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Parallel Quantum Solutions

Current Trends in Computational Chemistry 2001

Jackson, Mississippi
November 1-3, 2001





Conference

Agenda

Current Trends in Computational Chemistry 2001

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November 1-3, 2001



Thursday, November 1

12:00 - 6:00	Registration	
2:00 - 2:30	Opening Ceremony	
2:30 - 4:30	1st Session (S1)	3 Talks
4:30 - 4:50	Coffee Break	
4:50 - 6:00	2nd Session (S2)	2 Talks
6:00 - 8:00	First Poster Session (P1)	
8:00 - 8:30	Cocktails	
8:30 - 11:00	Banquet	Speaker: Dr. Walter Hollis, Deputy Under Secretary of the Army

Friday, November 2

8:00 - 9:00	Breakfast	
8:30 - 12:00	Registration	
2:00 - 4:00		
9:00 - 10:45	3rd Session (S3)	3 Talks
10:45 - 11:05	Coffee Break	
11:05 - 12:50	4th Session (S4)	3 Talks
12:50 - 1:05	Group Picture	
1:05 - 2:40	Lunch	
2:40 - 3:50	5th Session (S5)	2 Talks
3:50 - 4:10	Coffee Break	
4:10 - 5:20	6th Session (S6)	2 Talks
6:30 - 8:00	Dinner	
9:00 - 11:00	Second Poster Session (P2)	

Saturday, November 3

8:00 - 9:00	Breakfast	
8:30 - 12:00	Registration	
9:00 - 10:45	7th Session (S7)	3 Talks
10:45 - 11:05	Coffee Break	
11:05 - 12:15	8th Session (S8)	2 Talks
12:15 - 2:00	Lunch	
2:00 - 3:10	9th Session (S9)	2 Talks
3:10 - 3:40	Coffee Break	
3:40 - 4:50	10th Session (S10)	2 Talks
5:30 - 7:30	Third Poster Session (P3)	
8:00 - 11:00	Dinner	
	After Dinner Noble Lecture Series	Speaker: Dr. Herbert Hauptman
	Best Student Poster Award Presentation	

Thursday Sessions

1st Session

Session Chairman: **Cary F. Chabalowski**, *US Army Research Laboratory*

John A. Pople

Northwestern University

Theoretical Chemical Models for 3rd Row Elements

Ernest R. Davidson

Indiana University

The Cope Rearrangement in Theoretical Retrospect

Keiji Morokuma

Emory University

Potential Energy Surfaces and Dynamics of Nonadiabatic Processes in Photodissociation and Ion-Molecule Reactions

2nd Session

Session Chairman: **Szczepan Roszak**, *Wroclaw University of Technology*

Nicholas C. Handy

Cambridge University

Exchange and Correlation in Density Functional Theory

Jean-Louis Rivail

Université Henri Poincaré

Liquid State Quantum Chemistry, More on Continuum Models

Friday Sessions

3rd Session

Session Chairman: **Xavier Assfeld**, *Université Henri Poincaré*

Henry F. Schaefer III
University of Georgia

Radical Anions of DNA Base Pairs

Jack Simons
University of Utah

Unusual Negative Molecular Ions and Dianions and
Chemical Bonds Involving Rydberg Orbitals

Istvan Hargittai
*Budapest University of
Technology*

Shifting Balance Between Computation and Experiment

4th Session

Session Chairman: **Jane Murray**, *University of New Orleans*

Peter Pulay
University of Arkansas

Local Electron Correlation

Clifford Dykstra
Indiana University

Intermolecular Electrical Effects

J.V. Ortiz
Kansas State University

A Trajectory of Electron Propagator Theory

5th Session

Session Chairman: **Eric Perpete**, *Facultés Universitaires Notre-Dame de la Paix*

William H. Miller
*University of California at
Berkeley*

Using Semiclassical Theory to Add Quantum Effects to
Classical Molecular Dynamics Simulations

Donald Truhlar
University of Minnesota

Reaction Kinetics by Direct Dynamics

6th Session

Session Chairman: **Mihail Atanasov**, *Philipps-Universität Marburg*

William Jorgensen
Yale University

Computational Studies for Protein-Ligand Binding and Drug
Design

Harold Scheraga
Cornell University

Search for an Efficient Global Optimization Procedure for
Protein Folding

Saturday Sessions

7th Session

Session Chairman: **Ilya Kaplan**, *Kansas State University*

Krishnan Raghavachari
Agere Systems

Electronic Structure Studies of Semiconductor Surface Chemistry

George C. Schatz
Northwestern University

Electrodynamics of Metal Nanoparticles and Nanostructured Materials

Gernot Frenking
Philipps-Universität Marburg

Insight into the Chemical Bond of Transition Metal Complexes

8th Session

Session Chairman: **Roberto Cammi**, *Università degli Studi di Parma*

Yasuyuki Ishikawa
University of Puerto Rico

Relativistic Many-Body Perturbation Theory for Many-Electron Systems

Andrzej Sadlej
Nicolaus Copernicus University

Let's Go Relativistic Once Again: Interactions Between Relativistic Subsystems

9th Session

Session Chairman: **Alejandro Toro-Labbe**, *Pontificia Universidad Católica de Chile*

Peter Politzer
University of New Orleans

Computational Characterization of Energetic Materials

Joseph S. Francisco
Purdue University

The Atmospheric Chemistry of Halogens: Insights from Computational Chemistry

10th Session

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

Kimihiko Hirao
University of Tokyo

Research Activities of Theoretical Chemistry Group at the University of Tokyo: Recent Advances in Multireference Based Perturbation Theory and Relativistic Molecular Theory

William Lester, Jr.
University of California at Berkeley

Overview of Quantum Monte Carlo Developments for the Past Decade



Abstracts
*of oral & poster
presentations*

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