PHYS

DIVISION OF PHYSICAL CHEMISTRY

Final Program, 222nd ACS National Meeting --Chicago, Illinois-- August 26-30, 2001

R. M. Stratt, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

QM/MM Methods (see *Division of Computers in Chemistry* , Sun, Mon, Tue, Wed, page X)

Radiation Research: From the Science Laboratory to the Real World (see *Division of Chemical Education* , Tue, Wed, Thu, page X)

State of the Art: Semiconductor and Metal Nanoparticles for Light Energy Conversion (see *Division of Chemical Education* , Mon, Tue, page X)

Rowland Award Symposium (see *Division of Nuclear Chemistry & Technology* , Mon, Tue, Wed, page X)

(see *Division of Polymer Chemistry* , , page X)

Three-Dimensional Silicon-Oxygen Cages (polyhedral oligomeric silsesquioxanes, POSS): Materials for the 21st Century (see *Materials Chemistry Secretariat* , Sun, Mon, Tue, page X)

Three Dimensional Silicon-Oxygen Cages (Polyhedral Oligomeric Silsesquioxanes): Materials for the 21st Century (see *Division of Polymer Chemistry* , Tue, page X)

SOCIAL EVENT:
Social Hour: Wed

BUSINESS MEETING: Sun

SUNDAY MORNING

Section A

Unknown Site
Unknown Room

What Can We Really Learn About Condensed Phases from Clusters?

Solvation Effects on Molecular and Electronic Structure (Spectroscopy)

B. C. Garrett and D. Ray, *Organizer*
T. S. Zwier, *Presiding*

8:00 — 1. Cluster spectroscopy and its molecular-scale insight to solvation effects. **T. S. Zwier**

8:20 — 2. Incipient charge redistribution in clusters: An exploratory study. **D. W. Pratt**

9:00 — 3. Probing the solvation of complex and multiply charged anions in the gas phase using photodetachment photoelectron spectroscopy. **L. Wang**, X. Wang, X. Yang

9:40 — 4. Selective interactions in cluster ion complexes. **J. M. Lisy**, C. A. Corbett, B. Forinash

10:00 — Intermission.

10:20 — 5. Comparison of excess electron relaxation dynamics in water and water clusters. **M. Johnson**

11:00 — 6. Ice particles: Surface properties and interactions with adsorbates. **V. Buch**, J. P. Devlin, N. Uras, J. Sadlej

11:40 — 7. Heterogeneous effects in liquid structure and dynamics. **J. Cao**

Section B

Unknown Site
Unknown Room

Computational Chemistry in the Undergraduate Curriculum

I

Cosponsored with Division of Chemical Education, and Division of Computers in Chemistry
H. Jonsson, *Organizer*
F. Rioux, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:40 — 8. Computational chemistry, broadly defined, across the undergraduate curriculum **W. F. Coleman**

9:20 — 9. Computational chemistry in the undergraduate curriculum: Dreams and practice. **T. J. Zielinski**

10:00 — Intermission.

10:20 — 10. Computational methods throughout the curriculum at Duquesne University. **J. D. Madura**

11:00 — 11. WebMO: Visualizing computational chemistry on the world wide web. **W. F. Polik**, J. R. Schmidt

11:40 — 12. From wetlabs to weblabs: Enhancing learning in Physical Chemistry labs using the web. **T. K. Whittingham**, R. J. Magyar, K. Burke

Section C

Unknown Site
Unknown Room

Molecular Electronics

Molecular Nanostructures I

P. Avouris, *Organizer*
M. A. Ratner, *Organizer, Presiding*

8:20 — 13. Current flow in molecular nanostructures. **S. Datta**, A. W. Ghosh, P. Damle

9:00 — 14. Carbon nanoelectronics. **P. L. McEuen**

9:40 — 15. High efficiency electrophosphorescent OLEDs. **P. I. Djurovich**, V. Adamovich, M. E. Thompson, C. Adachi, M. A. Baldo, S. R. Forrest, R. C. Kwong

10:00 — Intermission.

10:20 — 16. Long-range energy and electron transfer in oligomers, on surfaces, and in films M. Sykora, S. Trammell, J. Yang, C. Fleming, J. Papanikolas, **T. J. Meyer**

11:00 — 17. Molecular electronics circuitry and scaling. **J. Heath**, M. Diehl, K. Nielson, F. Stoddart, Y. Luo, A. Star, J. Jeppesen

Section D

Unknown Site
Unknown Room

Three-Dimensional Silicon-Oxygen Cages: Materials for the 21st Century

Cosponsored with Division of Inorganic Chemistry, Division of Polymer Chemistry, and Materials Chemistry Secretariat
M. S. Gordon and M. Banaszak Holl, *Organizer*
M. Banaszak Holl, *Organizer, Presiding*

8:20 — 18. Ab initio study of silsesquioxanes. **T. Kudo**, M. S. Gordon

9:00 — 19. First principles study of silsesquioxanes. **R. Pandey**

9:40 — 20. Conformations of POSS monomers in the gas phase. **M. T. Bowers**

10:20 — Intermission.

10:40 — 21. Nuclear quantum effects in hydrogen transfer reactions for the synthesis of polyhedral oligomeric silsesquioxanes. **S. Hammes-Schiffer**, S. P. Webb, T. Iordanov

11:20 — 22. Atomic hydrogen in silsesquioxane cages: Results and hypotheses. **I. Carmichael**, R. M. Macrae, M. Paech

SUNDAY AFTERNOON

Section A

Unknown Site
Unknown Room

What Can We Really Learn About Condensed Phases from Clusters?

Solvation Effects on Reactions - Reaction Dynamics, Time-Resolved Solvation

B. C. Garrett and D. Ray, *Organizer*
D. G. Truhlar, *Presiding*

1:40 — 23. Chemical dynamics in the condensed phase. **D. G. Truhlar**

2:00 — 24. What can clusters tell us about proton transport in water? **G. A. Voth**

2:40 — 25. Solvation effects on dynamics in anion clusters. **D. M. Neumark**, A. V. Davis, R. Wester, A. E. Bragg

3:20 — Intermission.

3:40 — 26. Solvent-induced dynamics in size-selected cluster anions. **W. C. Lineberger**, R. Parson, T. Sanford, M. A. Thompson, S. Y. Han, A. Sanov, N. Delaney, J. Faeder

4:20 — 27. Solvation dynamics in mixed bulk liquids and clusters. **B. M. Ladanyi**

5:00 — 28. Dynamical tests of the nucleation kinetics of water. **G. K. Schenter**, S. M. Kathmann, B. C. Garrett

Section B

Unknown Site
Unknown Room

Computational Chemistry in the Undergraduate Curriculum

II

Cosponsored with Division of Chemical Education, and Division of Computers in Chemistry
F. Rioux, *Organizer*
H. Jonsson, *Organizer, Presiding*

1:40 — 29. Using computation and visualization in physical chemistry. **M. L. Caffery**

2:20 — 30. Computational experiments in the chemistry curriculum. **Z. L. Gasyna**

3:00 — 31. Computational chemistry in the physical chemistry curriculum. **J. M. Smith**

3:20 — Intermission.

3:40 — 32. Visualizing quantum mechanics: A dynamic base for teaching chemical bonding. **R. Kosloff**, G. Ashkenazi

4:20 — 33. Integrating quantum mechanical simulations into the undergraduate chemistry curriculum. **G. Ashkenazi**, R. Kosloff

5:00 — 34. Lewis structures and localized orbitals: What is the nature of the P-O bond? **J. M. Brom**

Section C

Unknown Site
Unknown Room

Molecular Electronics

Molecular Transport I

M. A. Ratner, *Organizer*
P. Avouris, *Organizer, Presiding*

1:40 — 35. Carbon nanotube based for molecular computing. **C. M. Lieber**

2:20 — 36. Carbon nanotube field-effect transistors and logic devices. **R. Martel**, V. Derycke, J. Appenzeller, P. H. -. Wong, P. Avouris

3:00 — 37. Measuring and controlling molecular-scale properties for molecular electronics. **P. S. Weiss**, J. M. Tour, D. L. Allara

3:40 — Intermission.

4:00 — 38. Carbon nanotube molecular wires: Recent progress in synthesis, characterization and devices **H. Dai**

4:40 — 39. Carbon nanotubes as field emission device and electromechanical sensor: Results from first-principles simulations. **A. Maiti**, J. Andzelm, N. Tanpipat, P. von Allmen

Section D

Unknown Site
Unknown Room

Three-Dimensional Silicon-Oxygen Cages: Materials for the 21st Century

II

Cosponsored with Division of Inorganic Chemistry, Division of Polymer Chemistry, and Materials Chemistry Secretariat
M. Banaszak Holl, *Organizer*
M. S. Gordon, *Organizer, Presiding*

1:40 — 40. Ti-containing silsesquioxanes: NMR properties and acidity. **J. A. Tossell**

2:20 — 41. Spherosiloxane cluster-based monolayers on gold and silicon surfaces. **M. M. Banaszak Holl**, K. Nicholson, K. Schneider

3:00 — 42. Photochemistry in thin silsesquioxane films. **H. Dai**

3:40 — Intermission.

