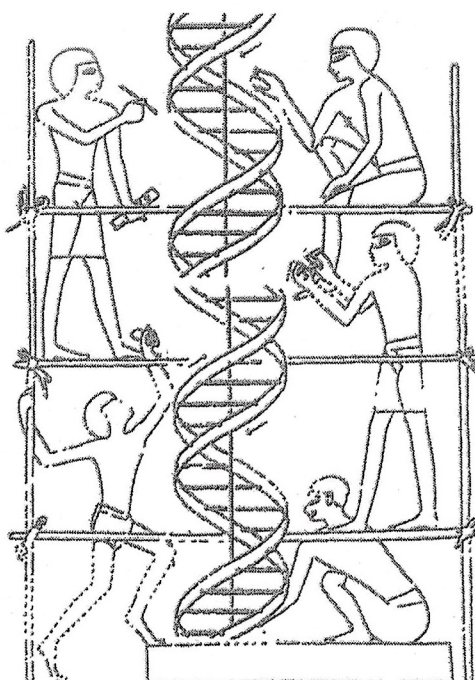


Modelling and Design of Molecular Materials



Program Book of Abstracts

Wrocław, September 16–20, 2004

MODELLING AND DESIGN OF MOLECULAR MATERIALS

workshop

organized in Wrocław, Poland on September 16-20, 2004

by

Molecular Modeling Laboratory (MML)
Wrocław University of Technology (WUT), Wrocław, Poland

NSF Computational Center
for Molecular Structure and Interactions (CCMSI)
Jackson State University (JSU), Jackson, MS, USA

Charles University in Prague, Czech Republic

Polish Chemical Society (PTCh)

Wrocław Center of Supercomputing and Networking (WCSS)

<http://mml.ch.pwr.wroc.pl/workshop/>

Sponsored by
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and

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and Support and Federal Relations

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WORKSHOP PROGRAM

September 16, 2004 (THURSDAY)

16.00 - 20.00 REGISTRATION **Patio in B-4 building –
crossing of Smoluchowskiego & Łukasiewicza streets**

September 17, 2004 (FRIDAY)

8.00 - 9.00 REGISTRATION **Patio in B-4 building**

9.00 WORKSHOP OPENING **Aula in B-4 building**

SESSION I - MODELING BIOMOLECULAR STRUCTURE

chair – P. Politzer

Aula in B-4 building

9.10 - 9.45 M.J. Ondrechen (Northeastern University, Boston, MA, USA)
Thematics: Prediction of Protein Active Sites

9.45 - 10.20 K. Zakrzewska (Institut de Biologie Physico-Chimique, Paris, France)
Theoretical Studies of DNA-protein Recognition

10.20 - 10.55 J. Koča (Masaryk University, Brno, Czech Republic)
*Exploring Multidimensional Energy Surfaces Related to Conformational
Search and Molecular Docking*

10.55 - 11.10 COFFEE BREAK **Patio in B-4 building**

SESSION II - MODELLING BIOMOLECULAR STRUCTURE

chair - B. Lesyng

Aula in B-4 building

11.10 - 11.45 S. Filipek (International Institute of Molecular and Cell biology, Warsaw,
Poland)
*Organization of rhodopsins in membrane and interactions with other
proteins*

11.45 - 12.20 J. Ciarkowski (University of Gdańsk, Poland)
*Modeling Neurohypophyseal Hormones to Signalling Mechanisms in
GPCRs*

12.20 - 12.55 L. Piela (University of Warsaw, Poland)
Theoretical Model of Prions

SESSION III - MODELLING CHEMICAL REACTIONS

chair - P. Kafarski

Aula in B-4 building

- 15.00 - 15.35 A. Mulholland (University of Bristol, UK)
Computational Enzymology: QM/MM Modelling of Enzyme-Catalyzed Reactions
- 15.35 - 16.10 P. Paneth (Technical University of Łódź, Poland)
Modeling of Enzymatic Reactions Based on Isotope Effects
- 16.10 - 16.45 A. Michalak (Jagiellonian University, Cracow, Poland)
Theoretical Modeling of the Polymerization and Copolymerization Processes Catalyzed by Late-transition-metal Complexes
- 16.45 - 17.00 COFFEE BREAK **Patio in B-4 building**

SESSION IV - MODELLING BIOMOLECULAR STRUCTURE

chair - M.J. Ondrechen

Aula in B-4 building

- 17.00 - 17.30 B. Lesyng (University of Warsaw, Poland)
Overview of Microscopic and Mezosopic Modeling Tools and Models
- 17.30 - 17.45 T. Andruniów (Università di Siena, Italy)
QM/MM and Car-Parrinello Molecular Dynamics Studies on Reaction Paths of Photoswitchable Oligopeptide
- 17.45 - 18.00 T. Kuliński (Institute of Bioorganic Chemistry PAN, Poznań, Poland)
The Mechanism of the Structure Formation and Dynamics of Functional RNA Hairpins: MD Studies Compared to NMR Structural Data
- 19.00 - 21.00 POSTER SESSION I - posters from P-1 to P-20 **Patio in B-4 building**

