Schedule of Events

Thursday, June 15

4:00-8:00 P.M.	Registration, Lobby of the Physics Research Building
6:00-8:00 P.M.	Poster Session A, Lobby of Physics Research Building Pizza and soft drinks will be served.

Friday, June 16

8:45-8:55 A.M.	Welcoming Remarks
8:55-10:20 A.M.	Talk Session 1, Christopher M. Hadad, presiding
10:20-10:50 A.M.	Coffee break
10:50-11:50 A.M.	Talk Session 2, Jean M. Standard, presiding

LUNCH BREAK – Information about places to eat lunch can be found at the end of the program

1:20-2:45 P.M.	Talk Session 3, Xiche Hu, presiding
2:45-3:15 P.M.	Coffee break
3:15-4:30 P.M.	Talk Session 4, Lichang Wang, presiding
4:30-6:00 P.M.	Free time
6:00-10:00 P.M.	Reception, Conference Dinner and Poster Session B, Fawcette Center, Olentangy River Road

Saturday, June 17

8:45-10:25 A.M.	Talk Session 5, H. Bernhard Schlegel, presiding
10:25-10:55 A.M.	Coffee break
10:55-11:55	Talk Session 6, Srinivasan S. Iyengar, presiding

LUNCH BREAK

1:20-2:45	Talk Session 7, John M. Herbert, presiding

All of the talks will be given in 1000 McPherson Laboratory

Abstracts for Invited and Contributed Talks

Talk Session 1

Friday, June 16, 8:45 A.M. – 10:20 A.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – Christopher M. Hadad, The Ohio State University

8:45-8:55 Welcoming Remarks
Anne B. McCoy, Organizer
Prabir K. Dutta, Chair Department of Chemistry, Ohio State

8:55-9:35 T1-1 INVITED LECTURE
Current-driven dynamics in molecular-scale electronics
Tamar Seideman, Northwestern University

9:35-9:50 T1-2
Surface enhanced Raman scattering (SERS) for pyridine on gold clusters
Christine M. Aikens and George C. Schatz, Northwestern University

9:50-10:05 T1-3
Description of Phosphate Hydrolysis Reactions with QM/MM Methods and the SCC-DFTB Model
Yang Yang and Qiang Cui, University of Wisconsin-Madison

10:05-10:20 T1-4
Computation of the NMR chemical shift of single-walled carbon nanotubes
Jochen Autschbach, SUNY Buffalo

Talk Session 2

Friday, June 16, 10:50 A.M. – 11:50 A.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – Jean M. Standard, Illinois State University

10:50-11:05 T2-1
Molecular Dynamics Simulations of the Hydrolysis of Paraoxon by Phosphotriesterase Uning Combined QM/MM Potentials.
Kin-Yiu Wong and Jiali Gao, University of Minnesota, Twin Cities

11:05-11:20 T2-2
Computational studies of metalla crown ethers via GridChem
Scott R. Brozell and Sudhakar Pamidighantam
Ohio Supercomputer Center

11:20-11:35 T2-3
Computational Binding Free Energy Analysis of HIV-1 Protease-Inhibitor Complexes
Kitiyaporn Wittayanarakul,[1,2] Pornthep Sompornpisut,[1] Supot Hannongbua[1] and Michael Feig[2]
(1) Chulalongkorn University and (2) Michigan State University

11:35-11:50 T2-4
Synthesis of molecular hydrogen in the interstellar medium
Herma M. Cuppen and Eric Herbst, The Ohio State University

Talk Session 3

Friday, June 16, 1:20 P.M. – 2:45 P.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – Xiche Hu, University of Toledo

1:20-2:00 T3-1 INVITED LECTURE
Studies of long-range proton transfers in biomolecules with QM/MM methods
Qiang Cui, University of Wisconsin-Madison

2:00-2:15 T3-2
Applying Molecular Dynamics to Understand Signal Transduction: Recognition of TRPC6 by FKBP12
Peng Tao, John C. Hackett and Christopher M. Hadad
The Ohio State University

2:15-2:30 T3-3
PH_3 Adsorption on In-rich Indium Phosphide Surfaces: Evidence of Stable Dative Bond Formation at RT
Ujjal Das and Krishnan Ravhavachari, Indiana University

2:30-2:45 T3-4
Effective Fragment Potential: A General Approach to Intermolecular Interactions: Theory and Applications to π–π bonding
Lyudmila V. Slipchenko, Toni Smith and Mark S. Gordon
Iowa State University

Talk Session 4

Friday, June 16, 3:15 P.M. – 4:30 P.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – Lichang Wang, Southern Illinois University, Carbondale

