Conference program

June 23, 2008 (Monday)

14:00-21:00 Registration - lobby of LAS Hotel

June 24, 2008 (Tuesday)

8:00-9:00 Registration - lobby of LAS Hotel
9:00-9:15 Conference opening

Session I **Advances in computational methods** (chair: J. Sauer)

9:15-9:55 **L1:** T. Wesołowski (Geneva, Switzerland)
Embedding quantum chemical system in orbital-free environment: recent formal developments and applications in multi-level simulations
9:55-10:35 **L2:** M. Meuwly (Basel, Switzerland)
Atomistic simulations for complex systems with chemical accuracy
10:35-10:50 Cofee break

Session II **Modeling zeolite materials** (chair: Z. Latajka)

10:50-11:30 **L3:** R. van Santen (Eindhoven, The Netherlands)
Molecular recognition in heterogenous catalysis

11:30-12:10 **L4:** J. Sauer (Berlin, Germany)
Hydrocarbon reactions in zeolites by hybrid QM/QM and QM/MM methods

12:10-12:25 **L5:** P. Boulet (Marseille, France)
Adsorption into the MFI zeolite of cyclic molecule of biological relevance. Investigations by Monte Carlo simulations

12:25-12:40 **L6:** B. Szyja (Eindhoven, Netherlands)
Study of the silica-water-SDA interactions during the initial stages of zeolite synthesis

12:40-14:40 Lunch break

Session III **Interactions in molecular materials** (chair: A. Tachibana)

14:40-15:15 **L7:** J. S. Murray (Cleveland, OH, USA)
σ–hole bonding – a widely occurying directional noncovalent interaction

15:15-15:50 **L8:** H. Cheng (Air Products & Materials Inc., Allentown, PA, USA)
Predictive atomistic simulations for design and development of novel materials for semiconductor applications

15:50-16:25 **L9:** O. Shishkin (Kharkov, Ukraine)
Non-conventional intermolecular interactions in molecular complexes and crystals

16:25-17:00 **L10:** S. Grabowski (Łódź, Poland)
The enhancement of X-H..pi hydrogen bonds - the study of cooperativity effects

17:00-17:15 Cofee break

17:15-19:15 Poster session A (P1-P26)

June 25, 2008 (Wednesday)

Session IV **Modeling chemical reactions** (chair: T. Brinck)

9:00-9:35 **L11:** A. Toro-Labbe (Santiago, Chile)
The reaction force analysis. Application to catalytic processes

9:35-10:10 **L12:** P. Politzer (New Orleans, LA, USA)
The reaction force constant

10:10-10:45 **L13:** P. Paneth (Łódź, Poland)
Modeling of enzymatic reactions based on isotope effects

10:45-11:00 **L14:** Z. Flisak (Opole, Poland)
Modeling Multidentate Ligands in Coordinative Olefin Polymerization Catalysts

11:00-11:15 Coffee break

Session V **Protein Dynamics** (chair: A. Liwo)

11:15-11:50 **L15:** T. Clark (Erlangen, Germany)
QM/MM Molecular Dynamics Calculations of Electronic Properties
11:50-12:25 **L16:** A. Koliński (Warsaw, Poland)
Multiscale modeling of protein structure, dynamics and interactions
12:25-12:40 **L17:** A. Sikorski (Warsaw, Poland)
Thermodynamic properties of polypeptide chains. The comparison of some Monte Carlo techniques
12:40-14:40 Lunch break

Session VI **Protein structure prediction** (chair: A. Koliński)

14:40-15:20 **L18:** A. Godzik (La Jolla, CA, USA)
Structural genomics – surveying the unknown regions of protein structure space
15:20-16:00 **L19:** A. Liwo (Gdańsk, Poland)
Prediction of structure and simulation of dynamics of protein folding with the mezoscopic UNRS force field
16:00-16:15 Coffee break

Session VII **Properties of molecular materials** (chair: T. Clark)

16:15-16:50 **L20:** R.A. Poirier (St.John's, Canada)
Interesting properties and applications of the average inter-particle distance
16:50-17:25 **L21:** A. Tachibana (Kyoto, Japan)
Stress tensor description of chemical bonds - formulation of non-classical bond order concept
17:25-18:00 **L22:** Z. Latajka (Wrocław, Poland)
Quantum nature of proton transfer in H-bonded mono- and di-carboxylic acid crystals - path integrals molecular dynamics studies
18:00-18:35 **L23:** B. Kuchta & L. Firlej (Marseille, France)
Modeling of alkanes adsorbed on graphite
18:35-18:50 **L24:** J. C. Wojdeł (Barcelona, Spain)
Influence of cations and water molecules on electron structure of Prussian blue analogues
19:00-21:00 Conference grill

