Lehrstuhl für Theoretische Chemie

Ruhr-Universität Bochum

www.theochem.ruhr-uni-bochum.de

Theoretical Chemistry Colloquia (SS 2010)

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

21. 04. 2010	no colloquium
Special date **Tu 27.** 04. 2010 11:15, NC 5/99	**Christian Schön**, MPI für Festkörperforschung, Stuttgart *Providing solid state chemistry with a theoretical foundation: employing energy landscapes for crystal structure prediction and the modeling of amorphous compounds* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
05. 05. 2010	**Georg Jansen**, Theoretische Organische Chemie, Universität Duisburg-Essen *Description of intermolecular interactions with density functional- and perturbation theory-based approaches* (Joint seminar with FOR 618 "Aggregation")
12. 05. 2010	**Thomas Dittrich**, Departamento de Fisica, Universidad Nacional de Colombia, Bogota *Complex quantum dynamics in phase space - making sense of Wigner functions*
19. 05. 2010	Title to be announced
02. 06. 2010	**Antonio Rizzo**, Institute for chemical and physical processes, National Research Council, Pisa *Linear and Nonlinear Absorption Spectra: Vibrational and Confirmation Effects* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
09. 06. 2010	**Daniel Sebastiani**, Fachbereich Physik, Freie Universität Berlin *Interplay of first-principles molecular dynamics and theoretical spectroscopy in complex systems: More than the sum of the components* (Joint seminar with FOR 618 "Aggregation")
Special date **Tu 15.** 06. 2010 11:15, NC 5/99	**Pavel Mach**, Department of Biophysics and Molecular Physics, Comenius University, Bratislava *Beryllium - hydrogen clusters, what can theory contribute* (Joint seminar with SFB 558 "Heterogeneous Catalysis")
23. 06. 2010	**Gerald Knizia**, Institut für Theoretische Chemie, Universität Stuttgart *A tensor framework for implementing general quantum chemistry algorithms*
30. 06. 2010	**Dmitry Ganyushin**, Institut für Physikalische und Theoretische Chemie, Universität Bonn *A spin-orbit coupled complete active space self-consistent field approach* (Speaker Exchange Program Bonn / Bochum)
07. 07. 2010	no colloquium
14. 07. 2010	**Sebastian Höfener**, Lehrstuhl für Theoretische Chemie, Institut für Physikalische Chemie, Universität Karlsruhe *Analytic calculation of first-order molecular properties at the MP2-F12 level*
21. 07. 2010	**Jozef Noga**, Slovak Academy of Science, Bratislava *An exact reformulation of SCF methods via variational coupled-cluster singles - an alternative way to diagonalization-free algorithms using non-unitary transformations*

gez. Die Dozenten der Theoretischen Chemie

Visitors are welcome to the seminar.