

Conference and workshop program

September 10, 2006 (Sunday)

- 16.00-20.00 Registration - Entrance to B-4 building
(corner of Smoluchowskiego & Łukasiewicza Streets)
16.00-20.00 Welcome reception

September 11, 2006 (Monday)

- 8.00-9.00 Registration - Entrance to B-4 building
9.00-9.10 Workshop opening - Room 409 B-4 building

SESSION I - Room 409 B-4 building (Chair - J. Leszczyński)

- 9.10-10.00 **L1:** W. Minor - *Structural Genomics Changes the Molecular
Modeling Approach*
10.00-10.45 **L2:** T. Brinck - *Computational Design of New Enzyme Catalysts*
10.45-11.00 Coffee break

SESSION II - Room 409 B-4 building (Chair - G. Náray-Szabó)

- 11.00-11.40 **L3:** A. Koliński - *Modeling Protein Structure and Interactions in
Reduced Conformational Space*
11.40-12.20 **L4:** L. Piela - *Theoretical Model of Conformational Autocatalysis*
12.20-13.00 **L5:** B. Lesyng - *Causality Analysis - A Strategy for the Analysis of
Molecular Dynamics Data*
13.00-15.00 Lunch break

SESSION III - Room 409 B-4 building (Chair - T. Brinck)

- 15.00-15.45 **L6:** G. Náray-Szabó - *On the Mechanism of Action of Enzymatic
Phosphate Hydrolysis*
15.45-16.30 **L7:** P. Paneth - *Application of Different QM/MM Schemes to Studies
of Enzyme-Catalyzed Reactions*
16.30-17.00 *FQS POLAND software presentation*
17.00-17.15 Coffee break

SESSION IV - Rooms 448 & 446 B-4 building

- Optional session for participants registered earlier
17.15-18.45 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*

SESSION V - 4th floor B-4 building

- 19.30-21.00 Poster session A (P2-P6, P8-P11, P13-P14, P16-P28, P30-P38, P56)

September 12, 2006 (Tuesday)

- SESSION VI - Room 409 B-4 building** (Chair - L. Piela)
- 9.00-9.45 **L8:** H. Cheng - *Design and Development of Efficient Hydrogen Storage Materials to Enable the Hydrogen Economy*
- 9.45-10.30 **L9:** W. Grochala - *Towards the "Hydrogen economy" Dream – Catalysis of the Homo- and Heterolytic Splitting of the H₂ Molecule*
- 10.30-11.00 **L10:** B. Kuchta - *Adsorption and Phase Transitions in Nanopores*
- 11.00-11.15 Coffee break
- SESSION VII - Room 409 B-4 building** (Chair - P. Paneth)
- 11.15-11.50 **L11:** P. Politzer - *Halogen Bonding as a Basis for the Design of New Materials*
- 11.50-12.25 **L12:** C. Ramseyer - *Modelling of Ionic Channels at the Molecular Level: Achievements and Perspectives*
- 12.25-13.00 **L13:** A. Miniewicz - *Design of Photochromic Polymers and Liquid Crystals for Dynamic Holography*
- 13.00-15.00 Lunch break
- SESSION VIII - Room 409 B-4 building** (Chair - C. Ghio)
- 15.00-15.40 **L14:** J. Leszczyński - *Nerve Agents - How To Uncover Their Characteristics and Not Get Killed?*
- 15.40-16.20 **L15:** I. Majerz - *Isotope Effects in Strong Hydrogen Bonds*
- 16.20-17.00 **L16:** J. Burda - *Computational Approach to Anticancer Metallodrugs*
- 17.00-17.15 Coffee break
- SESSION IX - Rooms 448 & 446 B-4 building**
Optional session for participants registered earlier
- 17.15-19.00 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*

September 13, 2006 (Wednesday)

- 9.30-10.00 Panorama Raclawicka Gallery tour (Purkyniego Street)
optional upon request
- 10.00-13.00 Wrocław sightseeing (starting from Panorama Raclawicka Gallery)
optional upon request, free
- SESSION X - Rooms 448 & 446 B-4 building**
Optional session for participants registered earlier
- 15.15-19.00 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*
- 19.30-21.00 Conference reception - Museum of Architecture (Bernardyńska Street)