3:15-3:30 T4-1
Large Amplitude Quantum Mechanics in Polyatomic Hydrides: A Particle on a Sphere Model for XH_n
Michael P. Deskevich and David J. Nesbitt, University of Colorado/ JILA

3:30-3:45 T4-2
Computing Spectroscopic Properties from Quantum Wavepacket *Ab Initio* Dynamics Simulations
Isaiah C. Sumner, Jacek Jakowski and Srinivasan S. Iyengar
Indiana University

3:45-4:00 T4-3
Accurately solving the electronic Schrödinger equation of small atoms and molecules using explictily correlated (r_{12}-) multi-reference methods
Robert J. Gdanitz, North Carolina A&T State University

4:00-4:15 T4-4
Single Molecule Transistors: a computational study of gating field and contact geometry effects
Trilisa M. Perrine and Barry D. Dunietz, University of Michigan

4:15-4:30 T4-5
Testing the two-state model of nanoconfined solvents: The conformational equilibrium of ethylene glycol in amorphous silica pores
Tolga S. Gulmen and Ward H. Thompson, University of Kansas

Conference Dinner, Reception and Poster Session B

Fawcette Center for Tomorrow
2400 Olentangy River Road

6:00-6:30	Cash bar and reception
6:30-7:30	Dinner
7:30	INVITED TALK
	Zigs and Zags in Quantum Chemistry
	Russell M. Pitzer, The Ohio State University

Followed by the poster session. Please plan to put up your posters before dinner. The listing of the posters can be found after this section.

Zigs and Zags in Quantum Chemistry

Russell M. Pitzer
Department of Chemistry
The Ohio State University
Columbus, Ohio 43210

In the application of quantum mechanics to chemistry, many approaches have been put forward over the years. Some have developed usefully and others have foundered. The availability of substantial computers starting in the 1960s had a huge influence on the field. The path to the most used types of computational theories done today has by no means been a straight one. At Ohio State a mythical figure named Chemman protects all graduate students from dangers such as dead-end projects.

Talk Session 5

Saturday, June 17, 8:45 A.M. – 10:25 A.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – H. Bernhard Schlegel, Wayne State University

8:45-9:25 T5-1 INVITED LECTURE
Quantum Monte Carlo: Higher Accuracies for Larger Systems
James B. Anderson, Pennsylvania State University

9:25-9:40 T5-2
DFT study of Carbohydrates: A comparison between the epimers of glucose
Udo Schnupf, J. L. Willett and Frank A. Momany, USDA/NCAUR/ARS

9:40-9:55 T5-3
Structure and spectroscopy of hydrated-electron clusters
John M. Herbert, The Ohio State University

9:55-10:10 T5-4
Polynitrogen Species: Fuel or Fizzle?
Jonathan M. Mullin and Mark S. Gordon, Iowa State University

10:10-10:25 T5-5
Quantum Wavepacket *Ab Initio* molecular dynamics: an approach for quantum dynamics in large systems
Jacek Jakowski, Isaiah Sumner, Xiaohu Li and Srinivasan S. Iyengar
Indiana University

Talk Session 6

Saturday, June 17, 10:55 A.M. – 11:55 A.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – Srinivasan S. Iyengar, Indiana University

10:55-11:10 T6-1
Indentification of Active Species in Ti-doped Sodium Aluminum Hydride Surfaces
Jianjun Liu and Qingfeng Ge, Southern Illinois University, Carbondale

11:10-11:25 T6-2
Theoretical Treatment of π–π Stacking Interactions in Ligand-Protein Complexs
Xiche Hu, Hui Yang and Yaohua Han, University of Toledo

11:25-11:40 T6-3
Vibrational spectra of methyl-terminated silicon (111) survaces using cluster models as well as periodic unit cells
Glen A. Ferguson and Krishnan Raghavachari, Indiana University

11:40-11:55 T6-4
Theory of Current-Induced Dynamics in Molecular Junctions
Ryan P. Jorn and Tamar Seideman, Northwestern University

Talk Session 7

Saturday, June 17, 1:20 P.M. – 2:45 P.M.
1000 McPherson Laboratory, 140 West 18th Ave.

