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Current Trends in Computational Chemistry 2002

Jackson, Mississippi
November 1-2, 2002

CONFERENCE AGENDA

Current Trends in Computational Chemistry 2002

Jackson, Mississippi
November 1-2, 2002

Friday, November 1

7:30 – 9:00	Continental Breakfast	
8:00 – 12:00	Registration	
9:00 – 9:30	Opening Ceremony	**Dr. Ronald Mason** *Jackson State University, President* **Dr. Jeffery Holland** *US Army ERDC, Laboratory Director* **Dr. William McHenry** *Institutions for Higher Learning, Asst. Commissioner for Academic Affairs* **Dr. Robert W. Whalin** *U.S. Army Research Lab, Director*
9:30 – 10:30	1st Session (S1)	Buckingham lecture
10:30 – 11:00	Coffee Break	
11:00 – 12:30	2nd Session (S2)	2 Talks
12:30 – 12:40	Group photo	
12:40 – 2:00	Lunch	
2:00 – 3:30	3rd Session (S3)	2 Talks
3:30 – 4:00	Coffee Break	
4:00 – 5:30	4th Session (S4)	2 Talks
6:00 – 8:00	First Poster Session (P1)	
8:00 – 9:30	Dinner After-dinner Noble Lecture Series	*Speaker:* **Magdolna Hargittai** Eötvös University

Saturday, November 2

8:00 – 9:00	Continental Breakfast	
8:30 – 11:00	Registration	
9:00 – 10:30	5th Session (S5)	2 Talks
10:30 – 11:00	Coffee Break	
11:00 – 1:00	Second Poster Session (P2)	
1:00 – 2:30	Lunch	
2:30 – 4:00	6th Session (S6)	2 Talks
4:00 – 4:30	Coffee Break	
4:30 – 6:30	Third Poster Session (P3)	
7:00 – 8:00	Cocktails	
8:00 – 11:00	Banquet Best Student Poster Award Presentation	*Speaker:* **Dr. Roosevelt Johnson** *National Science Foundation*

Buckingham Lecture

Session Chairman: **Peter Politzer**, *University of New Orleans*

David Buckingham
University of Cambridge

Polarizability and Hyperpolarizability

2nd Session

Session Chairman: **Andrzej Wierzbicki**, *University of South Alabama*

David A. Case
The Scripps Research Institute

Macromolecular Simulations Using Continuum Solvent Models

Andreas Klamt
COSMOlogic

COSMOtherm: The Bridge between Quantum Chemistry and Fluid Phase Thermodynamics

3rd Session

Session Chairman: **Jan Labanowski**, *Ohio Supercomputer Center*

Roberto Car
Princeton Materials Institute
Princeton University

First-principles Molecular Dynamics: Current Achievements and Perspectives

Yuko Okamoto
Institute for Molecular Science

Free Energy Calculations in Protein Folding by Generalized-Ensemble Simulations

4th Session

Session Chairman: **Eric Fisher**, *University of Illinois at Springfield*

Jean-Marie André
University of Namur

Does Deterministic Chaos Play a Role in Chemistry?

Piotr Piecuch
Michigan State University

Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods

5th Session

Session Chairman: **Jerome Karle**, *Naval Research Laboratory*

Peter J. Rossky
University of Texas

The Coupling of Environmental and Electronic Dynamics in Excited State Relaxation

Srinivasan Iyengar / **Gregory A. Voth**
University of Utah

Atom-centered Density Matrix Propagation (ADMP): A New Approach to *ab initio* Molecular Dynamics

6th Session

Session Chairman: **Jiande Gu**, *Chinese Academy of Sciences*

Kwang Soo Kim
Center for Superfunctional Materials

De novo Design of Functional Nano-materials and Molecular Devices

Margaret Hurley
US Army Research Laboratory

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