September 14, 2006 (Thursday)

SESSION XI - Aula B-4 building (Chair - P. Kafarski)

- 9.00-9.40 **L17:** L. Hua - *What controls enantioselectivity of carbonyl reductase?*
9.40-10.20 **L18:** C. Ghio - *Computational Prediction of Regio- and Stereoselectivities in the Hydroformylation of Chiral Olefins*
10.20-10.45 **L19:** N. Mishra - *A Theoretical Study of the Comparative Binding Affinities of PAILL towards Monosaccharides*

10.45-11.00 Coffee break

SESSION XII - Aula B-4 building (Chair - L. Komorowski)

- 11.00-11.40 **L20:** T. Wesolowski - *First-principles Treatment of the Interface Between the Orbital and Orbital-free Levels of Description in Multi-scale Modelling*
11.40-12.25 **L21:** A. Tachibana - *A New Energy Density Visualization Scheme for External Field Effects on Molecular Systems*
12.25-13.00 **L22:** A. Daini - *The Effect of Interaction Range and Anisotropy on Surface Tension*

13.00-15.00 Lunch break

SESSION XIII - Aula B-4 building (Chair - Z. Latajka)

- 15.00-15.40 **L23:** J. Sauer - *Treating Dispersion Effects in Extended Systems by Hybrid MP2:DFT calculations: Hydrocarbons on Catalyst Surfaces*
15.40-16.20 **L24:** J. Wojdel - *Computational Modelling of Double Metal Cyanide Catalyst for Propoxylation Reaction*
16.20-17.00 **L25:** E. Broclawik - *CYP 3A4: Modelling Substrate Binding and Electronic State of Oxyferryl Active Site Helps to Understand Reactivity*

17.00-17.15 Coffee break

SESSION XIV - Rooms 448 & 446 B-4 building

- Optional session for participants registered earlier
17.15-19.00 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*

SESSION XV - 4th floor B-4 building

- 19.30-21.00 Poster session B (P1, P3, P7, P12, P15, P17, P29, P31, P39-P55, P57-P58, P59)

September 15, 2006 (Friday)

SESSION XVI - Aula B-4 building (Chair - J. Sauer)

- 9.00- 9.35 **L26:** M. Cieplak - *Stretching to Understand Proteins*
9.35-10.10 **L27:** S. Grabowski - *Characteristics of a Wide Spectrum of
Dihydrogen Bonded Materials*
10.10-10.45 **L28:** H. Dodziuk - *Why Are Strained Hydrocarbons Worth Studying?*
10.45-11.00 Coffee break

SESSION XVII - Aula B-4 building (Chair - J. Burda)

- 11.00-11.35 **L29:** P. Cysewski - *Accuracy of Gas Phase Acidities of Carboxylic Acids Predicted by Direct Scaling of Harmonic Vibrational Frequencies from *ab initio* Calculations - A Perspective for Precise *pKa* Estimation*
11.35-12.00 **L30:** Z. Vokáčová - *NMR Parameters in RNA Molecules and Their Correlation with Molecular Structure*
12.00-12.20 **L31:** M. Pavelka - *Quantum Chemical Study of Cu(I)/Cu(II) Cations in a Peptide Environment*
12.30 Farewell - main campus building (A-1)
photograph of workshop participants on the stairs