4:00 — 43. Molecular dynamics simulations of POSS-containing polymers. **B. L. Farmer**, R. J. Berry, R. K. Bharadwaj

4:40 — 44. Insertion mechanism of N_2 and O_2 into T_n(n= 8, 10, 12)-silsesquioxanes framework **B. L. Tejerina**, M. S. Gordon

MONDAY MORNING

Section A

Unknown Site
Unknown Room

What Can We Really Learn About Condensed Phases from Clusters?

Intermolecular Interactions

B. C. Garrett and D. Ray, *Organizer*
G. Scoles, *Presiding*

8:00 — 45. Overview of what we learn from clusters about the role of three-body forces in condensed matter systems. **G. Scoles**

8:20 — 46. Development of transferable interaction potentials for water: The lessons learned from clusters. **S. S. Xantheas**, C. J. Burnham

9:00 — 47. Water pair potential from spectroscopic experiments. **C. J. Leforestier**, L. B. Braly, R. S. Fellers, C. Keoshian, R. J. Saykally

9:40 — 48. Nucleation kinetics and thermodynamics: From clusters to condensed phases. **S. M. Kathmann**, G. K. Schenter, B. C. Garrett

10:00 — Intermission.

10:20 — 49. Infrared spectroscopy of complexes in helium nanodroplets: A step towards the condensed phase. **K. Nauta**, B. E. Applegate, D. T. Moore, R. E. Miller

11:00 — 50. Dynamics and reactions in water and ice. **I. Ohmine**

11:40 — 51. From water clusters to ice polymorphs. **C. J. Burnham**, S. S. Xantheas

Section B

Unknown Site
Unknown Room

Computational Chemistry in the Undergraduate Curriculum

III

Cosponsored with Division of Chemical Education, and Division of Computers in Chemistry
H. Jonsson and F. Rioux, *Organizer*
A. Grushow and M. L. Caffery, *Presiding*

8:20 — 52. Agony and ecstasy of using molecular dynamics to teach physical chemistry. **S. M. Auerbach**

9:00 — 53. Computational physical chemistry for the undergraduate curriculum: Maple-assisted applications. **M. V. Scarlete**

9:40 — 54. Computer simulations of chemical dynamics. **P. L. Holt**, **S. L. Cooke**

10:00 — Intermission.

10:20 — 55. Molecular modeling as a teaching-learning tool in organic chemistry. **G. O. Spessard**

11:00 — 56. Computational assignments in organic chemistry: An evolution. **C. P. Schaller**, K. J. Graham, J. B. Klassen

Section C

Unknown Site
Unknown Room

Molecular Electronics

Molecular Transport II

P. Avouris and M. A. Ratner, *Organizer*
R. T. Hayes, *Presiding*

8:20 — 57. Electrical conductance of individual small molecules. **N. D. Lang**, P. Avouris

9:00 — 58. Microscopic switching of a molecular memory device. **D. Tomanek**

9:40 — 59. Molecular switch strategies for covalently linked trichromophoric systems based on photoinduced electron and triplet-triplet energy transfers. **R. T. Hayes**, M. R. Wasielewski

10:00 — Intermission.

10:20 — 60. Conformational changes, charging, and electrical conduction in molecular wires **G. Kirczenow**, E. Emberly

11:00 — 61. Toward single-molecule electronic devices. **J. Michl**, T. F. Magnera, J. R. Smith, J. Pecka, A. Reisinger, M. Trujillo, J. R. Miller, J. P. Kirby

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Ionization

S. L. Guberman, *Organizer*
M. R. Flannery, *Presiding*

8:05 — Introductory Remarks.

8:20 — 62. State-selected associative ionization as a probe of the molecular dissociative channels. **X. Urbain**

9:00 — 63. Associative ionization with cold atoms. **O. Dulieu**

9:20 — 64. Molecular autoionization and predissociation as "Inverse" dissociative recombination. **R. N. Zare**, I. M. Konen, R. Zhao

10:00 — Intermission.

10:20 — 65. Mode-dependent vibrational autoionization in ammonia. **S. T. Pratt**, J. A. Bacon, C. A. Raptis

11:00 — 66. Impulsive photodissociation dynamics. **R. Kosloff**

11:30 — 67. Dissociative recombination of slow electrons and molecular oxygen ions in the strong laser field. **M. G. Golubkov**, G. V. Golubkov, A. N. Romanov

Section E

Unknown Site
Unknown Room

Signal Processing in Chemistry

Methods of Spectral Analysis

V. Mandelshtam and A. J. Shaka, *Organizer*
J. C. Hoch, *Presiding*

8:30 — Introductory Remarks.

8:40 — 68. Fourier analysis by maximum entropy. **R. Silver**

9:20 — 69. Filter-Diagonalization for chemistry. **D. Neuhauser**, S. Anderson

10:00 — 70. RRT: The Regularized Resolevent Transform for high resolution spectral analysis. **J. Chen**, A. J. Shaka, V. A. Mandelshtam

10:20 — Intermission.

10:40 — 71. New methods of signal processing with application to theoretical and experimental signals arising in chemical studies. **H. S. Taylor**

11:20 — 72. Recent advances in multiscale signal/image representation. **D. Donoho**

Three-Dimensional Silicon-Oxygen Cages (polyhedral oligomeric silsesquioxanes, POSS): Materials for the 21st Century

I

Cosponsored with Materials Chemistry Secretariat
See Page X

State of the Art: Semiconductor and Metal Nanoparticles for Light Energy Conversion

Optical Effects in Metal Nanoparticles

Cosponsored with Division of Chemical Education
See Page X

MONDAY AFTERNOON

Section A

Unknown Site
Unknown Room

What Can We Really Learn About Condensed Phases from Clusters?

Thermodynamic Properties and Phase Transitions

B. C. Garrett and D. Ray, *Organizer*
R. S. Berry, *Presiding*

1:20 — 73. Thermodynamics of small systems: How is it different? **R. S. Berry**

1:40 — 74. Connections between structure, thermodynamics, and dynamics of finite systems and bulk material **D. J. Wales**

2:20 — 75. Melting behavior of Lennard-Jones and water clusters. **K. D. Jordan**

3:00 — 76. Symmetry in order-disorder phase changes of molecular clusters. **A. Proykova**, S. Pisov, R. S. Berry

3:20 — Intermission.

3:40 — 77. Fundamental properties of bulk water from cluster data. **J. V. Coe**

4:20 — 78. Large water clusters as a stage in the condensed phase connection. **J. P. Devlin**, V. Buch, J. Sadlej

5:00 — 79. Calorimetric properties of an interconnected array of benzene clusters. **E. Roduner**, G. Zhao, B. Gross, H. Dilger

Section B

Unknown Site
Unknown Room

Computational Chemistry in the Undergraduate Curriculum

IV

Cosponsored with Division of Chemical Education, and Division of Computers in Chemistry
F. Rioux and H. Jonsson, *Organizer*
J. D. Madura and T. J. Zielinski, *Presiding*

1:40 — 80. Introducing molecular modeling to organic, inorganic, and bio-chemists **J. H. Jensen**

2:20 — 81. Molecular modeling in the general chemistry laboratory. **M. Azam**, M. A. Parker

2:40 — 82. Computer lab exercises based on Mathematica in general chemistry. **H. Jonsson**

3:00 — Intermission.

3:20 — 83. Structure, thermodynamics, and kinetics: Computer modeling **R. L. DeKock**

4:00 — 84. Integrated computational and experimental research for honors general chemistry at Duquesne University. **J. D. Evanseck**

Section C

Unknown Site
Unknown Room

Molecular Electronics

Molecular Nanostructures II

P. Avouris and M. A. Ratner, *Organizer*
M. C. Lonergan, *Presiding*

1:40 — 85. Manipulation and analysis of DNA molecules in nanofluidic systems. **H. G. Craighead**, S. W. P. Turner, J. Han, M. Cabodi

2:20 — 86. Monodisperse nanocrystals as molecular-scale electronic building blocks. **C. B. Murray**, C. T. Black, S. Sun

3:00 — 87. Novel biosensors based on force discrimination between molecules. **R. J. Colton**, C. L. Cole, M. P. Malito, M. M. Miller, M. Natesan, M. A. Piani, P. E. Sheehan, C. R. Tamanaha, L. J. Whitman

3:40 — Intermission.

4:00 — 88. Polyelectrolyte mediated redox chemistry and interfaces between dissimilarly doped conjugated polymers. **M. C. Lonergan**, B. Langsdorf, C. Cheng

4:20 — 89. Self assembly and electrical characterization of metal nanowires for nanoscale and molecular electronics. **T. Mayer**, T. E. Mallouk, S. Goldstein, C. D. Keating, T. N. Jackson

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Molecular dissociation dynamics

S. L. Guberman, *Organizer*
A. F. Wagner, *Presiding*

1:40 — 90. Dynamics of three-body dissociative recombination of dihydrides. **S. Datz**, C. R. Vane, R. Thomas, S. Rosén, M. Larsson, W. van der Zande

2:20 — 91. Photodissociation and unimolecular dissociation of molecules. **R. Schinke**

3:00 — 92. Three body kinematical correlation in the dissociative recombination of H_3^+. **D. Zajfman**, D. Strasser, L. Lammich, S. Krohn, M. Lange, H. Kreckel, J. Levin, D. Schwalm, A. Wolf

3:40 — Intermission.

