Conference program

September 10, 2012 (Monday)

15:00-21:00	Registration - lobby of building A-1, Wyb. Wyspiańskiego 27

September 11, 2012 (Tuesday)

8:00-9:00	Registration (continued)
9:00-9:10	Conference opening - Aula on the first floor of building A-1
Session 1	**Advances and applications of computational methods** (chair: A. Toro-Labbé)
9:10-9:40	**L1:** A. Laganà (Perugia, Italy) *Cooperative modeling and design on the computer grid*
9:40-10:10	**L2:** T. Wesołowski (Genève, Switzerland) *Revealing the bonding pattern from the molecular electron density using single exponential decay detector (SEDD): an orbital-free alternative to the electron localization function (ELF)*
10:10-10:40	**L3:** W. Grochala (Warszawa, Poland) *Molecules and solids that refuse to exist*
10:40-11:10	**L4:** Z. Latajka (Wrocław, Poland) *Xenon compounds - theoretical studies and the nature of bonding*
11:10-11:25	Coffee break
Session 2	**Modeling molecular materials** (chair: M. Yáñez)
11:25-11:55	**L5:** T. Clark (Erlangen, Germany) *From molecules to devices: modeling "soft" electronics*
11:55-12:25	**L6:** B. Szyja (Münster, Germany) *Mechanochemical bond breaking by MD simulation*
12:25-12:55	**L7:** A. Michalak (Kraków, Poland) *Theoretical study in the dehydrogenation of ammonia borane by transition metal complexes for fuel cell applications*
12:55-15:00	Lunch break

Session 3 **Modeling interactions in molecular materials** (chair: T. Clark)

15:00-15:30 **L8:** M. Yáñez (Madrid, Spain)
Modulating chemical properties and forming new materials through non-covalent interactions

15:30-16:00 **L9:** J. Murray (Cleveland, USA)
σ-hole bonding and beyond

16:00-16:30 **L10:** J. Koča (Brno, Czech Republic)
Recent progress in computational chemistry of protein/carbohydrate interactions

16:30-16:50 **L11:** M. Mitoraj (Kraków, Poland)
Non-covalent interactions from an ETS-NOCV perspective

16:50-17:10 **L12:** M. Jabloński (Toruń, Poland)
Theoretical insight into the nature of the intermolecular charge-inverted hydrogen bond

17:10-17:30 Cofee break

17:10-19:00 Poster session A (P1-P45) - lobby of building A-1

September 12, 2012 (Wednesday)

Session 4 **Advances and applications of computational methods** (chair: J. Sauer)

9:00-9:30 **L13:** A. Tachibana (Kyoto, Japan)
Chirality and stress tensor of electron

9:30-10:00 **L14:** A. Toro-Labbé (Santiago de Chile)
Towards a theory of chemical reactions and reaction dynamics

10:00-10:30 **L15:** P. Politzer (New Orleans, USA)
The Reaction force constant: some observations

10:30-10:50 **L16:** J. Jaque (Santiago de Chile)
Synchronicity in chemical reactions: a reaction force constant analysis

10:50-11:05 Coffee break

Session 5 **Modeling molecular materials** (chair: Z. Latajka)

11:05-11:35 **L17:** J. Sauer (Berlin, Germany)
Towards predictions of energies and free energies for molecule-surface interactions with chemical accuracy

11:35-12:05 **L18:** B. Kuchta (Marseille, France)
Numerical design of new porous open carbon frameworks (OCF) for hydrogen storage

12:05-12:35 **L19:** O. Shishkin (Kharkov, Ukraine)
Topology of intermolecular interactions as basis for analysis of structure and properties of molecular crystals

12:35-12:55 **L20:** A. Sikorski (Warszawa, Poland)
Diffusion in a crowded environment: simulation within the frame of the dynamic lattice liquid (DLL)

12:55-15:00 Lunch break

15:00-15:20 Panorama Art Gallery show

15:30-17:30 Wrocław sightseeing with a guide

17:30-19:00 Centennial Hall Discovery Center show and Japanese Garden

19:15-22:15 Conference Dinner

September 13, 2012 (Thursday)

Session 6 **Modeling biomolecules** (chair: N. Richards)

9:00-9:30 **L21:** W. Minor (Charlottesville, USA)
Experiment and modelling: competitive or complementary approaches to structural biology ?

9:30-10.00 **L22:** J. Polański (Katowice, Poland)
Mining molecular databases for fragonomics based exploration of the architecture of drugs

10.00-10:30 **L23:** J. Gu (Shanghai, P.R. China)
Electron attachment to biomolecules: from nucleobase to DNA

10:30-11:00 **L24:** P. Paneth (Łódź, Poland)
An MP2-based extention of chlorine isotope effects limits; challenge for the experiment

11:00-11:15 Coffee break

Session 7 **Modeling biomolecules** (chair: P. Paneth)

11:15-11:45 **L25:** J. Burda (Prague, Czech Republic)
Study on the ruthenium(II) and platinum(II) complexes and their interactions in cellular environment

11:45-12:15 **L26:** J. Korchowiec (Kraków, Poland)
Molecular modeling studies of model monolayers

12:15-12:35 **L27:** P. Dominiak (Warszawa, Poland)
Electron density and electrostatic properties of biomacromolecules from a database of pseudoatomic densities

12:35-12.55 **L28:** D. Rutkowska-Żbik (Kraków, Poland)
Theoretical modeling ofchlorophyls and their derivatives as potential therapeutic agents

12:55-13:15 **L29:** Ł. Pepłowski (Toruń, Poland)
Molecular dynamics studies of synaptic adhesion neurolignin/neurexin complexes

13:15-15:00 Lunch break

15:00-17:00 Poster session B (P46-P91) - lobby of building A-1

Session 8 **Workshop - computer laboratory 50 in building A-2** (chair: W. Bartkowiak)

17:00-20:00 **L30:** R. Zaleśny and R. Góra (Wrocław, Poland)
Computational methods to determine electric dipole properties of molecules and their aggregates

September 14, 2012 (Friday)

Session 9 **Modeling biomolecules and drug design** (chair: W. Minor)

9:00-9.30 **L31:** N. Richards (Gainesville, USA)
Computing and evaluating absolute free energy differences for protein loop conformational changes

9:30:-10:00 **L32:** J Grembecka (Ann Arbor, USA)
Structure-based development of small molecule inhibitors for acute leukemia

10:00-10.30 **L33:** T. Cierpicki(Ann Arbor, USA)
Challenges in structure based design of protein-protein interaction inhibitors

10:30-11:00 **L34:** S. Filipek (Warszawa, Poland)
Recent structures and novel activation mechanisms of GPCRs

11.00-11:15 Coffee break

Session 10 **Modeling materials and biomolecules** (chair: J. Burda)

11:15-11:40 **L35:** P. Cysewski (Bydgoszcz, Poland)
Color predictions from first principle quantum chemistry computations

11:40-12:05 **L36:** T. Kuliński (Poznań, Poland)
Structural adaptation in nucleic acids-protein functional complexes studied by computational methods

12:05-12:25 **L37:** Z. Futera (Prague, Czech Republic)
Reaction mechanism of Ru(II) piano-stool complexes; QM/MM study

12:25-12:45 **L38:** D. Plewczyński (Warszawa, Poland)
MetaDock: enzyme substrate identification using protein-ligand docking

12:45-13:05 **L39:** S. Rai (Hyderabad, India)
Electronic structure based insights into proline tagged with gold nano clusters

13:05 Conference closing