International Symposium on Theoretical and Computational Chemistry

Max-Planck-Institut für Kohlenforschung
Mülheim an der Ruhr, Germany
28 February - 2 March 2010

Program

Sunday, 28 February 2010

12:00 - 18:00	**Registration**
13:45 - 14:00	**Opening remarks** **Alois Fürstner (Max-Planck-Institut für Kohlenforschung, Mülheim)**
14:00 - 14:40	**Is There Anything New in Electron-Pair Bonding? Charge-Shift Bonding and its Manifestations** **Sason Shaik (Hebrew University, Jerusalem)**
14:40 - 15:20	**Explicitly correlated local coupled-cluster methods: Approaching the CCSD(T) basis set limit for enzyme reactions** **Hans-Joachim Werner (University of Stuttgart)**
15:20 - 16:00	**Homoatomic Clusters** **Reinhart Ahlrichs (Karlsruhe Institute of Technology)**
16:00 - 16:30	**Coffee Break**
16:30 – 17:10	**Constrained-Pairing Mean-Field Theory** **Gustavo Scuseria (Rice University, Houston)**
17:10 – 17:50	**The Fundamental and Approximate Symmetries of Space, Time and Matter and the Dynamics of their Violations in the Spectroscopy and Kinetics of Molecules and Clusters** **Martin Quack (ETH Zürich)**
18:00 – 20:00	**Poster session** **Drinks and snacks provided**
20:00	**Group meeting (separate invitation)**

Monday, 1 March 2010

08:00 - 18:00	**Registration**
08:30 - 09:10	**Multi-Scale Methods for the Investigation of Biological Structures and Processes** **Marcus Elstner (Karlsruhe Institute of Technology)**
09:10 - 09:50	**QM/MM Simulations of Organic and Enzymatic Reactions** **William L. Jorgensen (Yale University, New Haven)**
09:50 - 10:30	**Reactivity and Selectivity in Organic and Biological Chemistry: QM and QM/MM Studies** **Jeremy N. Harvey (University of Bristol)**
10:30 - 11:00	**Coffee break**
11:00 - 11:40	**Usages of Theoretical Spectroscopy** **Frank Neese (University of Bonn)**
11:40 - 12:20	**Interplay of Theory and Experiment in Rotational Spectroscopy** **Jürgen Gauss (University of Mainz)**
12:30 - 14:00	**Lunch break**
14:00 - 14:40	**Environment and Substitution Effects on the Triplet Generation in Flavins** **Christel Marian (University of Düsseldorf)**
14:40 - 15:20	**On-the-Fly Non-Adiabatic Dynamics: Program Development and Application to Photochemical and Photobiological Simulations** **Hans Lischka (University of Vienna)**
15:20 - 16:00	**ONIOM Studies of Photochemical Processes and Chemical Reactions of Biomolecular Systems in Proteins** **Keiji Morokuma (Kyoto University)**
16:00 - 16:30	**Coffee break**
16:30 - 17:10	**Force-field development for computer simulation of biomolecular systems: the GROMOS case** **Wilfred van Gunsteren (ETH Zürich)**
17:10 - 17:50	**Efficient and Stable Hartree-Fock Exchange in Periodic Systems** **Jürg Hutter (University of Zürich)**

17:50 - 18:30 **Approximating CASSCF with increasingly perfect coupled cluster models for strong correlations -- perfect pairs, quadruples and hextuples**
Martin Head-Gordon (University of California, Berkeley)

19:00 **Dinner (separate invitation)**

Tuesday, 2 March 2010

08:00 - 09:00 **Registration**

08:30 - 09:10 **From Donor-Acceptor Complexes to Gallium Nitride Nanorods**
Henry F. Schaefer (University of Georgia, Athens)

09:10 - 09:50 **Insights into Uranyl(VI) Chemistry from CPMD Simulations**
Michael Bühl (University of St. Andrews)

09:50 - 10:30 **Oxidative Dehydrosulfurization and Selective Bond Activation by "Roll-over" Cyclometalated Pt(II) Complexes: Theory and Experiment in Concert**
Helmut Schwarz (Technical University of Berlin)

10:30 - 11:00 **Coffee break**

11:00 - 11:40 **Selective Oxidation of C-H Bonds by Vanadium Oxides - Clusters in the Gas Phase and Supported on SiO_2 and CeO_2**
Joachim Sauer (Humboldt University of Berlin)

11:40 - 12:20 **The Chemistry of Divalent Carbon(0) Compounds and Heavier Homologues - A Challenge for Theory and Experiment**
Gernot Frenking (University of Marburg)

12:20 - 12:30 **Closing remarks**
Walter Thiel (Max-Planck-Institut für Kohlenforschung, Mülheim)

12:30 **Lunch and departure**

Session chairs

Sunday, 28 February 2010

14:00 – 16:00 **Max Holthausen (University of Frankfurt)**

16:30 – 17:50 **Michael Filatov (University of Groningen)**

Monday, 1 March 2010

08:30 – 10:30 **Johannes Kästner (University of Stuttgart)**

11:00 – 12:20 **Sergei Yurchenko (Technical University of Dresden)**

14:00 – 16:00 **Stephan Sauer (University of Copenhagen)**

16:30 – 18:30 **Hans Martin Senn (University of Glasgow)**

Tuesday, 2 March 2010

08:30 – 10:30 **Tell Tuttle (University of Strathclyde)**

11:00 – 12:20 **Vidar Jensen (University of Bergen)**