Session Chair – John M. Herbert, The Ohio State University

1:20-2:00 T7-1 INVITED TALK
On the Role of Electrostatics and Polarization in Water Models
Kenneth D. Jordan, Albert DeFusco, Jun Cui and Thomas Sommerfeld
University of Pittsburgh

2:00-2:15 T7-2
Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice
Chris Knight and Sherwin J. Singer, The Ohio State University

2:15-2:30 T7-3
Entanglement and Electron Correlation in Quantum Chemistry Calculations
Sabre Kais, Purdue University

2:30-2:45 T7-4
Completely Renormalized Coupled-Cluster and MRCI Studies of the Thermal Stereomutations of Cyclopropane
Armagan Kinal, Michael J. Mcguire, Marta Wloch and Piotr Piecuch, Michigan State University

Abstracts for Poster Presentations in Poster Session A

Poster Session A

PA-1 DNA binding drugs by intercalation – molecular modeling study

Mircea N. Barbuceanu and L. E. Vijan, University of Pitesti

PA-2 Parameterization of Atomic Two-Body and Three-Body Potentials using Evolutionary Strategies

Brian C. Barnes and Lev D. Gelb, Washington University in St. Louis

PA-3 Adjustments to the Potential Surface of Ozone

Andrew E. Berke, Grand Valley State University

PA-4 Exploration of hydrogen transfer and dissociation mechanisms of Al_2H_4
Catherine J. Che, Jianjun Liu and Qingfeng Ge, Southern Illinois University, Carbondale

PA-5 NO_2 on Bare and Al_2O_3-supported BaO (100) Clusters: A First Principles Study

Lei Cheng and Qingfeng Ge, Southern Illinois University, Carbondale

PA-6 Simulations of Neutral and Protonated Water Clusters with the SCC DFTB Electronic Structure Method: applications to $(H_2O)_{21}H^+$, $(H_2O)_{22}H^+$, and $(H_2O)_8$

Tae Hoon Choi and Kenneth D. Jordan, University of Pittsburgh

PA-7 Multireference configuration interaction claculations for the $F(^2P) + HCl \rightarrow HF + Cl(^2P)$ reaction: a correlation scaled ground state ($1^2A'$) potential energy surface

Michael P. Deskevich and David J. Nesbitt, JILA and University of Colorado

PA-8 Density Functional Calculations on 3-Hydroxykynurenine

Brendan C. Dutmer and Thomas M. Gilbert, Northern Illinois University

PA-9 On the nature of the $(H_2O)_7^-$ cluster

Li Feng and Kenneth D. Jordan, University of Pittsburgh

PA-10 Efficient quantum chemical modeling of silicon and silicon oxide surface chemistry using pseudoatoms

Ryan D. Fenno, Hrant P. Hratchian and Krishnan Raghavachari, Indiana University-Bloomington

PA-11 On the keto-enol tautomerization of malonaldehyde

Mark A. Freitag, Trenton L. Pruden, David R. Moody, James T. Parker and Marcel Fallet, Creighton University

PA-12 Exploring ABAD/Ligand Interactions with MD Simulation

Xiaoxia Ge, Weill Medical College of Medical Science, Cornell University

PA-13 Computational Chemistry Grid: Production Cyberinfrastructure for Computational Chemistry

James E. Giuliani, Ohio Supercomputer Center

PA-14 Nanoscale confined light: metal nanoparticles,thin films and nanoholes

Tae-Woo Lee,[(a)] Xiwen Wang,[(b)] George C. Schatz[(b)] and Stephen K. Gray, [(a)] (a)Argonne National Laboratory and (b)Northwestern University

PA-15 A Model for the Water-Amorphous Silica Interface

Ali A. Hassanali and Sherwin J. Singer, The Ohio State University

PA-16 Spectroscopic and Computational Studies of the Non-Aqueous Solvation of n-Octanol and Ethanol

Carrigan J. Hayes Lori M. Levering, Karen M. Callahan, Heather C. Allen and Christopher M. Hadad, The Ohio State University

PA-17 The effect of dynamics, temperature and nuclear quantum effects on the spectroscopy of small and medium sized clusters

Yong He, Xiaohu Li, Virginia Teige and Srinivasan S. Iyengar
Indiana University

PA-18 Diffusion Monte Carlo studies of CH_5^+ structure

Charlotte E. Hinkle and Anne B. McCoy, The Ohio State University

PA-19 Theoretical Studies on Hydrogen-bonding in $X^-(H_2O)$ (X = F, Cl and Br)

Samantha Horvath and Anne B. McCoy, The Ohio State University; Joseph R. Roscioli and Mark A. Johnson, Yale University

PA-20 Including Anharmonicity in the Calculation of Rate Constants. 2. The $OH+H_2$ Reaction

Alan D. Isaacson, Miami University

PA-21 Quantum Wavepacket *Ab Initio* Molecular Dynamics: efficient quantum dynamics for large systems through time-dependent, deterministic sampling