4:00 — 93. Molecular photodissociation and dissociative recombination. **G. G. Balint-Kurti**, J. N. Harvey, A. Brown

4:40 — 94. Electronic accessibility of product channels in photodissociation: Implications for dissociative recombination processes. **L. J. Butler**

Section E

Unknown Site
Unknown Room

Signal Processing in Chemistry

Quantum Dynamics and Control

A. J. Shaka, *Organizer*
V. Mandelshtam, *Organizer, Presiding*

1:40 — 95. Optimal Hamiltonian identification: The synthesis of quantum optimal control and inversion. **H. Rabitz**

2:20 — 96. Toward molecular logic machines using pump-probe spectroscopy. **F. Remacle**

3:00 — Intermission.

3:20 — 97. Self-adaptive filtering methods in numerical path integration. **J. D. Doll**, D. L. Freeman

4:00 — 98. New methods and applications of numerical inversion of the Laplace transform. **E. Pollak**

4:40 — 99. Spectral analysis of Chebyshev signals in calculating bound and resonance levels of polyatomic molecules. **H. Guo**

State of the Art: Semiconductor and Metal Nanoparticles for Light Energy Conversion

Semiconductor Nanostructures

Cosponsored with Division of Chemical Education
See Page X

Rowland Award Symposium

Atmospheric Chemistry I

Cosponsored with Division of Nuclear Chemistry & Technology
See Page X

MONDAY EVENING

Unknown Site
Unknown Room

Sci-Mix

R. M. Stratt, *Presiding*

8:00 - 10:00

205, 207, 213, 216-217, 221-222, 225-226, 229, 233, 237, 240, 243-245, 251-252, 255-256, 263, 266-267, 269, 273-275, 282-283, 286-287, 291, 295, 300-301, 303, 312, 314, 316, 321, 326, 330, 332, 336, 338, 343-347, 355, 357. See subsequent listings.

Clusters and Aerosols.

Gas-Phase Spectroscopy and Dynamics.

Condensed-Phase Spectroscopy and Dynamics.

Quantum Chemistry and Dynamics.

Molecular Electronics and Electronic Materials.

Colloids, Surfaces, Interfaces, and Nanoscale Materials

Biophysical Chemistry.

General Physical Chemistry.

TUESDAY MORNING

Section A

Unknown Site
Unknown Room

What Can We Really Learn About Condensed Phases from Clusters?

Properties of Solids - Evolution of the Metallic State and Crystal Growth

B. C. Garrett and D. Ray, *Organizer*
J. Jellinek, *Presiding*

8:00 — 100. Properties of solids: Evolution of the metallic state and crystal growth. **J. Jellinek**

8:20 — 101. Growth and reactivity of metals, metal compounds, and alloys: Evolution of the nanoscale and bulk condensed state **A. W. Castleman Jr.**

9:00 — 102. Understanding solids using clusters and quantum tunneling of magnetization in cluster-solids. **S. N. Khanna**

9:40 — 103. Is the stability of Mg_4 a "chemical" effect? **G. Scoles**

10:00 — Intermission.

10:20 — 104. Bond energies of molecular fragments to metal clusters. **P. B. Armentrout**, R. Liyanage

11:00 — 105. Photoelectron spectroscopy of cluster anions. **K. H. Bowen Jr.**

11:40 — 106. Electronic and structural evolution of transition metal clusters from anion photoelectron spectroscopy. **S. Liu**, H. Zhai, L. Wang

Section B

Unknown Site
Unknown Room

Computational Chemistry in the Undergraduate Curriculum

V

Cosponsored with Division of Chemical Education, and Division of Computers in Chemistry
F. Rioux and H. Jonsson, *Organizer*
W. F. Coleman and R. L. DeKock, *Presiding*

8:20 — 107. Undergraduate introduction to computational chemistry through research projects. **A. L. Parrill**, P. K. Bridson, T. R. Cundari

9:00 — 108. Using a computer to learn NMR spectroscopy. **A. Grushow**, A. J. Brandolini

9:40 — 109. Site-wide access: Computational chemistry for every undergraduate. **G. D. Purvis III**

10:00 — Intermission.

10:20 — 110. NBO 5.0: New frontiers of localized analysis for NMR properties and transition metal bonding **F. Weinhold**

11:00 — 111. Use of computers in the undergraduate physical chemistry course. **H. Metiu**

11:40 — 112. Computer-assisted learning in quantum chemistry. **F. Rioux**

Section C

Unknown Site
Unknown Room

First Principles Simulation of Chemical Dynamics

I

Cosponsored with Division of Computers in Chemistry
R. Car and T. J. Martínez, *Organizer, Presiding*

8:20 — 113. First principles dynamics related to combustion. **E. A. Carter**, R. L. Hayes, A. Andersen

9:00 — 114. Car-Parrinello simulations of the disordering of ice and dissociation of HCl, relevant to stratospheric chemistry Y. Mantz, F. M. Geiger, L. T. Molina, M. J. Molina, **B. Trout**

9:20 — 115. Modeling liquids under pressure and in a biological environment. **G. Galli**

10:00 — Intermission.

10:20 — 116. Dynamical processes of reactions, excitations, and transport in nanoscale systems: Clusters,

wires, and DNA **U. Landman**

11:00 — 117. Dynamical density functional study of the multistep CO insertion into zirconium-carbon bonds anchored to a calix[4]arene moiety. **F. De Angelis**, S. Fantacci, A. Sgamellotti, N. Re

11:20 — 118. Adsorption and diffusion at metal oxide surfaces. **A. Selloni**

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Theory

S. L. Guberman, *Organizer, Presiding*

8:20 — 119. Wave packet studies of dissociative recombination. **A. E. Orel**

9:00 — 120. Stark mixing in dissociative recombination. **M. R. Flannery**, D. Vrinceanu

9:40 — 121. Analytical treatment of the K-matrix integral equation. **H. Nakamura**

10:20 — Intermission.

10:40 — 122. Extension of the quantum defect theory and its application to electron and molecular ion collisions. **H. Takagi**

11:20 — 123. Channel mixing effects in dissociative recombination and related processes. I. F. Schneider, **A. Suzor-Weiner**

Section E

Unknown Site
Unknown Room

Signal Processing in Chemistry

NMR data processing

V. A. Mandelshtam, *Organizer*
A. J. Shaka, *Organizer, Presiding*

8:20 — 124. Practical aspects of applying linear prediction to NMR spectroscopy. **H. Gesmar**, J. J. Led

9:00 — 125. XFT: Extended Fourier Transform, multi-dimensional NMR spectral estimation **G. S. Armstrong**, V. A. Mandelshtam

9:20 — 126. Maximum Entropy processing of NMR diffusion experiments: Application to molecular interaction measurements. **M. A. Delsuc**, T. Gostan, T. E. Malliavin

10:00 — Intermission.

10:20 — 127. Constant time NMR signals processed by the Filter Diagonalization Method. **A. A. De Angelis**, J. Chen, V. A. Mandelshtam, A. J. Shaka

10:40 — 128. Nonlinearity of linear prediction. **J. C. Hoch**, A. S. Stern

11:20 — 129. "Parallel" processing of several FIDs by the filter diagonalization method: Identifying signals in noisy data. **J. E. Curtis**, V. A. Mandelshtam, A. J. Shaka

11:40 — Concluding Remarks.

Rowland Award Symposium

Nuclear and Radiochemistry I

Cosponsored with Division of Nuclear Chemistry & Technology
See Page X

State of the Art: Semiconductor and Metal Nanoparticles for Light Energy Conversion

Photochemical Solar Cells

Cosponsored with Division of Chemical Education
See Page X

TUESDAY AFTERNOON

Section A

Unknown Site
Unknown Room

What Can We Really Learn About Condensed Phases from Clusters?

Heterogeneous Catalysis

B. C. Garrett and D. Ray, *Organizer*
B. C. Gates, *Presiding*

1:40 — 130. Supported metal cluster catalysts: Progress and perspectives. **B. C. Gates**

2:00 — 131. Clusters on oxides: A coupled system. N. Nilius, N. Ernst, **H. Freund**

2:40 — 132. Density functional studies of heterogeneous catalysts by means of cluster models. **N. Rösch**

3:20 — Intermission.

3:40 — 133. How different are mechanisms of chemical reactions on atoms and clusters compared to their bulk analogs? **U. Heiz**, S. Abbet, H. Häkkinen, U. Landman, G. Pacchioni

4:20 — 134. Nanocluster catalyzed reactions. **H. Hakkinen**, U. Landman

5:00 — 135. Band gap evolution in the (MgO)n (n=1-5) clusters and instability of the polar (111) surface of MgO. **M. S. Gutowski**, P. Skurski, X. Li, L. Wang

Section B

Unknown Site
Unknown Room

Physical Chemistry of Gas-Particle Interactions

I-Overview

V. H. Grassian, *Organizer*
J. T. Roberts, *Organizer, Presiding*

1:35 — Introductory Remarks.

1:40 — 136. Steady state homogeneous nucleation rate and primary particle size distribution. **R. B. McClurg**

2:20 — 137. Surface segregation of bromine in bromide doped NaCl: Implications for particle chemistry and the seasonal variations in Arctic ozone. **J. C. Hemminger**, S. Ghosal, K. Inazu

3:00 — Intermission.

