



## *Organizing Committee*

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Robert Baylot	U.S. Army Engineer Research and Development Center
Cary F. Chabalowski	U.S. Army Research Laboratory
William A. Lester, Jr.	University of California at Berkeley
Jerzy Leszczynski (Chairman)	Jackson State University
David Magers	Mississippi College
Gerald Maggiora	Pfizer, Inc.
Donald G. Truhlar	University of Minnesota

## *Staff*

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Shonda Allen	Jackson State University
Del Bagwell	U.S. Army ERDC
Olexandr Isayev	Jackson State University
Tracye Lewis	Jackson State University
Yevgeniy Podolyan	Jackson State University
Ilya Yanov	Jackson State University

## *Support*

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National Science Foundation (CREST Program)  
U.S. Army Engineer Research and Development Center  
Army High Performance Computing Research Center  
Parallel Quantum Solutions

*Current Trends in Computational Chemistry 2003*

*Jackson, Mississippi  
October 31 - November 1, 2003*





# Conference Agenda

*Current Trends in Computational Chemistry 2003*  
*Jackson, Mississippi*  
*October 31 - November 1, 2003*



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## Friday, October 31

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7:30 – 9:00	Continental Breakfast	
8:00 – 12:00	Registration	
9:00 – 9:30	Opening Ceremony	<b>Dr. Ronald Mason</b> <i>Jackson State University, President</i> <b>Dr. Vipin Kumar</b> <i>AHPCRC, Director</i> <b>Dr. Jeffery Holland</b> <i>US Army ERDC, Laboratory Director</i>
9:30 – 10:30	1 <sup>st</sup> Session (S1)	Davidson lecture
10:30 – 11:00	Coffee Break	
11:00 – 12:30	2 <sup>nd</sup> Session (S2)	2 Talks
12:30 – 12:40	Group photo	
12:40 – 2:00	Lunch	
2:00 – 3:30	3 <sup>rd</sup> Session (S3)	2 Talks
3:30 – 4:00	Coffee Break	
4:00 – 6:00	First Poster Session (P1)	
7:00 – 8:00	Cocktails	
8:00 – 10:00	Banquet	<i>Speaker: Dr. Donald E. Thompson</i> <i>Div. of Human Resource Development</i> <i>National Science Foundation</i>

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## Saturday, November 1

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8:00 – 9:00	Continental Breakfast	
8:30 – 11:00	Registration	
9:00 – 10:30	4 <sup>th</sup> Session (S4)	2 Talks
10:30 – 11:00	Coffee Break	
11:00 – 1:00	Second Poster Session (P2)	
1:00 – 2:00	Lunch	
2:00 – 3:30	5 <sup>th</sup> Session (S5)	2 Talks
3:30 – 4:00	Coffee Break	
4:00 – 5:30	6 <sup>th</sup> Session (S6)	2 Talks
5:30 – 7:30	Third Poster Session (P3)	
8:00 – 10:00	Dinner	
	After-dinner Noble Lecture Series	<i>Speaker: Dr. Isabella L. Karle</i>
	Best Student Poster Award Presentation	<i>Naval Research Laboratory</i>



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**Davidson Lecture**Session Chairman: **Peter Pulay**, *University of Arkansas*

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**Ernest R. Davidson**  
*University of Washington*

Radicals and Molecular Magnets

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**2<sup>nd</sup> Session**Session Chairman: **Suely Black**, *Norfolk State University*

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**Sally L. Price**  
*University College London*

The Computer Prediction of Organic Crystal Structures — Progress, Problems and Polymorphism

**Chen Wang**  
*Chinese Academy of Sciences*

Weak Forces in Building Molecular Nanostructures

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**3<sup>rd</sup> Session**Session Chairman: **Henry Kurtz**, *University of Memphis*

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**Laurence E. Fried**  
*Lawrence Livermore National Laboratory*

Molecular Thermochemistry via Path Integral Monte Carlo

**Mark Pederson**  
*Naval Research Laboratory*

Simulation of Molecular Magnets within Density Functional Theory

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**4<sup>th</sup> Session**Session Chairman: **Jane Murray**, *University of New Orleans*

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**Jan Linderberg**  
*Aarhus University*

The Reaction Simplex. A Computational and Conceptual Tool

**Shigeki Kato**  
*Kyoto University*

RISM-SCF Studies of Chemical Reactions in Solutions

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**5<sup>th</sup> Session**Session Chairman: **David Close**, *East Tennessee State University*

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**Georgii M. Zhidomirov**  
*Boskov Institute of Catalysis*

Structure, Chemisorption and Catalytic Activity of Multivalent Metal Oxide Species in High Silica Zeolites

**Joachim Sauer**  
*Humboldt University*

Calculations on Transition Metal Oxides — From Gas Phase Clusters to Solid Catalysts

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**6<sup>th</sup> Session**Session Chairman: **Jerome Karle**, *Naval Research Laboratory*

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**Bogumil Jeziorski**  
*University of Warsaw*

Density Functional Theory Approach to Van der Waals Interactions via Symmetry-Adapted Perturbation Expansion

**Walter Kohn**  
*University of California at Santa Barbara*

Van der Waals Energies and Time-Dependent Density Functional Theory

