PHYS Technical Program
227TH National ACS Meeting
Anaheim, CA
March 28-April 1, 2004

SUNDAY MORNING
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Nuclear Dynamics

D. M. Jonas, *Organizer, Presiding*
8:20 - 1. Hydrogen bond dynamics probed with vibrational echo correlation spectroscopy. **M. D. Fayer**, T. Steinel, J. B. Asbury

9:00 - 2. Vibrational echo correlation spectroscopy as a new probe of complex dynamics and mixtures. **J. B. Asbury**, T. Steinel, M. D. Fayer

9:20 - 3. X-ray absorption spectroscopy of solvated iron pentacarbonyl measured with an ultrafast laser-driven x-ray source. **C. Rose-Petruck**, T. Lee, F. Benesch, Y. Jiang

9:50 - 4. 3D view of signal generation and propagation in femtosecond four-wave mixing. **N. Belabas**, D. M. Jonas

10:20 - Intermission.

10:40 - 5. "2-D Polarizability response measurements of solvation and simulation of mid-IR pulse propagation in dense liquids. **N. F. Scherer**

11:20 - 6. Photoacid-base neutralization reactions studied with ultrafast infrared spectroscopy. M. Rini, O. F. Mohammed, B. Magnes, A. Usman, **E. T. J. Nibbering**, E. Pines

Section B
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Photodissociation of Ions and Radicals

H. Reisler, *Presiding*
8:00 - 7. Argon Pre-dissociation Infrared Spectroscopy of trapped intermediates in the O- + CH4 -> OH- + CH3 reaction. **G. H. Weddle**, E. G. Diken, E. A. Price, S. A. Corcelli, J. M. Headrick, M. Johnson

8:20 - 8. Dissociative photodetachment studies of acetate and formate anions. **R. E. Continetti**, Z. Lu

9:00 - 9. Probing the effects of molecular conformation on ionization dynamics using threshold ionization techniques. **C. E. H. Dessent**, M. S. Ford, X. Tong, K. Muller-Dethlefs

9:40 - 10. Photodissociation of the OH and SH radicals. **D. H. Parker**

10:20 - Intermission.

10:40 - 11. State-to-state photodissociation dynamics of OH radical via the A^2S^+ state: Fine-structure distributions of the $O(^3P_J)$ product. **W. Zhou**, Y. Yuan, **J. Zhang**

11:00 - 12. Rotationally resolved infrared spectroscopy of the hydroxymethyl radical (CH_2OH). **L. Feng**, J. Wei, H. Reisler

11:20 - 13. Imaging mechanistic pathways in photodissociation. **C. Vallance**, M. Brouard, M. J. Bass, A. P. Clark, B. Martinez Haya

Section C
Unknown Site -- Unknown Room
Mass Spectrometry of Biopolymers: From Model Systems to Ribosomes
Proteomics and High-Throughput Methods
Cosponsored with ANYL

R. Orlando, *Presiding*
8:20 - 14. Mass Spectrometric Approaches for Comprehensive, Quantitative and Ultra-sensitive High Throughput Proteomics. **R. D. Smith**

9:00 - 15. Dynamic proteome profiling of Drosophila early development stages and B cell biogenesis using metabolic labeling. **A. J. R. Heck**, E. P. Romijn, M. Monti, J. Krijgsveld

9:40 - 16. Developing IM-MS as a proteomics-mass spectral imaging tool. **D. H. Russell**

10:20 - Intermission.

10:40 - 17. Towards comprehensive proteomics of cells. **J. Yates**

11:20 - 18. High throughput mass spectrometry for the identification and typing of biowarfare agents and pathogens associated with emerging infectious diseases: The TIGER approach. **S. A. Hofstadler**, D. J. Ecker, L. B. Blyn, R. Sampath, J. Drader, Y. Jiang, J. C. Hannis, T. Hall, M. Eshoo, J. McNeil, D. Robbins, D. Knize, K. Rudnick, E. Moradi, D. Moore, A. Desai, J. Penhune, D. Sofianos, N. Freed, K. Russell

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Clusters, Droplets and Cryogenic Matrices

R. Parson, *Organizer, Presiding*
8:00 - 19. Dynamics in helium nanodroplets. **K. K. Lehmann**

8:40 - 20. Fragmentation dynamics of ionized neon clusters in helium nanodroplets. **N. Halberstadt**, D. Bonhommeau, A. Viel

9:20 - 21. Path integral method to study rotations in doped helium clusters: application to He_N-OCS and He_N-N_2O. **P. N. Roy**, N. Blinov

9:40 - 22. Molecular dynamics in cryogenic quantum solids. **R. J. Hinde**

10:20 - Intermission.