Jacek Jakowski, Isaiah Sumner, Xiohu Li and Srinivasan S. Iyengar
Indiana University

PA-22 Ab-Initio Studies of the Geometries and Vibrational spectra of $NH_4^+(H_2O)_{4-6}$ Clusters

Glen R. Jenness and Kenneth D. Jordan, University of Pittsburgh

PA-23 Development of an Open Shell Effective Fragment Potential

Daniel D. Kemp and Mark S. Gordon, Iowa State University

PA-24 Time-dependent density functional theory modeling of the chiroptical properties of aromatic amino acids in solution

Matthew D. Kundrat and Jochen Auschbach, SUNY at Buffalo

PA-25 The Transferability of Aromaticity Between Aromatic and Antiaromtic Rings Connected by Hydrocarbon Chains

Daniel B. Lawson, University of Michigan-Dearborn

PA-26 Energy gradients in combined quantum mechanics, effective fragment potential and polarizable continuum model calculations

Hui Li and Mark S. Gordon, Iowa State University

PA-27 A theoretical study of the irreversible inhibition of matrix metalloproteinases

Jie Li, Thom Vreven, Sammy O. Meroueh, Sharhriar Mobashery and H. Bernhard Schlegel, Wayne State University

PA-28 Dynamics Within the Hydration Layer Surrounding a Protein: Origin of Slow Relaxation Dynamics

Tanping Li, Ali A. Hassanali, Dongping Zhong and Sherwin Singer
The Ohio State University

PA-29 Development of symmetry-adapted ab initio quantum wavepacket dynamics for condensed matter systems

Xiaohu Li and Srinivasan S. Iyengar, Indiana University-Bloomington

PA-30 Molecular Dynamics Simulations on the Amonium/Ammonia transport protein AmtB

Yuchun Lin and Yirong Mo, Western Michigan University

PA-31 Linear Bis(cyclopentadienyl) Actinide Complexes: A new class of organoactinides

Michael K. Mrozik,[1] Jason L. Sonnenberg,[2] Jaqueline L. Kiplinger and Bruce E. Bursten,[4] (1) The Ohio State University, (2) Wayne State University, (3) Los Alamos National Laboratory, (4) University of Tennessee

Abstracts for Poster Presentations in Poster Session B

Poster Session B

PB-1 Effect of Ti on hydrogen interaction in Ti-doped $LiBH_4$: A first principles study

Jianjun Liu and Qiangfeng Ge, Southern Illinois University, Carbondale

PB-2 Non-iterative Coupled-Cluster Methods Employing Multireference Perturbation Theory Wave Functions

Maricris D. Lodriguito, Marta Wloch and Piotr Piecuch,
Michigan State University

PB-3 *Ab initio* direct dynamics trajectory study of the $F^- + CH_3OOH$ reaction

Jose G. Lopez, Grigoriy Vayner, U. Lourderaj and William L. Hase Texas Tech; Theresa L. Windus and Wibe A. deJong, Pacific Northwest National Lab

PB-4 *Ab initio* study of carbon chains

Helena Masso,[(a)] Maria Luisa Senent,[(a)] Javier Goicoechea,[(a)] Jose Cernicharo,[(a)] Mahdi Hochlaf,[(b)] Pavel Rosmus,[(b)] Valera Veryazov,[(c)] Per-Ake Malmqvist,[(c)] and Bjorn Roos, (a) CSIC, Serrano, (b) Universite de Marne la Vallee, (c) Lund University.

PB-5 Structure and stability of the $(H_2O)_{21}$ and $(H_2O)_{20}H_2S$ clusters: Relevance of cluster systems to gas hydrate formation

Valerie N. McCarthy and Kenneth D. Jordan, University of Pittsburgh

PB-6 Simulation of Quantum Dynamics Under Chirped Laser Pulses

Porscha L. McRobbie, University of Michigan

PB-7 A Computational Study of Carbon Acid-Catalyzed Friedel-Crafts Acylation

Katie R. Mitchell-Koch, Mikhail V. Barybin and Ward H. Thompson, University of Kansas

PB-8 A Molecular-Level Perspective on Vibrational Dynamics in Liquids

Christine Morales and Ward H. Thompson, University of Kansas

PB-9 Calculation of Low-Lying Excited States of PaO^+ and PuO^+

Michael K. Mrozik,[(a)] Russel M. Pitzer[(a)] and Bruce E. Bursten,[(b)] (a) The Ohio State University, (b) University of Tennessee

PB-10 Molecular dynamics simulations of the coalescence of iridium clusters

Tiffany L. Pawluk and Lichang Wang, Southern Illinois University, Carbondale

PB-11 Spectroscopic Comparisons of Helium-Dihalogen Complexes: What Dictates the Spectral Structure?

