Conference program

July 4, 2010 (Sunday)

14:00-21:00 Registration - lobby of D-20 building, ul.Janiszewskiego 8

July 5, 2010 (Monday)

8:00-9:00 Registration (ctd.)

9:00-9:10 Conference opening

Session 1 **Modeling molecular materials for hydrogen storage** (chair: J. Murray)

9:10-9:40 **L1:** H. Cheng (Singapore)
Mechanistic study of hydrogen spillover in carbon based materials

9:40-10:10 **L2:** A. Tachibana (Kyoto, Japan)
Energy density concept: a stress tensor concept

10:10-10:40 **L3:** I. Cukrowski (Pretoria, South Africa)
Intramolecular steric H-H clashes or stabilising H-H bonds in transition metal complexes?

10:40-11:00 **L4:** B. Nemeth (Budapest, Hungary)
Amine- and phosphine-boranes

11:00-11:15 coffee break

Session 2 **Modeling molecular materials for nanotechnology** (chair: H. Cheng)

11:15-11:45 **L5:** M. Samoć (Wrocław, Poland)
Third-order nonlinear optical materials: practical issues and theoretical challenges

11:45-12:15 **L6:** W. Grochala (Warsaw, Poland)
Quantum modeling in suport of chemical intuition - case studies in inorganic chemistry

12:15-12:35 **L7:** D. Thompson (Cork, Ireland)
Harnessing molecular motion for materials design

12:35-14:30 Lunch break

Session 3 **Advances in computational methods** (chair: Z. Latajka)

14:30-15:00 **L8:** B. Lesyng (Warsaw, Poland)
Causality analysis of proton transfer processes in molecular systems - a novel methodological approach

15:00-15:20 **L9:** D. Rohr (Łódź, Poland)
Efficient calculation of isotope effects for large molecules

15:20-15:40 **L10:** M.P. Mitoraj (Kraków, Poland)
A combined charge and energy decomposition scheme for analysis of chemical bonds and reaction paths

15:40-16:00 **L11:** P. Szarek (Wrocław, Poland)
The self-capacitance density of atoms and molecules based on electron cloud deformation analysis

16:00-16:15 Cofee break

Session 4 **Modeling biomolecules** (chair: V. Moliner)

16:15-16:45 **L12:** S. Filipek (Warsaw, Poland)
Modeling of G-Protein coupled receptors and shared mechanisms of their activation

16:45-17:15 **L13:** P. Cysewski (Bydgoszcz, Poland)
Environmental influences on the aromaticies of nucleobases and aminoacids

17:15-19:00 Poster session A (P1-P33)

July 6, 2010 (Tuesday)

Session 5 **Drug design** (chair: S. Filipek)

9:00-9:30 **L14:** A. Lodola (Parma, Italy)
Understanding structure-activity relationship of FAAH inhibitors by QM/MM mechanistic modelling

9:30-10.00 **L15:** J. Grembecka (Ann Arbor , USA)
Development of small molecules targeting menin-MLL interaction in leukemia

10:00-10:30 **L16:** T. Cierpicki (Ann Arbor, USA)
NMR in rational drug design for protein-protein interactions

10:30-10:50 **L17:** D. Plewczyński (Warsaw, Poland)
VoteDock: the consensus docking metod for prediction of protein ligand-interactions

10:50-11:05 coffee break

Session 6 **Modeling chemical reactions** (chair: P. Politzer)

11:05-11:35 **L18:** J. Murray (Cleveland, USA)
Reaction force analyses of energetic molecule decomposition

11:35-12:05 **L19:** J. Burda (Prague, Czech Republic)
The thermodynamic and kinetic description of reactions of the organometallic complexes

12:05-12:35 **L20:** Z. Latajka (Wrocław, Poland)
Proton transfer dynamics in strong hydrogen bonded systems

12:35-14:30 Lunch break

Session 7 **Modeling interactions in molecular materials** (chair: K. Ghio)

14:30-15:00 **L21:** P. Politzer (New Orleans, USA)
Some applications of molecular volumes in materials science

15:00-15:30 **L22:** O. Shishkin (Kharkov, Ukraine)
Structural properties of nucleic acid bases in polar environment

15:30-16.00 **L23:** S. Roszak (Wrocław, Poland)
Resonance Raman spectra in detecting nerve agents

16:00-16:20 **L24:** V. Andruschenko (Praha, Czech Republic)
Simulations of nucleic acid vibrational spectra

16:20-16:35 Coffee break

16:35-18:30 Poster session B (P34-P66)

July 7, 2010 (Wednesday)

Session 8 **Progress in predicting biomolecular structure** (chair: O. Shishkin)

9:00-9:45 **L25:** M. Neumann (France)
Crystal structure prediction of molecular compounds - beyond proof of concept

9:45-10.15 **L26:** J. Bujnicki (Warsaw, Poland)
RNA 3D structure prediction: from comparative to de novo modeling

10.15-10:45 **L27:** D. Gront (Seattle, USA)
Protein structure determination based on fragmentary experimental measurements

10:45-11:00 Coffee break

Session 9 **Modeling reaction mechanisms** (chair: T. Brinck)

11:00-11:30 **L28:** K. Ghio (Pisa, Italy)
Theoretical prediction of selectivities in nonreversible and reversible hydroformylation reactions catalyzed by unmodified Rh-carbonyls

11:30-12:00 **L29:** P. Kozłowski (Louisville,KY, USA)
How the Co-C Bond is cleaved in coenzyme B12-dependent mutases

12:00-12.30 **L30:** P. Paneth (Łódź, Poland)
Isotopic fractionation calculations of reactions between environment pollutants and permanganate

12:30-12:50 **L31:** T. Borowski (Kraków, Poland)
DFT studies on the reaction mechanizm of intra- and estradiol dioxygenases

14:30-16:30 Wrocław sightseeing

16:30-17:00 Panorama art gallery show

17:30-18:30 Boat trip along Odra river

19:00 Conference dinner

July 8, 2010 (Thursday)

Session 10 **Catalyst and biocatalyst design** (chair: P. Paneth)

9:00-9.30 **L32:** K. Yoshizawa (Fukuoka, Japan)
Computational mutation of enzymatic reaction: QM/MM studies

9:30:-10:00 **L33:** T. Brinck (Stockholm, Sweden)
Promoting carbon-carbon formation - the Holy Grail in the design of enzymes and organocatalysts

10:00-10.30 **L34:** V. Moliner (Castellóe la Plana, Spain)
Theoretical design of new biological catalysts

10:30-11:00 **L35:** A. Michalak (Kraków, Poland)
Theoretical studies on the ethylene polymerization catalyzed by half-metalocene Ti(IV) complexes with arylo ligands

11.00-11:15 Coffee break

Session 12 **Modeling biomolecules II** (chair: J. Burda)

11:15-11:35 **L36:** A. Sikorski (Warsaw, Poland)
Properties of two-dimensional polymer-solvent systems. A Monte Carlo study

11:35-11:55 **L37:** T.S. Barata (London, United Kingdom)
Structural studies on glycosylated gen. 3.5 PAMAM dendrimers

11:55-12:15 **L38:** K. Mikulska (Torun, Poland)
Steered MD simulations of adhesive protein contactin

12:15-12:35 **L39:** M. Łaźniewski (Warsaw, Poland)
Squalene epoxidase as target for new hypocholesterolemic drugs

12:35-12:55 **L40:** M. Długosz (Warsaw, Poland)
Brownian dynamics study of the association between the 70S ribosome and elongation factor G

13:00 Conference closing