Conference posters

No.	Session	Main author	Title
P1	B	T. Borowski	<i>DFT Studies on the Reaction Mechanisms of Intra- and Extradial Dioxygenases</i>
P2	A	G. Brancolini	<i>Mechanism for DNA Triple Helix Formation: a Computational Study</i>
P3	B	E. Broniatowska	<i>PLDB - Protein Ligands DataBase</i>
P4	A	H. Chojnacki	<i>Multiple Proton Transfer in Some Molecular Systems. Implications for Crystalline Phases</i>
P5	A	P. Czeleń	<i>Molecular Dynamic Simulation of the Effects of Oxidative Damage on the Structure of Telomeric DNA</i>
P6	A	M. Doskocz	<i>Studies of Hydrogen Bonds in C-H...O=P by NMR Chemical Shifts and $3hJ(13C-31P)$ Spin-Spin Coupling. Correlation of Experimental and ab initio Data</i>
P7	B	M. Doskocz	<i>The Theoretical Study of Five Heterocyclic Derivatives of Carbazole – Monomers Electroconducting Polymers</i>
P8	A	M. Feliks	<i>Reactivation mechanisms for sarin-inhibited acetylcholinesterase by oxime: a model DFT study</i>
P9	A	M. Fiet	<i>Theoretical Study of Concerted Proton Transfer in the Ground Electronic State of the Double Hydrogen Bonded Formic Acid Dimer</i>
P10	A	Z. Futera	<i>Activation of Ruthenium(II) Complexes and their Interactions with DNA bases</i>
P11	A	P. Gauden	<i>CO₂ Sorption on N-, O-, and OH-substituted Carbonaceous Materials. A computational Chemistry Study</i>
P12	B	P. Gauden	<i>Argon Adsorption on Heterogeneous Carbon Surfaces: Accesible Pore volume and Width</i>
P13	A	A. Gorączko	<i>Modeling of Isotopomeric Molecular Clusters in Electron Ionisation Mass Spectra</i>
P14	A	H. Grebneva	<i>Causes of Rare Tautomer Forms Stabilization of DNA Bases Under Dimers Formation and DNA Synthesis</i>
P15	B	H. Grebneva	<i>Changes in Structure of DNA Bases as one of Reasons of the Untargeted UV-mutagenesis</i>
P16	A	D. Gront	<i>Optimizing the Parallel Tempering Monte Carlo method for biomolecular systems - insights from stat. thermodynamics</i>
P17	B	D. Gront	<i>BBQ - Backbone Building from Quadrilaterals: An Algorithm That Outperforms Existing Methods</i>
P18	A	R. Grzywa	<i>The Molecular Basis of Urokinase Inhibition: From the Analysis of Intermolecular Interactions to the Prediction of Binding Affinity</i>
P19	A	J. Handzlik	<i>DFT Study of Molybdena-silica System in Olefin Metathesis</i>
P20	A	K. Hernik	<i>cis-Diammine(oxalato)platinum(II) - a Cisplatin Analogue. Density Functional Study</i>
P21	A	J. Hładyszowski	<i>DFT Study of Dihexanoyle Phosphatidylcholine Monolayer</i>
P22	A	T. Jaroń	<i>DFT Studies of Novel Hypothetical Hydrides of Late Lanthanide Metals: Route to high-TC Superconductivity?</i>
P23	A	A. Kaczmarek	<i>Experimental and Theoretical Investigations of Spectroscopic Properties of Azobenzene Derivatives in 1,1,2-trichloroetan</i>
P24	A	J. Kamiński	<i>Accuracy of Various Approximations to the Non-additive Kinetic Functional in Exactly Solvable Cases</i>