3:20 — 138. Mass and thermal accommodation coefficients of $H_2O(g)$ on liquid water as a function of temperature. Y. Q. Li, **P. Davidovits**, Q. Shi, J. T. Jayne, C. E. Kolb, D. R. Worsnop

4:00 — 139. Thin film water. **G. E. Ewing**

4:40 — 140. Size and composition measurements of individual ultrafine particles by aerosol mass spectrometry. **M. V. Johnston**, D. B. Kane

Section C

Unknown Site
Unknown Room

First Principles Simulation of Chemical Dynamics

II

Cosponsored with Division of Computers in Chemistry
T. J. Martínez and R. Car, *Organizer*
G. Galli and A. I. Krylov, *Presiding*

1:40 — 141. First principles simulation beyond the Born-Oppenheimer approximation. **D. Marx**

2:20 — 142. Ab initio studies of cis-trans photoisomerization dynamics. **J. Quenneville**, T. J. Martínez

2:40 — 143. Reaction coordinate mapping for ultrafast photo-induced chemical reactions. **M. Olivucci**

3:00 — Intermission.

3:20 — 144. Density matrix treatment of collision- and photo-induced electronic energy and charge transfer. **D. A. Micha**

4:00 — 145. Pseudospectral ab initio methods for electronically excited states. **D. K. Malick**, T. Martinez

4:20 — 146. Coupled Electronic-Ionic Monte Carlo. **M. D. Dewing**, D. M. Ceperley

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Storage Rings

S. L. Guberman, *Organizer*
E. Herbst, *Presiding*

1:40 — 147. Studies of electron-molecular ion dissociative recombination using ion storage rings. **M. Larsson**

2:20 — 148. Dissociative recombination of atmospherically relevant ions. **W. J. van der Zande**

3:00 — 149. An electrostatic storage ring for the research of electron-ion collisions at KEK. **T. Tanabe**, K. Chida, K. Noda, I. Watanabe

3:20 — 150. Dissociative recombination of vibrationally excited levels of O_2^+. **P. C. Cosby**, J. R. Peterson, D. L. Huestis

3:40 — Intermission.

4:00 — 151. Electron collision studies on CN^+, HCN^+/HNC^+, CN^- and C_4^- **A. Le Padellec**

4:40 — 152. Electron induced vibrational cooling of the hydrogen molecular ions H_2^+ and D_2^+. **S. Krohn**, H. Kreckel, L. Lammich, M. Lange, D. Schwalm, D. Strasser, A. Wolf, D. Zajfman

Section E

Unknown Site
Unknown Room

Molecular Electronics

Molecular Electronics Concepts

M. A. Ratner, *Organizer*
P. Avouris, *Organizer, Presiding*

1:40 — 153. Influence of miniaturization of carbon nanotubes on their electronic and electrical transport properties. **A. Rochefort**

2:20 — 154. Molecular logic machines. **R. D. Levine**

3:00 — Intermission.

3:20 — 155. Multiporphyrin arrays as molecular electronic gates. **R. K. Lammi**, A. Ambroise, T. Balasubramanian, J. R. Diers, R. W. Wagner, D. F. Bocian, J. S. Lindsey, D. Holten

3:40 — 156. Catching molecular devices in action by determination of transient molecular structure using laser pump/x-ray probe XAFS. **L. X. Chen**, G. Jennings, T. Liu, D. V. Scaltrio, G. J. Meyer

4:00 — 157. Theoretical modeling of molecular electronic device elements. **R. Pati**, S. P. Karna

Radiation Research: From the Science Laboratory to the Real World

New Instruments and Techniques for Radiation Research

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Rowland Award Symposium

Atmospheric Chemistry II

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TUESDAY EVENING

Three Dimensional Silicon-Oxygen Cages (Polyhedral Oligomeric Silsesquioxanes): Materials for the 21st Century

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WEDNESDAY MORNING

Section A

Unknown Site
Unknown Room

Stereochemistry in Aligned Environments

I

D. J. Nesbitt, *Organizer*
A. M. Wodtke, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:40 — 158. Peter Andresen: An appreciation of his contributions to molecular physics. **R. Schinke**

9:20 — 159. Selective energy transfer: Geometric specificity. **C. Wittig**

10:00 — 160. Vibrationally-mediated dissociation of H_2O molecules inside $(H_2O)_2$ and Ar-H_2O complexes: Spectroscopy, dynamics, and alignment effects **S. Nizkorodov**, M. Ziemkiewicz, A. E. W.

Knight, T. L. Myers, O. Votava, D. J. Nesbitt

10:20 — Intermission.

10:40 — 161. Reaction of overtone excited methane with atomic chlorine: State-to-state differential cross sections and vector correlations. **Z. H. Kim**, H. A. Bechtel, R. N. Zare

11:20 — 162. State-selective photo-decomposition of ClNO in the region 295-355 nm. **D. Baugh**, E. Torres, B. Alleyne

11:40 — 163. Alignment and orientation in the H + H_2O Reaction. **G. C. Schatz**, D. Troya, G. Lendvay

Section B

Unknown Site
Unknown Room

Physical Chemistry of Gas-Particle Interactions

II-Nucleation, Theory and Experiment

V. H. Grassian and J. T. Roberts, *Organizer*
H. C. Allen, *Presiding*

8:20 — 164. Reactive systems at the onset of microsolvation. **K. R. Leopold**, D. L. Fiacco, S. W. Hunt, K. Higgins, C. S. Brauer, M. Craddock

9:00 — 165. Stability properties of C_n (n=1-6) dicationic carbon clusters. **A. F. Jalbout**, H. J. Hogreve

9:20 — 166. Size effect of hematite and corundum inclusions as heterogeneous nuclei for aqueous ammonium sulfate particles. **S. T. Martin**, J. Han, H. Hung

10:00 — Intermission.

10:20 — 167. Role for nitrate radical in gas-particle conversion for mixed biogenic and anthropogenic emissions. **J. B. Miller**

10:40 — 168. Hygroscopicity and volatility of nanoparticles studied by Nano TDMA. **H. Sakurai**, K. Park, M. Zuk, D. B. Kittelson, P. H. McMurry

11:00 — 169. Aerosols in prebiotic chemistry. C. M. Dobson, G. B. Ellison, **A. F. Tuck**, V. Vaida

Section C

Unknown Site
Unknown Room

First Principles Simulation of Chemical Dynamics

III

Cosponsored with Division of Computers in Chemistry
T. J. Martínez, *Organizer*
R. Car, *Organizer, Presiding*
K. Burke, *Presiding*

8:20 — 170. First-principle molecular dynamic simulations along the intrinsic reaction paths. **T. Ziegler**, A. Michalak

9:00 — 171. Size-consistent wave functions for bond-breaking: The equation-of-motion spin-flip model. **A. I. Krylov**

9:20 — 172. First-principles simulations of shock front propagation in liquid deuterium. **F. Gygi**, G. Galli

10:00 — Intermission.

10:20 — 173. Transition path sampling and the pathways to auto ionization of a water molecule in liquid water. **D. Chandler**, C. Dellago, P. Geissler

11:00 — 174. Long time scale dynamics using DFT and the Dimer method: Application to boron clustering in silicon. G. Henkelman, B. P. Uberuaga, **H. Jonsson**

11:20 — 175. Action-derived molecular dynamics: A powerful tool for investigating rare events. **D. Passerone**, D. Atkah, M. Parrinello

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Astrophysics and Ionospheres

S. L. Guberman, *Organizer*
N. Adams, *Presiding*

8:20 — 176. Dissociative recombination in planetary and cometary aeronomy. **T. E. Cravens**

9:00 — 177. Dissociative recombination in interstellar clouds. **E. Herbst**

9:40 — 178. Dissociative recombination and deuterium fractionation in interstellar clouds. **E. M. Roueff**

10:20 — Intermission.

10:40 — 179. Absolute cross sections for state-selected reactions of O^+ (^4S, ^2D, ^2P) **C. Ng**

11:20 — 180. Great enhancements in dissociative electron attachment to chlorine-containing molecules adsorbed on H_2O/NH_3 ice. **Q. Lu**, L. Sanche

11:40 — 181. Electronic dissociative recombination of an ion of astrophysical interest : Quantum chemical calculations. **D. Talbi**

Radiation Research: From the Science Laboratory to the Real World

Radiation Effects and Consequences

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Rowland Award Symposium

Spectroscopy and Modeling

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QM/MM Methods

Session 6

Cosponsored with Division of Computers in Chemistry
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WEDNESDAY AFTERNOON

Section A

Unknown Site
Unknown Room

Stereochemistry in Aligned Environments

II

A. M. Wodtke, *Organizer*
D. J. Nesbitt, *Organizer, Presiding*

1:40 — 182. Strong field molecular control. **P. B. Corkum**

2:20 — 183. On the control of external molecular modes with laser and STM fields. **T. Seideman**

3:00 — 184. Spectral hole-burning of dye-molecules in nanopores: Electric field and pressure effects. **B. J. Prince**, P. Geissinger

3:20 — Intermission.