September 18, 2004 (Saturday)

SESSION V - DESIGN AND SYNTHESIS OF NEW MOLECULAR MATERIALS

chair - L. Firlej

Aula in B-4 building

- 9.00 - 9.35 A. Clearfield (Texas A&M University, College Station, TX, USA)
Modeling and Design Based on Phosphonic Acids

- 9.35 - 10.10 V. Renugopalakrishnan (Florida International University, Miami, FL, USA and Harvard Medical School, Boston, MA, USA)
Cytochrome c Super Family Based Bionanosensors
- 10.10 - 10.45 P. Kafarski (Wrocław University of Technology, Poland)
From Inhibitors of LAP to Inhibitors of PAL – Lessons from Molecular Modeling and Experimental Interface
- 10.45 - 11.00 COFFEE BREAK **Patio in B-4 building**

SESSION VI – MODELING PROPERTIES OF MOLECULAR MATERIALS

chair - J. Ciarkowski

Aula in B-4 building

- 11.00 - 11.35 J.S. Murray (University of New Orleans, LA, USA)
Computed Surface Properties of Carbon, Boron/Nitrogen and Carbon/Boron/Nitrogen Nanotube Models
- 11.35 - 12.10 W. Grochala (University of Warsaw, Poland)
Superconductivity and the Grand Periodic Table of Chemical Elements. What Can we Learn from Diatomic and Triatomic Molecules?
- 12.10 - 12.45 J. Burda (Charles University, Prague, Czech Republic)
Solvation Barriers and Rate Constants for Hydration of Platinum and Palladium Square Complexes: An ab initio and DFT Calculations with Inclusion of PCM-COSMO Model

SESSION VII - MODELING PROPERTIES OF MOLECULAR MATERIALS

chair - A. Clearfield

Aula in B-4 building

- 15.00 - 15.35 T. A. Wesółowski (University of Geneva, Switzerland)
Computer Modelling Using the Orbital-free Embedding Formalism An Useful Tool for Interpretation of Spectroscopic Data
- 15.35 - 16.10 B. Kuchta (Université de Provence, Marseille, France)
Computer Simulations of Adsorption in Porous Materials
- 16.10 - 16.30 J. Wojdeł (Delft University of Technology, The Netherlands)
New Pragmatic Approach to Modeling Mixed-valence Molecular Materials
- 16.30 - 16.45 COFFEE BREAK **Patio in B-4 building**

September 20, 2004 (Monday)

SESSION IX - COMPUTATIONAL METHODS AND SOFTWARE PRESENTATIONS

chair - P. Paneth

Lecture hall 4.9 in B-4 building

- 9.00 - 9.45 A. Michalak (Jagiellonian University, Cracow, Poland)
Car-Parrinello Molecular Dynamics along Intrinsic Reaction Paths
- 9.45 - 10.00 M. Prokop (National Centre for Biomolecular Research, Brno, Czech Republic)
Triton – Graphic Software for Modelling Protein Mutants and Calculation Reaction Pathways
- 10.00 - 10.15 R. Góra (Wrocław University of Technology, Poland)
An Introduction into the Theory of Intermolecular Forces – from van der Waals Equation of State to State of Art Theories
- 10.15 - 10.30 G. Hill (Jackson State University, MS, USA)
Accuracy vs. Size: Addressing Computational Shortcomings in Biological Calculations
- 10.30 - 10.45 **COFFEE BREAK** **Cafeteria in B-4 building**
- 10.45 - 13.00 Accelrys software presentations: Life Sciences
Lecture hall 4.9 in B-4 building
- 10.45 - 13.00 Accelrys software presentations: Material Sciences
Lecture hall 4.9 in B-4 building

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- Marina Balakina P-2
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- Wojciech Bartkowiak P-3
Hydrogen bond effects on the electronic absorption spectrum and evaluation of non-linear properties of an aminobenzodifuranone exhibiting the largest positive solvatochromism
- Cesar C. Diaz P-4
Theoretical study of the alkaline-earth anionic clusters: Be- and Mg-
- Edyta Dyguda P-5
Ab initio prediction of binding affinity: determinants of phenylalanine ammonia-lyase inhibition
- Artur Giełdoń P-6
Residues responsible for recognition of antagonists by the vasopressin receptor. Molecular dynamics study.
- Andrzej Gorączko P-7
Prediction of the most abundant peak location in isotopomeric clusters of organic compounds
- Jerzy Hładyszowski P-8
Aggregation of dihexanoylphosphatidylcholine
- Jerzy T. Jodkowski P-9
Theoretical Study on Kinetics of the Reaction of CF₃ and NO₂
- Jakub Kamiński P-10
From van der Waals interactions to a chemical bond. An ab-initio study of the nature of interactions between the methyl cation and rare gas atoms.
- Karina Kubiak P-11
The role of posttranslational oxidation of cysteine in nitrile hydratases. Quantum-chemical study of changes in the electronic structure of active site ligands.
- Vitalina Kukueva P-12
Quantum-chemical research of elemental processes during flame inhibition
- Katarzyna Kulińska P-13
Conformational switching in RNA hairpins

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