No.	Session	Main author	Title
P25	A	M. Kluba	<i>Molecular Basis of Vampirism - Designing Anti-porphyrin Drugs</i>
P26	A	S. Kmiecik	<i>De Novo Simulations of Protein-folding Pathways in a Reduced Conformational Space</i>
P27	A	M. Kurciński	<i>Model of Three-dimensional Structure of the Vitamin D Receptor Bound with Peptide Ligand Mimicking Co-activator Sequence</i>
P28	A	M. Kwiatkowski	<i>A Clustering Based Approach to Adsorption Modeling</i>
P29	B	M. Kwiatkowski	<i>Computer Analysis of Nitrogen Adsorption Isotherms on Active Carbons by an Employment of the New LBET Class Models</i>
P30	A	D. Latek	<i>Theoretically Predicted Contacts and Sparse NMR Data in De novo Protein Structure Prediction</i>
P31	B	J. Lundell	<i>Quantum Chemical Studies of Xenon Insertion Compounds of Formic Acid</i>
P32	A	J. Lundell	<i>Computational Study of Formic Acid Dimers Involving the Higher-energy Conformer, cis-HCOOH</i>
P33	A	Ł. Maj	<i>Design of Ti/Si/H Clusters and Surfaces of Cubic TiSi for Heterolytic Addition of H₂</i>
P34	A	L. Michera	<i>Theoretical Study of Cisplatin Interactions with Glycine in Gas-phase and Implicit Water Solution – COSMO</i>
P35	A	P. Miszta	<i>Homology Modelling of G-protein Coupled Odorant Receptor AgOR1 from Malaria Mosquito Anopheles Gambiae</i>
P36	A	J. Mrázek	<i>Computational DFT Study of the Non-heme Iron Center of Photosystem II</i>
P37	A	J. Murray	<i>The Two Components of the Activation Energy</i>
P38	A	W. Niewodniczański	<i>Electronic Structure of Pyridinium N-phenolate Betaine Dye</i>
P39	B	S. Orłowski	<i>Locally Enhanced Sampling Molecular Dynamics Study of the Dioxygen Transport in Human Cytochrome c</i>
P40	B	A. Panczakiewicz	<i>Implementation of the QM/QM Method Based on the LocalSCF Algorithm</i>
P41	B	P. Paneth	<i>Continuum Solvent Models of Body Fluids on the Example of Serum</i>
P42	B	Ł. Peplowski	<i>Insights Into the Catalytic Activity of Industrial Enzyme Co-Nitrile Hydratase. Docking Studies of Nitriles and Amides</i>
P43	B	J. Pietkiewicz	<i>Glycolytic enzyme enolase as a plasminogen receptor: in vitro interaction and theoretical modeling.</i>
P44	B	Y. Pivak	<i>Defect Transport Modelling in Monoclinic La(2-x)Pr(x)Ti(2-y)Nb(y)SiO(9+d)</i>
P45	B	M. Radoń	<i>Peculiarities of the Electronic Structure of Cytochrome P450 Active Site (Compound I) - DFT and CASPT2 Modeling</i>
P46	B	P. Rejmak	<i>Cu(I) Sites in Faujasite and their Interactions with the CO Molecule - Theoretical Studies</i>
P47	B	M. Rostkowski	<i>Charge Localization in Monothiophosphate Monoanions</i>
P48	B	D. Rutkowska-Zbik	<i>Preliminary Theoretical Studies on TiO₂ Anatase System</i>
P49	B	J. Sebek	<i>Modeling of Circular Dichroism Spectra of Flexible Peptides in Water Solutions with Using Molecular Dynamics and Quantum Mechanics</i>
P50	B	W. Szczepanik	<i>Linear Response Kohn-Sham Equations with Constrained Electron Density Applied to a Nonheme Fe(IV)=O Complex</i>
P51	B	B. Szyja	<i>Modeling the Adsorption of Aromatic Compounds on a TiO₂/SiO₂ Catalyst</i>

No.	Session	Main author	Title
P52	B	K. Świderek	<i>Modeling Properties of Iridium Complexes</i>
P53	B	M. Ullrich	<i>Modelling of Transition States in Stereoselective Addition of Diethylzinc to Benzaldehyde Catalyzed by N,S-camphor Based Catalysts</i>
P54	B	Z. Velkov	<i>Predicted Antioxidant Activity of Amide and , Thioamide of o-Coumaric Acid</i>
P55	B	P. Wielgus	<i>Theoretical Description of Ge/Si Microclusters</i>
P56	A	M. Wiśniewski	<i>On the Reactivity of Curved Carbon Nanostructures to Amidogen</i>
P57	B	M. Wiśniewski	<i>Towards the Reactivity of Carbon to Izelectronic (Cl- and K+) Adsorbates</i>
P58	B	T. Zimmermann	<i>The Interactions of Platinum Complexes with Sulfur-Containing Amino Acids; Theoretical Calculations</i>
P59	B	A. Zwiefka	<i>Study of Binding of Pseudomonas aeruginosa Alginate by Toll-Like 4 and CD18 Receptors</i>