Program last updated: Tuesday, 29 June 2010

The 8th European Conference on Computational Chemistry

25-28 August 2010, Lund, Sweden

Wednesday 25 August

in Palaestra lecture hall

The organizers reserve the right to make alterations in the program

12.30-14.00	**Registration**
14.00-14.15	*Conference opening and welcome*

Session 1 *Materials and multiscale modelling*

14.15-15.15	*(PL)* **William Goddard**, California Institute of Technology, USA *First-Principles Based Theory and Applications to Energy, Materials, Pharma, Catalysis, and Water*
15.15-15.35	*(OC)* **Stefano Evangelisti,** University of Bologna, Italy *Beryllium Chains on Graphene Nanoislands*
15.35-15.55	*(OC)* **Gianluca Malavasi**, University of Modena and Reggio Emilia, Italy *Bioactive phospho-silicate glasses: a molecular dynamics simulation study using rigid ion and core shell models*
15.55-16.25	**Coffee**
16.25-16.55	*(KL)* **Kersti Hermansson**, Uppsala University, Sweden *Title to be announced*
16.55-17.15	*(OC)* **XueQing Zhang**, Eindhoven University of Technology, The Netherlands *Kinetic Monte Carlo modeling of initial stage zeolite synthesis*
17.15-17.45	***Inga Fischer-Hjalmars Award ceremony*** **Na Lin**, University of Tromsö, Norway *Vibrationally Resolved Multi-Photon Absorption and Dichroism*
18.00-19.30	**Poster session 1 and refreshments**

Thursday 26 August

in Palaestra lecture hall

Session 2	***Biological chemistry***
09.00-09.45	*(PL)* **Walter Thiel**, Max-Planck-Institut für Kohlenforschung, Germany *Theoretical Studies of Enzymatic Reactions*
09.45-10.05	*(OC)* **Lubomir Rulíšek**, Academy of Sciences of the Czech Republic, Czech Republic *QM/MM and Multireference Calculations of Reaction Mechanisms of Redox-Active Metalloproteins*
10.05-10.25	*(OC)* **Leif Eriksson,** School of Chemistry, National University of Ireland, Ireland *SLC25A43: From gene sequence to protein function*
10.25-10.50	**Coffee**
10.50-11.20	*(KL)* **Berk Hess**, Stockholm University, Sweden *The state of the art in bio-molecular simulation*
11.20-11.40	*(OC)* **Judith Sponer**, Academy of Sciences of the Czech Republic, Czech Republic *Quantum Chemical Studies on the Prebiotic Chemistry of Nucleic Acids*
11.40-12.10	*(KL)* **Michal Pitonak**, Comenius University, Bratislava, Slovak Republic *Many-body effects in DNA base pairs interactions at highly correlated* ab initio *level*
12.10-13.40	**Lunch**
Session 3	***Homogeneous catalysis***
13.40-14.25	*(PL)* **Feliu Maseras**, ICIQ, Spain *Enantioselective hydrogenation: a new twist to old mechanisms*
14.25-14.45	*(OC)* **Michael Hall**, Texas A&M University, USA *Mechanism of Electrocatalytic Hydrogen Production in Models for Iron-Iron Hydrogenase: A Density Functional Theory Study of Proton Dissociation Constants and Electrode Reduction Potentials*
14.45-15.05	*(OC)* **John Slattery**, The University of York, UK *The ligand-assisted proton shuttle (LAPS) mechanism in organometallic transformations involving alkynes*
15.05-15.30	**Coffee**
15.30-16.00	*(KL)* **John McGrady**, University of Oxford, UK *Water oxidation catalysis – some insights from computational chemistry*
16.00-16.20	*(OC)* **Pietro Vidossich**, Universitat Autònoma de Barcelona, Spain Ab-initio *molecular dynamics modeling of water oxidation by mononuclear Ru and Ir catalysts*
16.20-16.40	*(OC)* **Christophe Raynaud**, Université Montpellier, France *C-H oxidation by Mn porphyrins: A theoretical study on the nature of the active species and the reaction*
16.40-17.00	*(OC)* **Timofei Privalov**, Royal Institute of Technology, Sweden *Involvement of Seven-Coordinate Ru-centers in Catalytic Water Oxidation: Rationalization of Mono- and Bi-Nuclear Pathways*
17.00-19.00	**Poster session 2 and refreshments**

Friday 27 August

In Palaestra lecture hall

Session 4 *Soft matter*

09.00-09.45	*(PL)* **Martien Cohen Stuart**, Wageningen University, the Netherlands *From atoms to hydrogels: how can modelling contribute to understanding Soft Matter?*
09.45-10.05	*(OC)* **Aatto Laaksonen**, Stockholm University, Sweden *Computer modelling and simulations of porous materials*
10.05-10.25	*(OC)* **Alessandro Magliano**, University of Rome, Italy *Molecular dynamics study of aggregation of amyloidogenic peptides in explicit water*
10.25-10.50	**Coffee**
10.50-11.20	*(KL)* **Martin Nilsson Jacobi**, Chalmers University of Technology, Sweden *Estimating effective force fields in dissipative particle dynamics*
11.20-11.40	*(OC)* **Cesare Mollica**, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland *Defeating the efficiency of both quantum and classical simulations with accurate semiclassics [1]*
11.40-12.00	*(OC)* **Joakim Stenhammar**, Lund University, Sweden *Bulk simulation of polar liquids in cubic and spherical symmetry*
12.20-14.00	**Lunch**

Session 5 *Computational chemistry on alternative platforms*

13.40-14.25	*(PL)* **Tod Martinez**, Stanford, USA *Electronic Structure and First Principles Dynamics on Graphical Processing Unit*
14.25-14.45	*(OC)* **Allesandro Constantini**, University of Perugia, Italy *Grid Enabled Molecular Simulations: from Quantum Mechanics to Molecular Dynamics*
14.45-15.15	*Keynote contribution* **Ron Dror**, D. E. Shaw Research, USA *Long simulations of GPCRs on a specialized molecular dynamics machine*
	Free afternoon
19.00-	**Banquet dinner at Grand Hotel**

Saturday 28 August

in Palaestra lecture hall

Session 6 *Photochemistry and photobiology*

09.00-09.45	*(PL)* **Massimo Olivucci**, Bowling Green State University, USA & University of Siena, Italy *Computational Photochemistry and Beyond*
09.45-10.05	*(OC)* **Ines Corral**, Universidad Autónoma de Madrid, Spain *O-O homolysis vs. singlet oxygen generation: two competing deactivation pathways in excited model endoperoxides*
10.05-10.25	*(OC)* **Bernhard Sellner**, University of Vienna, Austria *The Photodynamics of Azomethane – A Nonadiabatic Surface-Hopping Study*
10.25-10.50	**Coffee**
10.50-11.20	*(KL)* **Leticia Gonzalez**, Friedrich-Schiller-Universität Jena, Germany *Photochemistry, dynamics, and control of molecular devices*
11.20-11.40	*(OC)* **Luis Serrano-Andrés**, University of Valencia, Spain *Photochemistry and Quantum Chemistry: the New Frontiers*
11.40-12.10	*(KL)* **Lynn Kamerlin**, University of Southern California, USA *The Use of Multiscale Approaches to Model Ultra (and Not So) Fast Biological processes*
12.10-	**Conference closing**

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