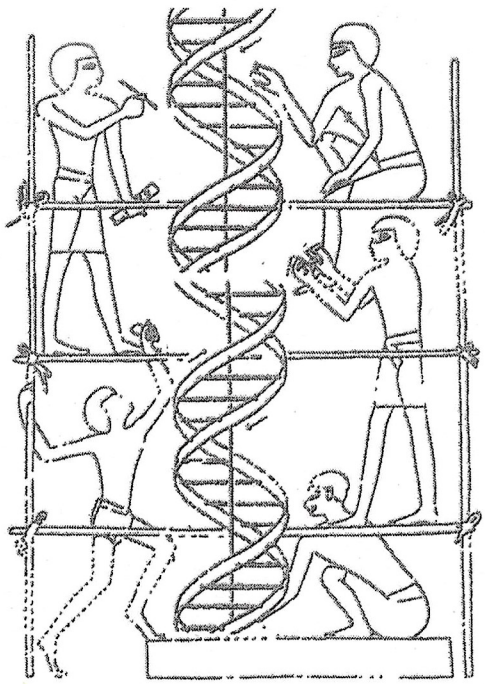
Modelling and Design of Molecular Materials



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

Wrocław University of Technology

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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 Łódz, 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 Mezoscopic 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.Wesołowski (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 ReactionPathways

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

Index of posters