June 26, 2008 (Thursday)

9:00-15:30 Excursions (A – Szrenica mountain, B – uranium mines & Wang temple)

Session VIII **General session** (chair: S. Roszak)

15:30-16:45 Fujitsu Poland workshop session
Tools for computational chemistry
16:45-17:00 Coffee break
17:00-19:00 Poster Session B (P27-P53)

June 27, 2008 (Friday)

Session IX **Protein design** (chair: P. Paneth)

9:00-9:40 **L25:** M. Ramos (Porto, Portugal)
Computational mutagenesis and drug discovery

9:40-10:20 **L26:** T. Brinck (Stockholm, Sweden)
Computational search and design of new enzyme activities

10:20-11:00 **L27:** J. Koca (Brno, Czech Republic)
In silico mutagenesis to improve protein binding affinity and selectivity

11:00-11:15 Coffee break

Session X **Modeling biomaterials** (chair: P. Tchounwou)

11:15-11:55 **L28:** P. Kozłowski (Louisville, KY, USA)
The Co-C bond cleavage in cobalamin-dependent methioninine synthase: a theoretical study

11:55-12:15 **L29:** D. Plewczyński (Warsaw, Poland)
Evaluation of various protein-ligand docking programs

12:15-12:30 **L30:** P. Sharma (Hyderabad, India)
Modelling the noncovalent interactions at the metabolite binding site in purine riboswitches

12:30-12:45 **L31:** S. Sharma (Hyderabad, India)
Design of laser pulses for selective vibrational excitation of amino N-H bond of adenine and A-T base pair using Optimal Control Theory

12:45-14:45 Lunch break

Session XI **Drug design I** (chair: P. Kafarski)

14:45-15:20 **L32:** P. Tchounwou (Jackson, USA)
Molecular pharmacology of arsenic trioxide and the cure of acute promyelocytic leukemia

15:20-15:55 **L33:** S. Guccione (Catania, Italy)
Identification of novel scaffolds leading to small molecule DNA polymerase-beta inhibitors with potential in neurodegenerative and oncology disorders

15:55-16:30 **L34:** V. Kuzmin (Odessa, Ukraine)
The hierarchical QSAR technology for virtual screening and drug design

16:30-16:45 Coffee break

Session XII **Drug design II** (chair: V. Kuzmin)

16:45-17:20 **L35:** J. Burda (Prague, Czech Republic)
Electronic Properties and Reaction Mechanisms of Selected Anticancer Metallodrugs

17:20-17:45 **L36:** L. Berlicki (Wroclaw, Poland)
Computer-aided design of inhibitors of amino acids biosynthesis

17:45-18:00 **L37:** T. Zimmermann (Praha, Czech Republic)
Reaction of cisplatin aquation products with cysteine and methionine at constant pH

18:00-18:15 **L38:** E. Muratov (Odessa, Ukraine)
Consensus prediction of aqueous solubility of military compounds

Session XII **Special lecture folowed by conference dinner** (chair: J. Leszczyński)

18:30-19:00 **L39:** P.Drożdżewski (Wrocław, Poland)
Normal vibrations and music harmony

June 28, 2008 (Saturday)

Session XIV **Nucleic acids I** (chair: J. Murray)

9:00-9:40 **L40:** P. Hobza (Prague, Czech Republic)
Accurate stabilization energies of DNA base pairs

9:40-10:20 **L41:** J. Rak (Gdansk, Poland)
Single strand breaks in DNA induced by low energy electrons. Possible mechanisms

10:20-11:00 **L42:** J. Sponer (Brno, Czech Republic)
RNA base pairing and RNA building blocks

11:00 -11:15 Coffee break

Session XIV **Nucleic acids II** (chair: J. Burda)

11:15-11:50 **L43:** P. Cysewski (Bydgoszcz, Poland)
The post-SCF complete basis set quantum chemistry characteristics of the energetic heterogeneity of stacking interactions in crystallographic DNA.

11:50-12:05 **L44:** Z. Vokáčová (Praha, Czech Republic)
Probing the structure and dynamics of RNA dinucleoside monophosphates (ApA, ApC, CpA, CpC) with NMR spectroscopy)

12:05-12:45 **L45:** J. Leszczyński (Jackson, MS, USA)
Common convenient misconceptions: theory versus experiment

12:45-13:00 Conference closing