3:40 — 185. Deceleration, trapping, and storing neutral dipolar molecules **G. Meijer**

4:20 — 186. Manipulating molecules via combined electrostatic and pulsed nonresonant laser fields. **B. Friedrich**

Section B

Unknown Site
Unknown Room

Physical Chemistry of Gas-Particle Interactions

III-Interfacial Chemistry

J. T. Roberts and V. H. Grassian, *Organizer*
C. J. Pursell, *Presiding*

1:40 — 187. Gas-particle interactions relevant to organic atmospheric aerosols. **V. Vaida**

2:20 — 188. Reactive uptake of atmospheric oxidants by proxies for organic aerosols: Uptake coefficients, gas phase, and surface bound products **Y. Rudich**

3:00 — 189. "Hydrocarbon films as models for organic aerosols". **X. Zhang**, E. B. Jochnowitz, T. G. Lindeman, S. Simpson, B. Ellison

3:20 — Intermission.

3:40 — 190. Uptake of SO_2, H_2O_2 and Oxygenated Organics by Ice Surfaces under Conditions of the Free Troposphere **J. Abbatt**, O. Sokolov, S. Clegg

4:20 — 191. Reactivity and biological activity of PAH on respirable particles. **R. Kristovich**, P. Dutta, H. C. Allen, W. J. Waldman, M. V. Williams, J. F. Long

4:40 — 192. High-temperature surface chemistry of soot nanoparticles. **K. J. Higgins**, H. Jung, D. B. Kittelson, J. T. Roberts, M. R. Zachariah

Section C

Unknown Site
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First Principles Simulation of Chemical Dynamics

IV

Cosponsored with Division of Computers in Chemistry
T. J. Martínez and R. Car, *Organizer*
M. Olivucci and S. Hammes-Schiffer, *Presiding*

1:40 — 193. Photochemistry from first principles Quantum molecular dynamics. **M. Ben-Nun**, T. J. Martinez

2:20 — 194. Mixed quantum-classical dynamics via interacting trajectories: A method for performing ab-initio non-adiabatic molecular dynamics. **J. Schofield**

2:40 — 195. Extended space Car-Parrinello molecular dynamics. **N. Marzari**, R. Car

3:00 — Intermission.

3:20 — 196. Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. **H. B. Schlegel**, J. M. Millam, S. S. Iyengar, G. A. Voth, A. D. Daniels, G. E. Scuseria, M. J. Frisch

4:00 — 197. Mixed molecular orbital and multiconfiguration valence bond (MOVB) approach for simulation of chemical reactions in solution. **J. Gao**, Y. Mo

4:20 — 198. New methods for performing mixed plane wave based ab initio and classical force field calculations. **G. J. Martyna**, M. E. Tuckerman, D. Yarne

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Dissociative Recombination of H_3^+

S. L. Guberman, *Organizer, Presiding*

1:40 — 199. Help!!! Theory for H_3^+ recombination badly needed **T. Oka**

2:20 — 200. Importance of Jahn-Teller coupling in the dissociative recombination of H_3^+ by low energy electrons. **C. H. Greene**, V. Kokoouline, B. D. Esry

3:00 — 201. Branching ratio in the dissociative recombination of polyatomic ions. **D. Strasser**, J. Levin, H. B. Petersen, O. Heber, A. Wolf, D. Schwalm, D. Zajfman

3:20 — 202. Quantum dynamical study of H_3^+ recombination. **M. Tashiro**, S. Kato

3:40 — Intermission.

4:00 — 203. Coupling bound states to continua in neutral triatomic hydrogen. **H. Helm**

4:40 — 204. Recombination of H_3^+ and D_3^+ with electrons: Low limit of the recombination rate coefficient. **J. Glosik**, R. Plasil, V. Poterya, P. Kudrna, M. Tichy, A. Pysanenko

Radiation Research: From the Science Laboratory to the Real World

Radiation-Induced Interfacial Processes

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Rowland Award Symposium

Atmospheric Chemistry III

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WEDNESDAY EVENING

Unknown Site
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Physical Chemistry Poster Session

R. M. Stratt, *Organizer, Presiding*

7:30 - 10:00

Clusters and Aerosols.

205. A structural study of $(AlN)_n$, $(GaN)_n$, and $(InN)_n$ (n= 3 - 6): from N-N dominated molecules to Metal-N dominated solid-like clusters **A. K. Kandalam**, R. Franco, A. Costales, M. A. Blanco, R. Pandey

206. Ab initio and DFT studies of sulfur trioxide-water complexes. **J. M. Standard**, D. H. Pulsifer

207. Computation of geometrical and electrostatic parameters for a cluster model of silica. **M. Collins**, E. Demchuck, T. A. Holme

208. First principles calculations of vibrations in van der Waals clusters. **L. E. Fried**, K. R. Glaesemann

209. IR optical studies of model tropospheric organic aerosols. A. M. Potscavage, E. M. Lucchetta, **R. F. Niedziela**

210. Knudsen cell and FT-IR studies of NO2 on soot and HNO3 on oxide and carbonate particles. **H. A. Al-Abadleh**, V. H. Grassian

211. Knudsen cell study of SO_2 reactivity on mineral oxide powders. **C. R. Usher**, V. H. Grassian

212. Knudsen cell study of the heterogeneous reaction of gaseous nitric acid on iron oxide. **C. J. Pursell**, E. E. Frinak, M. A. Tolbert

213. Laboratory studies of heterogeneous atmospheric chemistry on mineral and carbonaceous aerosols. **A. Preszler Prince**, J. L. Wade, V. H. Grassian, P. D. Kleiber, M. A. Young

214. Modeling the optoelectronic properties of porous silicon using ab initio cluster calculations. **J. D. Head**

215. Molecular modeling (PM3) of the solvation of atrazine dimers. **Z. Meng**, W. R. Carper

216. Nonlinear optical studies of particle surface structure: application to atmospheric aerosol chemistry. **G. Ma**, E. L. Hommel, R. L. Kristovich, H. C. Allen

217. Observation of resonant two-photon photodetachment of water cluster anions via femtosecond photoelectron spectroscopy. **E. A. Woronowicz**, A. R. Keimowitz, G. H. Weddle, J. M. Weber, M. A. Johnson

218. Photodissociation spectroscopy of size-selected alkaline earth ions solvated by ammonia: $Sr^+(NH_3)_n$, $Sr^+(ND_3)_nD_m$, and $Mg^+(NH_3)_n$ J. I. Lee, D. C. Sperry, A. J. Midey, **J. M. Farrar**

219. Photoelectron spectroscopy of solvated doubly charged dicarboxylate anions. **X. Yang**, X. Wang, L. Wang

220. Quantum molecular dynamics simulations of solid-like water pentamers: Evidence for a rigid-flexible phase transition. **W. B. Bosma**, M. Rhodes

221. Quantum Monte Carlo studies of doped small helium clusters: Structural motifs in quantum solvation. **R. J. Hinde**, L. Warren, W. O. Klein, B. K. Taylor

222. Reactions in supercritical CO_2: Neutralization, electron capture, and formation of CO_2 anion clusters **K. Takahashi**, H. Kamata, S. Sawamura, N. Dimitrijevic, D. Bartels, C. Jonah

223. Solvent reorganization from a cluster perspective. **L. A. Posey**

224. Structure and dynamics of molecular ions in size-selected clusters. S. Shin, **E. Cho**

225. Supersonic expansion conformational studies of dipeptide analogues and their water clusters. **A. Longarte**, B. C. Dian, S. Merciers, T. S. Zwier

226. Water clusters of tryptamine and 3-indolepropionic acid: The role of water bridges in directing the confomational preferences of flexible biomolecules. J. R. Carney, **B. C. Dian**, T. S. Zwier

Gas-Phase Spectroscopy and Scattering.

227. Coupled-cluster ab initio multiple spawning dynamics simulation of the electronic spectra of ethylene. **K. K. Baeck**, M. Ben-Nun, T. J. Martinez

228. Creating rotational wavepackets using picosecond laser pulses. **S. Unny**, L. Zhu, R. J. Gordon, A. Cornea, W. A. Schroeder, T. Seideman

229. Dissociative recombination of NO^+. **A. Petrignani**, F. Hellberg, S. Rosen, R. Thomas, A. Neau, M. Larsson, W. van der Zande

230. Dissociative recombination of protonated dimer ions. **J. Glosik**, R. Plasil, P. Zakouril, V. Poterya

231. Electron collisions on C_4^-: Detachment and dissociation. **A. Le Padellec**, F. Rabilloud, D. Pegg, K. Andersson, D. Hanstorp, A. Neau, M. Larsson, F. Hellberg, R. Thomas

232. Electronic spectroscopy of a cis-amide dimer and its hydrated complexes. **J. R. Cable**, A. V. Fedorov

233. Evaluation and compilation of the laboratory spectroscopy of H_3^+. **C. M. Lindsay**, B. J. McCall

234. Investigating the three-body fragmentation dynamics of triatomic molecules using dissociative recombination and theoretical calculations. **R. D. Thomas**, S. Rosén, A. M. Derkatch, F. Hellberg, M. Larsson, S. Datz, R. N. Dixon, W. J. van der Zande

235. Investigation of the CN + C_2H_6 and CN + CH_4 exothermic reactions via state resolution of the HCN products. E. Carrasquillo-Molina, **T. He**, J. Adamson

236. Ion imaging studies on the ionic dissociation channels in the photodissociation of CS2 at 193 nm at low pulse energies. **D. Xu**, J. Huang, **W. M. Jackson**

