

Organizing Committee

Steven Davis	University of Mississippi
Jerzy Leszczynski (Chairman)	Jackson State University
David H. Magers	Mississippi College
Svein Saebo	Mississippi State University

Staff

Shonda Allen	Jackson State University
Olexandr Isayev	Jackson State University
Tracye Lewis	Jackson State University
Yevgeniy Podolyan	Jackson State University

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**ARMY HIGH PERFORMANCE COMPUTING
RESEARCH CENTER**



Schedule of Events

Friday, March 26, 2004		
Workshop on High Performance Computing of Large Molecular Systems		
Registration	12:00 noon – 2:00 p.m. 4:00 p.m. – 5:00 p.m.	
Lunch	12:30 p.m. – 1:55 p.m.	
Opening Remarks (Jerzy Leszczynski)	1:55 p.m. – 2:00 p.m.	
1 st Session	Andrzej Sadlej	2:00 p.m. – 3:00 p.m.
	Apurba Bhattacharjee	3:00 p.m. – 3:20 p.m.
	Mohammad Qasim	3:20 p.m. – 3:40 p.m.
	Mark Zottola	3:40 p.m. – 4:00 p.m.
Coffee Break	4:00 p.m. – 4:30 p.m.	
2 nd Session	Michael McKee	4:30 p.m. – 4:50 p.m.
	Jaroslav Burda	4:50 p.m. – 5:10 p.m.
	David Close	5:10 p.m. – 5:30 p.m.
	Carlos Crespo-Hernández	5:30 p.m. – 5:50 p.m.
Dinner	6:30 p.m. – 8:00 p.m.	
Poster Session	9:30 p.m. – 11:00 p.m.	



Saturday, March 27, 2004			
Breakfast (provided by hotel)		8:00 a.m. – 9:00 a.m.	
Registration		8:00 a.m. – 9:00 a.m. 10:30 a.m. – 11:30 p.m.	
3 rd Session	Steven Davis	9:00 a.m. – 9:20 a.m.	
	David Magers	9:20 a.m. – 9:40 a.m.	
	Ras Pandey	9:40 a.m. – 10:00 a.m.	
	Bidhan Saha	10:00 a.m. – 10:20 a.m.	
Coffee Break		10:20 a.m. – 10:50 a.m.	
4 th Session	William Adams	10:50 a.m. – 11:10 a.m.	
	Svein Saebo	11:10 a.m. – 11:30 a.m.	
	Manoj Shukla	11:30 a.m. – 11:50 a.m.	
	Andrzej Wierzbicki	11:50 a.m. – 12:10 p.m.	
Lunch		1:00 p.m. – 2:30 p.m.	
5 th Session	Ernest Davidson	2:30 p.m. – 3:30 p.m.	
	Gregory Tschumper	3:30 p.m. – 3:50 p.m.	
Coffee Break		3:50 p.m. – 4:10 p.m.	
6 th Session	Michael Lee	4:10 p.m. – 4:30 p.m.	
	Leonid Gorb	4:30 p.m. – 4:50 p.m.	
	Jamal Musaev	4:50 p.m. – 5:10 p.m.	
Dinner		7:30 p.m. – 9:00 p.m.	



Oral Presentations

1st Session

Session Chairman:

Danuta Leszczynska
Florida State University

Andrzej Sadlej	Two as Good as Four: Relativistic Theory for Electrons Only
Apurba Bhattacharjee	In Silico Pharmacophore Development and Identification of Antimalarial Agents by Three-Dimensional Multi-Conformer Database Searches
Mohammad Qasim	Using CL-20 as the Model, UV/VIS/FTIR Spectrophotometry Supports Theoretical Predictions as to Initial/Intermediate Steps in Chemical Transformation of Cyclic and Cage Cyclic Nitramines
Mark Zottola	Qinghaosu-Based Antimalarials — Mechanism of Activation and Inhibition

2nd Session

Session Chairman:

Peter Politzer
University of New Orleans

Michael McKee	Computational Modelling of Nitrogenase
Jaroslav Burda	Cisplatin Hydration: Thermodynamics and Kinetics Study
David Close	DFT Calculations of the Deamination of Cytosine
Carlos Crespo-Hernández	<i>Ab Initio</i> Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution

3rd SessionSession Chairman: *Frances Hill*
Army High Performance Computing Research Center

Steven Davis	Stabilities, Strain Energies, and Isomerization Barriers of Some trans-Cycloalkenes
David Magers	Conformational Flexibility in Naphthylquinoline Derivatives
Ras Pandey	Roughness of the Film Growth on an Adsorbing Substrate with Kinetic Reactions in an Aqueous Solution of Hydrophobic and Polar Groups
Bidhan Saha	Electron Impact Ionization at Intermediate and High Energies

4th SessionSession Chairman: *W. Andrzej Sokalski*
Wroclaw University of Technology

William Adams	Understanding Intermolecular Perturbation Theory
Svein Saebo	Efficient AO-Formulation of MP2-Gradients
Manoj Shukla	Theoretical Study of Excited States of Nucleic Acid Bases: Electronic Transitions, Geometries and Interaction with Water Molecules
Andrzej Wierzbicki	Molecular Modeling of Crystal Growth Control in Biological Systems

5th SessionSession Chairman: *Eric Fisher*
University of Illinois at Springfield

Ernest Davidson	Momentum Space Chemistry
Gregory Tschumper	Guiding Chemical Reaction Path Searches with Graph Theory

6th SessionSession Chairman: *Louis Carlacci*
Army High Performance Computing Research Center

Michael Lee	Evaluation of Implicit Solvent Models
Leonid Gorb	Combined <i>ab Initio</i> Molecular Dynamics and Quantum-Chemical Studies of Selected Chemical Processes of Biological Importance
Jamal Musaev	Theoretical Prediction of a New Dinitrogen Reduction Process: The Utilization of Four Dihydrogen Molecules and Zr ₂ Pt ₂ Cluster

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