Sara E. Ray and Anne B. McCoy, The Ohio State University

PB-12 Computational studies on the mechanism of human tyrosyl phosphodiesterase

Brooke E. Richardson and Alan C. Goren, Transylvania University

PB-13 Oxidative Dehalogenation of Perhalogenated Benzenes by Cytochrome P450

John C. Hackett, Toby T. Sanan and Christopher M. Hadad,
The Ohio State University

PB-14 Theoretical study of complex forming $CH+H_2 \rightarrow CH_2+H$

Jordi Mayneris,[1,2] Amaia Saracibar,[3,4] Evelyn Goldfield,[3] Miguel Gonzalez,[2] Ernesto Garcia,[4] and Stephen K. Gray[1], (1) Argonne National Laboratory, (2) Universitat de Barcelona, (3) Wayne State University, (4) Universidad del Pais Vasco

PB-15 Very Large Scale CI Calculations Using Nonlinear Basis Functions

Ron L. Shepard, Argonne National Laboratory

PB-16 Molecular Simulations of Electrokinetically Driven Nanofluidic Phenomena

Yun Kyung Shin, Ali Hassanali and Sherwin J. Singer, The Ohio State University

PB-17 The Jahn-Teller Effect in the Ground and Excited States of the Tropyl Radical

Ilias Sioutis, Vadim L. Stakhursky, Gyorgy Tarczay and Terry A. Miller
The Ohio State University

PB-18 A Numerical Simulation of Nonadiabatic Electron Excitation in the Strong-Field Regime III. Polyacenes

Stanley M. Smith,[1] Xiaosong Li,[2] Alexei Markevitch,[3] Dmitri Momanov,[3] Robert J. Levis[3] and H. Bernhard Schlegel,[1] (1) Department of Chemistry, Wayne State University, (2) University of Washington, (3) Temple University

PB-19 Reactive potential energy surfaces built using distributed Gaussians

Jason L. Sonnenberg and H. Bernhard Schlegel, Wayne State University

PB-20 Structures of Undecagold Clusters: Ligand Effect

Kasi L. Spivey, Joseph I. Williams and Lichang Wang,
Southern Illinois University-Carbondale

PB-21 DFT Studies of Small Cu Clusters

Brian A. Stachowiak, Chasity B. Love and Lichang Wang
Southern Illinois University, Carbondale

PB-22 Computational studies of the Interaction of Sulfur Oxides with Ice Surfaces

Jean M. Standard, and Mary T. Van Der Hoven, Illinois State University, Normal

PB-23 Calculational Study on the Reduction of Nitro Aromatic Derivatives

Zhenjiao Tian and Christopher M. Hadad, The Ohio State University

PB-24 Quantum Chemical Studies of Phenol Oxidation using Co(salen) and Co(acacen) Catalysts

Kumar Vanka and Ward H. Thompson, University of Kansas

PB-25 Calculation of quantum mechanical time correlation functions in liquids via semiclassical methods

Francisco X. Vazquez and Eitan Geva, University of Michigan

PB-26 Initiating the Cl + HCl hydrogen exchange reaction by vibrational excitation of the HCl molecule

Gé W. M. Vissers and Anne B. McCoy, The Ohio State University

PB-27 DFT Studies of PtVFe Nanoparticles

Joseph I. Williams, and Lichang Wang, Southern Illinois University, Carbondale

PB-28 Experimental and Computational Studies of Tetrathiatriarylmethyl Radicals

Shijing Xia, Frederick A. Villamena, Jay L. Zweier and Christopher M. Hadad,
The Ohio State University

PB-29 Quantum Chemical Calculations of Intermolecular Interactions in Protein-Ligand Complexes

Hui Yang, Yaohua Han and Xiche Hu, University of Toledo

PB-30 The Water-Carbon Dioxide Interface Under Sub-Critical Conditions: A Molecular Simulation Study

Hui Zhang and Sherwin J. Singer, Ohio State University

PB-31 Exploring the quantum dynamics of the dissociative photodetachment of $(HOCO)^-$

Shesheng Zhang,[(a)] Dmitry M. Medvedev,[(b)] Evelyn M. Goldfield[(a)] and Stephen K. Gray[(b)], (a) Wayne State University, (b) Argonne National Laboratory

PB-32 Beta-peptide: from structure to phase behavior

Xiao Zhu, Arun Yethiraj and Qiang Cui, University of Wisconsin-Madison