237. Kinetic measurements of the quenching of CO_2 (010) by O atoms. **K. J. Castle**, E. S. Hwang, J. A. Dodd

238. Merged beam studies of the associative ionization process. **A. Le Padellec**, X. Urbain, T. Nzeyimana, E. Naji

239. Molecular symmetry and two-photon absorption. **Z. Xu**, Z. Wu, X. Bi, D. Wang

240. Photodissociating methyl vinyl ether to calibrate O + ethylene product branching and to test propensity rules for product channel electronic accessibility. **M. L. Morton**, **D. E. Szpunar**, L. J. Butler

241. Photodissociation dynamics of ozone using the analysis and denoising process of Raman Excitation Profiles. **E. S. Lotfi**, C. Kittrell, B. R. Johnson, J. L. Kinsey

242. Photodissociation of the CH2Br2+ at 355 nm using ion velocity imaging and time-of-flight mass spectroscopy. **J. Huang**, **D. Xu**, R. J. Price II, W. M. Jackson

243. Photoelectron spectra of diacetylene. **C. Ramos**, S. T. Pratt, T. S. Zwier

244. Product analysis for the reaction OH + D_2 using quasiclassical trajectories. **M. J. Lakin**, D. Troya, G. Lendvay, M. González, G. C. Schatz

245. Quasi-classical trajectory studies of the $NH(^3\Sigma^-)$ + H <--> $N(^4S)$ + H_2 reaction. **R. Z. Pascual**, G. C. Schatz, E. W. Ignacio

246. Rate constants and kinetic isotope effect for the 4-centered elimination of HF and HCl from checmically activated $CF_3CFClCH_3$ and $CF_3CFClCD_3$: A test of the 1,2-FCl rearrangement pathway for halocarbons **M. O. Burgin**, B. E. Holmes

247. Sensitivity of the extended STIRAP method of selective population transfer to coupling to background states. **V. Kurkal**, S. A. Rice

248. Spectroscopic identification of a novel catalytic reaction of hydrogen. **R. L. Mills**, J. Dong, J. He, B. Dhandapani, N. Greenig, W. Good, A. Voigt, S. Hicks, M. Nansteel

249. State-to-state differential cross sections of the reaction of overtone excited methane with atomic chlorine. Z. H. Kim, **H. A. Bechtel**, R. N. Zare

250. Study of isotope effects in the photoionization of HI and DI using phase lag spectroscopy. **A. Khachatrian**, R. Billotto, L. Zhu, R. J. Gordon, H. Lefebvre-Brion, T. Seideman

251. Study of the gas phase photochemistry of $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ using time resolved IR spectroscopy. **J. Wang**, E. Weitz

252. Supersonic jet spectroscopy of anthranilic acid. **C. A. Schehr**, D. H. Levy

253. Enigma of H_3^+ in diffuse interstellar clouds. **B. J. McCall**, T. Oka

254. Time cross correlation functions from resonant Raman excitation profiles: A direct inversion by maximum entropy. **F. Remacle**

255. Time-resolved studies of the vibrational state populations of $NO(X^2\Pi,V"=1\text{-}7)$ following NO_2 photodissociation at 193 nm using Fourier Transform IR Emission Spectroscopy **Y. Gong**, X. Chen, B. R. Weiner

256. Trajectory studies of S_N2 nucleophilic substitution .8: Central barrier dynamics for gas phase Cl^- + CH_3Cl **K. Song**, L. Sun, W. L. Hase

257. Unimolecular rate constants and kinetic isotope effects for decomposition of chemically activated $CF_2BrCF_2CH_3$ and $CF_2BrCF_2CD_3$: Evidence for a novel 1,2-FBr interchange **C. E. Lisowski**, G. L. Heard, B. E. Holmes

258. Vibrational signatures in gas-phase diffraction patterns. **S. Ryu**, P. M. Weber, R. M. Stratt

Condensed-Phase Spectroscopy and Dynamics.

259. Amplitude and phase distortions of femtosecond mid-IR pulses in water: A 2-D pulse propagation study using cross-correlation frequency-resolved optical gating. **J. A. Gruetzmacher**, N. F. Scherer

260. Comparison of semi-classical treatments of the three-pulse echo. **S. J. Schvaneveldt**

261. Dispersive and dipolar interactions of acetone and acetonitrile in various solvents. **G. S. Devendorf**

262. Excited state dynamics of self-assemblies of metalloporphyrins and metallophthalocyanines. **A. Gusev**, M. A. J. Rodgers

263. Hydrated electron spectrum: From clusters to supercritical fluid†. **D. M. Bartels**, J. A. Cline, C. D. Jonah, K. Takahashi

264. Infrared excitation driven Jahn-Teller transformations in copper Tutton salt. Y. Cha, **H. L. Strauss**

265. Large electron transfer rate effects from the Duschinsky coupling of vibrations. **G. M. Sando**, K. G. Spears, P. T. Ruhoff, J. T. Hupp

266. Role of hydrogen bonding in the Ground and Excited-State Intramolecular proton transfer in 6,7,8-trimethyl-[2,3-b](4-amino-5-Benzoylthio)pyridine & 7,8-(cycloalkane)-[2,3-b](4-amino-5-Benzoylthio)pyridines: Evidence of tautomeric equilibria **I. A. Z. Al-Ansari**

267. Role of intramolecular electron transfer in fluorescence deactivation of 2-arylbenzotriazoles. N. J. Turro, **A. J. Maliakal**, G. Lem, R. Ravichandran, J. C. Suhadolnik, A. D. DeBellis, M. G. Wood, J. Lau

268. Solvation of ammonium ion in water with polarizable potentials : A molecular dynamics study. **T. Chang**, L. X. Dang

269. Solvent-assisted intramolecular vibrational relaxation of a linear triatomic molecule. **Y. Deng**, R. Stratt

270. Spectroscopic and computational study of 4-dimethylamino-4'-nitrostilbene. **J. M. Smith**, Y. Soo Hoo, B. Barker

271. Time correlation function approach to liquid phase vibrational energy relaxation: Dihalogen solutes in rare gas solvents. **S. A. Adelman**, D. W. Miller

272. Time-resolved resonance Raman investigation of photocyclopropanation reactions. D. L. Phillips, **K. H. Leung**, Y. Li

273. Time-resolved resonance Raman studies of the intramolecular charge transfer (ICT) state of 4-dimethylaminobenzonitrile (DMABN). **W. M. Kwok**, **C. Ma**, P. Matousek, A. W. Parker, D. Phillips, M. Towrie, W. T. Toner

274. Vibrational quantum level dependence of ultrafast electron-transfer rates. **T. W. Marin**, **K. G. Spears**, B. J. Homoelle

275. Vibrational spectrum of the hydronium ion: Comparison of experiment, simulation, and normal mode analysis **J. Kim**, U. W. Schmitt, G. A. Voth, N. F. Scherer

Equilibrium Thermodynamics and Statistical Mechanics.

276. Thermodynamic studies of ternary systems: III Me_4NCl-$(n\text{-}Bu)_4NCl$-H_2O at 25 °C. **D. M. Fox**, L. Leifer

277. Absolute single ion hydration enthalpies, entropies, and heat capacities: Using cluster data and ab initio calculations to remove the extra-thermodynamic assumption D. M. Bartels†, **J. V. Coe**

278. Multicanoncal ensemble with molecular dynamics. **S. Jang**, Y. Pak, E. Cho, S. Shin

279. Quantum effects in liquid water. **H. A. Stern**, B. J. Berne

Quantum Chemistry and Dynamics.

280. 1,2-FCl rearrangement of CF_3CH_2Cl: An alternative pathway for CF_2CHF production **P. T. Beaton**, G. Heard, B. E. Holmes

281. Ab initio calculations for the three-body C_2+H+H dissociative channel of acetylene. **A. M. Derkatch**, B. F. Minaev, M. Larsson

282. Ab initio calculations of pressure-induced polymorphism in ZnTe. **R. Franco**, P. Mori, E. Francisco, R. Pandey, J. M. Recio

283. Ab initio perturbed ion description of equation of state, phase transition, and reactivity in the alpha-Al_2O_3 **R. Franco**, J. M. Recio, L. Pueyo

284. Ab initio studies of bromine and iodine containing halocarbenes. **R. W. Quandt**, J. M. Standard, S. A. Drake

285. Bonding in an isoelectronic atrane series. **M. W. Schmidt**, S. Nagase, J. Kobayashi, K. Goto, T. Kawashima

286. Changing features of the molecular intrinsic characteristic contours of H2 molecule in the ground and first excited states calculated by an ab initio method. **D. Zhao**

287. Characterization of the bent F state of the CaOH radical by the H^v method. **C. M. Taylor**, R. K. Chaudhuri, K. F. Freed

288. Characterizing individual molecular bonds. **D. Pressler**

289. Concepts in the topology of the electron density in ionic materials: Accumulated experience. **A. Costales**, A. Martín Pendás, M. A. Blanco, P. Mori-Sánchez, V. Luaña

290. Full dimensional quantum study of resonance scattering for reaction: Li + HF -> H + LiF. **L. Wei**, D. G. Truhlar

291. Hypothesis on microirreversible catastrophe of chemical bond breaking and remaking processes. **Z. Yang**

292. Implementation of Table CI method and macroconfiguration concept in Second-Order Generalized Van Vleck Perturbation Theory (GVVPT2). **J. Song**, Y. G. Khait, M. R. Hoffmann

