

# Modeling and Design of Molecular Materials 2006

conference and workshop organized by

Molecular Modeling & Quantum Chemistry Group  
Institute of Physical & Theoretical Chemistry,  
Wroclaw University of Technology,  
Wroclaw, Poland

NSF Computational Center  
for Molecular Structure and Interactions  
Jackson State University, Jackson, MS, USA

Charles University in Prague, Czech Republic

Wroclaw Centre for Networking and Supercomputing

Wroclaw, POLAND, 10-15 September 2006

event sponsored by European Association for Chemical and Molecular Sciences and FQS Poland

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Meeting will be devoted to presentation of the contemporary computational methods and their applications in molecular modeling and design of molecular materials. Some lectures will be delivered by experimentalists involved in synthesis and testing of novel materials.

## Planned sessions:

- Structural genomics and biopolymer structure
- Modeling reactions and catalyst design
- Modeling molecular materials
- Bionanotechnology
- Design and synthesis of new molecular materials
- Workshop on Monte Carlo and statistics: modeling of molecular adsorption in nanoporous materials

## Proceedings:

Refereed conference contributions will be published in Journal of Molecular Modeling (indexed by ISI)

## Honorary Scientific Committee:

- T. Brinck – Royal Inst. Technol, Stockholm, Sweden
- J. Burda – Charles Univ., Prague, Czech Rep.
- S. Grabowski – Univ. of Lodz, Poland
- P. Kafarski – Wroclaw Univ. of Technology
- L. Komorowski – Wroclaw Univ. of Technology
- Z. Latajka – Wroclaw Univ., Poland
- J. Leszczynski – Jackson State Univ, USA – CHAIR
- T. Luty – President of Wroclaw Univ. of Technol.
- K. Maruszewski – Wroclaw Univ. of Technology
- G. Naray-Szabo – Lorand Eotvos Univ., Hungary
- V. Renugopalakrishnan – Harvard Univ., USA
- W. A. Sokalski – Wroclaw Univ. of Technology
- A. Tachibana – Kyoto Univ., Japan

## Important dates:

June 15, 2006 – Registration and early fee payment  
August 15, 2006 – Abstracts and late fee payment  
September 10-15, 2006 – Meeting (following immediately  
6th European Conference on Computational Chemistry  
Tale, Slovakia, 3-7 IX 2006  
<http://www.fns.uniba.sk/eucocc6/>)

## Tentative list of speakers:

- E. Broclawik – Krakow, Poland
- H. Cheng – Allentown, PA, USA
- M. Cieplak – Warsaw, Poland
- L. Firlej – Montpellier, France
- C. Ghio – Pisa, Italy
- S. Grabowski – Lodz, Poland
- W. Grochala – Warsaw, Poland
- S. Guccione – Catania, Italy
- A. Kolinski – Warsaw, Poland
- B. Kuchta – Marseille, France
- J. Leszczynski – Jackson, MS, USA
- A. Miniewicz – Wroclaw, Poland
- W. Minor – Charlottesville, VA, USA
- G. Naray-Szabo – Budapest, Hungary
- P. Paneth – Lodz, Poland
- L. Piela – Warsaw, Poland
- R. A. Poirier – St. John's, Newfoundland, Canada
- C. Ramseyer – Comte, France
- F. Raushel – College Station, TX, USA
- V. Renugopalakrishnan – Boston, MA, USA
- J. Sauer – Berlin, Germany
- A. Tachibana – Kyoto, Japan

Detailed information, program and registration form available on the WEB page  
<http://mml.ch.pwr.wroc.pl/workshop/>

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