, Departament de Fisica i Enginyeria Nuclear, Universitat Politecnica de Catalunya *Higher-order actions for path integral Monte Carlo simulations* (Joint seminar with FOR 618 "Aggregation")

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.