293. Molecular dynamics and the effective fragment potential method. **H. M. Netzloff**, M. S. Gordon, J. Sorenson, G. Merrill

294. Molecular electronic structure and magnetic properties of $Y_2Ti(\mu\text{-}X)_2TiY_2$ (X,Y=H,F,Cl,Br) isomers **C. M. Aikens**, M. S. Gordon

295. New ab initio potential energy surface for the Van der Waals complex: H2 + CN(A). **U. Schnupf**, M.

C. Heaven

296. Potential energy surface and IR spectrum of $Cl^-–H_2$ complexes. **R. P. Linnemann II**, R. J. Hinde

297. Practical embedding for ionic materials: Crystal adapted pseudopotentials for the MgO crystal. V. Luaña, J. M. Recio, A. Martín Pendás, **M. A. Blanco**, L. Pueyo, R. Pandey

298. Pressler's atom. **D. E. Pressler**

299. Reactions of 2,2'- dichlorodiethyl sulfide (mustard gas) in the water vapor and the solvent effect of water molecules **F. Tao**, K. H. Weber

300. Role of the deformation energy in bond energies for metal-olefin and metal-dinitrogen complexes. **D. L. Cedeño**, E. Weitz

301. Structure and relative energies of the conformers of n-butyl cyanide and n-butyl acetylene. **K. Atticks**, R. K. Bohn, H. H. Michels

302. Tetrazane: Hartree-Fock, Gaussian-2 and -3, and complete basis set predictions of some thermochemical properties of N_4H_6 **D. W. Ball**

303. Theoretical investigation of the reaction dynamics for the gas-phase system $NO + O_3 \rightarrow NO_2 + O_2$. **E. Vayner**, D. W. Ball

304. Theoretical study on the structural symmetry of some bis-adduct of the cation with two bases (D-A-D). H. Liao, **S. Chu**

305. Vibrational analysis and ionization potentials of XCH_3 (X=Be, Mg, Ca) calculated by hybrid density functional theory and high order ab initio methods **A. F. Jalbout**

306. Violating the octet rule? Concepts and examples from DFT studies of thiazyl trifluoride, nitrosyl trifluoride: Their structural isomers and the hydrogen analogues **M. Burtzoff**, L. Peter, D. Y. Zhang

Molecular Electronics and Electronic Materials.

307. Preparation and characterization of conducting polyaniline. **L. Qian**, **Z. Yan**, **Z. Liu**

308. Chemical and electrical properties of metal-insulator-metal thin film devices. **M. Biscotto**, J. Gallegos, M. Banaszak Holl, B. G. Orr, U. C. Pernisz

309. Dependence of the optical properties of poly(*p* -phenylene vinylene) on morphology. **T. G. Bjorklund**, C. J. Bardeen

310. Development and performance of photorefractive materials composed of conjugated polymeric thin films and doped nematic liquid crystals. **M. J. Fuller**, M. R. Wasielewski

311. Electron transfer through dendrimer wires. **C. Kalyanaraman**, D. G. Evans

312. Electron transport in conjugated oligomer SAMs. **M. S. Doescher**, M. L. Myrick

313. Exciton transfer or intramolecular vibrational relaxation? Exciton dynamics in poly(p-phenylene vinylene) studied by temperature-dependent femtosecond spectroscopy **S. Lim**, C. J. Bardeen

314. Photoluminescence of $YVO_4:Eu^{3+}$ thin films prepared by pulsed-laser deposition: Cross relaxation as an

index of Eu^{3+} concentration. **W. Kang**, **J. Park**

315. Picosecond luminescence dynamics of phenylethynylene dendrimers. **K. M. Gaab**, C. J. Bardeen

316. Resonance-enhanced diffraction-based sensing: Improved sensitivity and selectivity. **R. C. Bailey**, J. T. Hupp

317. Resonant tunneling and the substituent effects for the molecules exhibiting negative differential resistence in molecular electronic devices. **N. Matsunaga**, K. Sohlberg

318. Spatially resolved electrical properties of polyaniline. **S. Rane**, Y. Liau, M. K. Ng, L. Yu, N. F. Scherer

319. Towards a density functional theory of scattering. **A. Wasserman**, N. Maitra, K. Burke

320. Toward computing with molecules: Examples of molecular logic circuits. **F. Remacle**

321. Ultrafast and long-lived photoinduced charge separation in MEH-PPV/nanoporous semiconductor thin film composites. **N. A. Anderson**, E. Hao, X. Ai, G. G. Hastings, T. Lian

Colloids, Surfaces, Interfaces, and Nanoscale Materials

322. Novel method of the preparation of aluminum sol. **L. Qian**, **Z. Yan**, **X. Gao**

323. Effects of different silica gel on the synthesis of the different SAPOs. **Z. Wang**, Z. Yan

324. Anionic and upper-excited fluorescence of C_{60} encapsulated in Y zeolitic nanocavity. **O. Kwon**, H. Yoo, K. Park, **D. Jang**

325. Atomic oxygen erosion of decanethiol SAMs: A molecular beam and STM study. **B. Isa**, S. J. Sibener

326. Computational thermochemistry of the siting of Cu^{+} ions in zeolite ZSM-5. **D. A. Horner**, P. Zapol, L. A. Curtiss

327. Electrodynamic modelling of the tunable surface plasmon resonance spectra of silver nanoparticles. **E. A. Coronado**, G. C. Schatz

328. Energy transfer dynamics associated with Ne-atom collisions with the N-hexylathiolate self-assembled monolayer(SAM)/Au{111} surface. **T. Yan**, W. L. Hase

329. ESR study of the dynamics of trapped H and D atoms in silsesquioxane cages. **E. Roduner**, B. Gross, H. Dilger

330. Nonlinear optical properties of mono- and bimetallic nanoparticles: Effects of symmetry and structure. **R. C. Johnson**, J. T. Hupp

331. Preferential nucleation of metal nanoclusters on S(4x4)/W(111). **Q. Wu**, W. Chen, T. E. Madey

332. Reaction of acetylene on Si(001)-(2x1) and a report on the extension of the effective fragment potential method for the study of heterogeneous catalysis. **J. M. Rintelman**, M. S. Gordon

333. Self-assembled monolayers: Alkylsilanes on gold. **T. M. Owens**, K. T. Nicholson, M. M. Banaszak Holl, S. Süzer

334. Synthesis of mixed layers derived from functional silicon oxide clusters on gold. **K. T. Nicholson**, K. Z. Zhang, M. M. Banaszak Holl, F. R. McFeely, U. C. Pernisz

335. What is the rate-limiting step for alkane dehydrogenation in zeolite H-ZSM-5? **S. A. Zygmunt**, L. A. Curtiss, L. E. Iton, B. L. Bootz, A. W. Miller

Biophysical Chemistry.

336. Computational modeling studies of the interactions of β-peptides with each other and with the products of the nuclear oncogenes FOS and JUN. **F. N. Ngassa**, E. M. Nkabyo, S. H. Gellman, K. A. Thomasson

337. Electron super-exchange mechanism and the residual mobility of topa quinone in amine oxidases. **A. W. Masiukiewicz**

338. Formation of a new photo-induced oxygen isotope-sensitive intermediate during the reduction of O_2 by fully reduced cytochrome c oxidase. **J. F. Cerda**, D. A. Proshlyakov, G. T. Babcock

339. Interaction energies of acetylthiocholine with aromatic and polar solvent molecules. **C. A. Deakyne**, W. Zheng

340. Investigations of the peroxidase site Of Prostaglandin H synthase. **S. Seibold**, J. Cerda, R. Cukier, M. Garavito, W. Smith

341. Mixed quantum/classical molecular dynamics simulations of hydride transfer in dihydrofolate reductase. **P. K. Agarwal**, S. R. Billeter, S. Hammes-Schiffer

342. Model simulation of DNA melting dynamics. **G. Wu**, G. C. Schatz

343. Monte Carlo simulations of locally denatured, closed circular DNA at low salt concentration **C. A. Sucato**, D. C. Aspleaf, B. S. Fujimoto, J. M. Schurr

344. NMR studies of lung surfactant peptides SP-B_{1-25} and SP-B_{11-25}. **J. W. Kurutz**, K. Y. C. Lee

345. Peptide-based photoprobes, their aggregation, and inclusion complexation with cyclodextrin in water **X. Zhou**, G. Jones II

346. Solvation of a flexible biomolecule in the gas phase: The IR and ultraviolet spectroscopy of melatonin and its water clusters. **G. M. Florio**, T. S. Zwier

347. Spectroscopic study of pyrene-labled polypeptides: Aggregation and photoinduced electron transfer. **X. Zhou**, G. Jones II

348. Electronic structure of a model green fluorescent protein chromophore. **S. Olsen**, T. J. Martínez

General Physical Chemistry.

349. CeO_2 and MgO addition effects of nickel catalysts of dryreforming of methane. **Z. Yan**, R. Ding, X. Liu, L. Song

350. Design and optimization of zeolite for producing LPG and diesel in FCC process. **X. Liu**, Z. Yan

351. On-line TPSR, EPR, XPS, and UV-DRS studies of nickel catalysts of propylene oligomerization **Z. Yan**, L. Song, Q. Wang

352. Carbon dioxide laser initiated reactions: Capabilities and limitations. L. Jacobus, D. Miliano, C. W. Szakal, **B. D. Anderson**

353. Kinetics of the ligand exchange reaction in metal bipyridine complexes. **T. R. Brewer**, L. Kolopajlo

354. Novel oxygen sensor material based on a ruthenium bipyridyl complex encapsulated in hydrophobic zeolite Y. **P. Payra**, P. K. Dutta

355. Radiolysis of oxygenated and air-free aqueous benzene solutions as a method of detoxification. **R. J. Hanrahan**, L. L. Land

356. Radiolysis of water adsorbed on oxides. **J. A. LaVerne**, L. Tandon

357. Water radiolysis at elevated temperatures. **S. M. Pimblott**, M. Begusova

THURSDAY MORNING

Section A

Unknown Site
Unknown Room

Stereochemistry in Aligned Environments

III

D. J. Nesbitt and A. M. Wodtke, *Organizer*
C. Wittig, *Presiding*

8:20 — 358. Molecular orientation in liquid helium nanodroplets studied by high resolution infrared laser spectroscopy. **R. E. Miller**, K. Nauta, D. Moore, P. Stiles

9:00 — 359. Alignment of planar molecules in supersonic expansions: Experiments, quantum mechanical theory, and use for measuring anisotropic intermolecular forces **V. Aquilanti**, D. Cappelletti, F. Pirani

9:40 — 360. Chemical impurities in a quantum solid. **D. T. Anderson**

10:00 — Intermission.

10:20 — 361. Photon- and electron-induced localized atomic reaction of aligned chlorobenzenes with Si(111)7x7 and Si(100)2x1. P. Lu, **J. C. Polanyi**, D. Rogers

11:00 — 362. Aligned chemistry of single molecules on surfaces. **L. J. Lauhon**, W. Ho

11:40 — 363. Molecular tracer dynamics in monolayer crystals at the solid-liquid interface. **D. F. Padowitz**, D. M. Sada, E. L. Kemer

Section B

Unknown Site
Unknown Room

Physical Chemistry of Gas-Particle Interactions

IV-Experimental Advances in Particle Science

J. T. Roberts, *Organizer*

V. H. Grassian, *Organizer, Presiding*

9:00 — 364. Reactions of ozone with organic aerosols analyzed by single-particle time-of-flight mass spectrometry. G. Smith, C. Hauser, **T. Baer**, R. E. Miller, E. Woods III

9:40 — 365. Ammonium sulfates in Houston: Automated time-tagged archiving of field collected aerosols for laboratory single particle analysis. **J. P. Cowin**, A. Laskin, M. J. Iedema

10:00 — Intermission.

10:20 — 366. Atmospheric aerosol processing in the lab and the field as measured with an aerosol mass spectrometer. **D. R. Worsnop**, J. T. Jayne, M. Canagaratna, J. Jimenez, C. E. Kolb, J. Morris, P. Davidovits

11:00 — 367. Measurements of single particles from Atlanta using particle analysis by laser mass spectrometry (PALMS). **A. M. Middlebrook**, S. Lee, D. M. Murphy, D. S. Thomson

11:40 — 368. Time-resolved field study of chloride depletion and nitrate enrichment in sea salt aerosol using single particle analysis. **A. Laskin**, M. J. Iedema, J. P. Cowin

Section C

Unknown Site
Unknown Room

First Principles Simulation of Chemical Dynamics

V

Cosponsored with Division of Computers in Chemistry
T. J. Martínez and R. Car, *Organizer*
G. J. Martyna and D. Marx, *Presiding*

8:20 — 369. Time-dependent density functional theory in real time. **G. F. Bertsch**, K. Yabana

9:00 — 370. Electronic excited states in density functional theory. **K. Burke**

9:20 — 371. First-principles electronic structure simulations for very large systems. **D. Sanchez-Portal**, E. Artacho, A. Garcia, G. Fabricius, J. Gale, J. Junquera, P. Ordejón, J. M. Soler

10:00 — Intermission.

10:20 — 372. Incorporating electronic and nuclear quantum effects in the dynamical simulation of proton and hydride transfer. **S. Hammes-Schiffer**

11:00 — 373. Nonadiabatic dynamics of the green fluorescent protein chromophore. **A. Toniolo**, M. Ben-Nun, T. J. Martinez

11:20 — 374. Molecular dynamics with quantum statistics: A path integral approach. **P. N. Roy**, N. Blinov

Section D

Unknown Site
Unknown Room

Dissociative Recombination of Molecules with Electrons

Afterglow Experiments

S. L. Guberman, *Organizer*
R. Johnsen, *Presiding*

8:20 — 375. Dissociative recombination of electrons and ions: The early experiments. **M. A. Biondi**

9:00 — 376. Optical spectroscopy of recombining ions in flowing afterglow plasmas. **R. Johnsen**

9:40 — 377. Technique for distinguishing and determining the origin of photon emissions from He^+/Ar^+ plasmas: Recombination emission with addition of OCS, CS_2 and H_2S **N. G. Adams**, T. Mostefaoui, L. M. Babcock

10:20 — Intermission.

10:40 — 378. Reactions of electrons with hydrocarbon cations: From linear alkanes to aromatic species. **C. Rebrion-Rowe**

11:20 — 379. Dissociative recombination of Xe_2^+ and XeH^+. **J. B. A. Mitchell**, R. H. Lipson

11:40 — 380. Dissociative recombination of the helium molecular ion. **K. Hardy**

Radiation Research: From the Science Laboratory to the Real World

Environmental and Other Real-World Applications

Cosponsored with Division of Chemical Education
See Page X

THURSDAY AFTERNOON

Section A

Unknown Site
Unknown Room

Stereochemistry in Aligned Environments

IV

D. J. Nesbitt and A. M. Wodtke, *Organizer*
G. C. Schatz, *Presiding*

1:20 — 381. Inorganic nanorods: Synthesis, alignment, properties **A. P. Alivisatos**

2:00 — 382. Laser desorption spectroscopy of biomolecular building blocks. **M. S. de Vries**

2:40 — 383. Semiconductor nanowires: Building blocks for nanoscale science and technology. **C. M. Lieber**

3:00 — Intermission.

3:20 — 384. Self-alignment of serine: Possible steps towards homochirogenesis. **R. G. Cooks**, K. J. Koch, W. A. Tao, M. N. Eberlin, F. C. Gozzo

4:00 — 385. Alignment at a solid-liquid interface and its implications on the double layer. **E. S. Yeung**, X. N. Xu, S. H. Kang, J. Zheng

4:40 — 386. Diffusion model for self-assembled monolayer formation in dip-pen nanolithography. **J. Jang**, G. C. Schatz, M. A. Ratner

5:00 — 387. Toward regular and sturdy 2-D grids. **J. Michl**, N. Varaksa, L. Pospisil, T. F. Magnera

Section B

Unknown Site
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Physical Chemistry of Gas-Particle Interactions

V-Spectroscopy, Bulk-Phase Chemistry and Small Volume Effects

J. T. Roberts and V. H. Grassian, *Organizer*
V. Vaida, *Presiding*

1:40 — 388. Kinetics of transfer of trace gases across the liquid interface. **M. Mozurkewich**

2:20 — 389. Broadband sum frequency generation: A new look at liquid surfaces relevant to tropospheric aerosols. **E. L. Hommel**, G. Ma, J. Schlegel, H. C. Allen

2:40 — 390. Collisions of ethanol, HCl, and HBr with organic surfactants on dilute sulfuric acid G. M. Nathanson, **J. R. Splan**, R. D. Torn

3:00 — Intermission.

3:20 — 391. Surface studies and instrumentation advances: Understanding heterogeneous chemistry at the molecular-level. **H. C. Allen**

3:40 — 392. Photoelectric charging of small aerosol particles: Theory and applications. **K. Siegmann**, H. C. Siegmann

Section C

Unknown Site
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First Principles Simulation of Chemical Dynamics

VI

Cosponsored with Division of Computers in Chemistry
R. Car, *Organizer*
T. J. Martínez, *Organizer, Presiding*

1:40 — 393. Electron nuclear dynamics. **N. Y. Ohrn**

2:20 — 394. Direct dynamics simulations of unimolecular and bimolecular reactions. **W. L. Hase**, K. Song, L. Sun, K. Bolton

3:00 — 395. Effect of the potential energy surface on the dynamics of weakly bound precursor complexes and new "black-blox" coupled-cluster methods for entire potential energy surfaces of reactive molecular systems. **P. Piecuch**, V. Spirko, R. Burcl, K. Kowalski, S. A. Kucharski, F. Mrugala, O. Bludsk‡

Section D

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Unknown Room

Dissociative Recombination of Molecules with Electrons

Electron Attachment

S. L. Guberman, *Organizer*
A. Orel, *Presiding*

1:40 — 396. Advances in the calculation of electron affinities. **T. H. Dunning**, T. van Mourik, K. A. Peterson

2:20 — 397. Dissociative electron attachment in gas and condensed phases. **I. I. Fabrikant**

3:00 — 398. Dissociative electron attachment at low temperatures with molecules and clusters. **B. R. Rowe**

3:20 — 399. Chiral recognition via excess electron attachment to the 1,3-butandiol/2-butanol complex: Ab initio study **A. F. Jalbout**, L. Adamowicz

3:40 — Intermission.

4:00 — Panel Discussion.

5:00 — Concluding Remarks.

Submit Final Program