10:40 - 23. Quasi-classical simulations of photodissociation and caging of hydrogen halides in a cryogenic rare gas environment. **P. Jungwirth**, P. Slavicek

11:20 - 24. Simulations of negatively-charged water clusters. **K. D. Jordan**, F. Wang

Section E
Unknown Site -- Unknown Room
Nanocrystals and Nanotubes
Nanocrystals and Nanotubes
Cosponsored with PRES

U. Banin and R. Weisman, *Presiding*
8:00 - 25. Nanotubes and Nanocrystals. **M. S. Dresselhaus**

8:40 - 26. Inorganic Nanotubes for Nanofluidic Applications. **P. Yang**

9:20 - 27. Optical studies of the mechanism of lasing in single cadmium sulfide nanowires. **R. Agarwal**, C. J. Barrelet, O. Hayden, C. M. Lieber

9:40 - 28. Nanowiring Enzymes to Carbon Nanotube Probes. **P. Collier**, M. J. Esplandiu, V. G. Bittner, I. R. Shapiro

10:00 - 29. Nanowire solar cells. **M. D. Law**, L. E. Greene, K. Kadnikova, J. Liu, J. M. J. Frechet, P. Yang

10:20 - Intermission.

10:40 - 30. Integration of colloidal nanocrystals into electrical devices. Y. Cui, **A. P. Alivisatos**

11:20 - 31. Electronics and mechanics with carbon nanotubes. **P. L. McEuen**

Section F
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

N. Halas, *Presiding*
8:20 - 32. Single molecule fluctuating chemical kinetics in zeptoliter volumes. **W. W. Webb**

9:00 - 33. Nanoscale Chemical and Materials Characterization with Near-Field Microscopy and Spectroscopy. **S. J. Stranick**, B. Chase, C. A. Michaels

9:40 - 34. Near-field optical interactions excited by a field enhancement effect. **A. Bouhelier**, M. R. Beversluis, L. Novotny

10:20 - Intermission.

10:40 - 35. Nanoscopic nonlinear optical interactions. **P. N. Prasad**, Y. Shen, P. Markowicz

11:20 - 36. Application of Solid Immersion Lens Techniques to High-Resolution Subsurface Microscopy and Thermal Imaging. **M. S. Unlu**, M. G. Eraslan, Z. Liu, A. N. Vamivakas, S. A. Thorne, S. B. Ippolito, B. B. Goldberg

SUNDAY AFTERNOON
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Electronic-Vibronic Dynamics

N. F. Scherer, *Presiding*
1:20 - 37. Sub-5fs spectroscopy. **T. Kobayashi**

2:00 - 38. Using femtosecond polarization spectroscopy to determine vibrational symmetry. **D. A. Farrow**, W. Qian, E. R. Smith, D. M. Jonas

2:20 - 39. Vibrational mode coupling via an external field as a control mechanism in SRS. **S. A. Malinovskaya**, P. R. Berman, P. H. Bucksbaum

2:40 - 40. Terahertz emission spectroscopy: From molecular monolayers to magnetic thin films. S. M. Harrel, J. M. Schleicher, E. Beaurepaire, **C. Schmuttenmaer**

3:20 - Intermission.

3:40 - 41. Ultrafast hydration dynamics of proteins. **D. Zhong**

4:00 - 42. Molecular structure and dynamics observed by ultrafast photoionization via Rydberg states. **P. M. Weber**, N. Kuthirummal, W. Cheng, J. L. Gosselin

4:20 - 43. Revealing reaction mechanisms from coherent wavepacket dynamics. **S. Lochbrunne**

Section B
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Acid Dissolution and Zwitter Ion Formation in Clusters

M. Johnson, *Organizer, Presiding*
1:20 - 44. The Influence of Solvation on the Dynamics of Cluster-Ion Reactions. **A. W. Castleman Jr.**

2:00 - 45. Molecular picture of solvent separated ion pairs in hydrogen bonded clusters: The role of water in forming effective bridges that stabilize charge separation*. **S. S. Xantheas**

2:40 - 46. Photoelectron Spectroscopy of Cluster Anions. **K. H. Bowen Jr.**

3:20 - Intermission.

3:40 - 47. Amino acid/halide clusters: Zwitterions vs. neutral structures. **S. R. Kass**

4:20 - 48. Molecular beams studies of elementary processes on ice surfaces: Can the ionic dissociation of HCl be spontaneous? **P. Ayotte**, M. Hébert, P. Marchand

5:00 - 49. Population-modulated electron attachment spectroscopy: A new route for size-selective characterization of neutral molecules and clusters. **W. H. Robertson**, E. G. Diken, M. A. Johnson

Section C
Unknown Site -- Unknown Room
Mass Spectrometry of Biopolymers: From Model Systems to Ribosomes
Glycobiology
Cosponsored with ANYL

J. A. Leary, *Presiding*
1:20 - 50. Profiling oligosaccharides diversity by infrared multiphoton dissociation. **C. B. Lebrilla**

2:00 - 51. Partitioning of solvent effects and intrinsic interactions in the association of biological complexes. **J. S. Klassen**, E. N. Kitova, D. R. Bundle

2:40 - 52. Studying protein carbohydrate interactions with mass spectrometry and molecular dynamics. **R. Orlando**, D. A. King, C. Bergman, R. J. Woods, J. Barnes

3:20 - Intermission.

3:40 - 53. Optimizing mass spectrometry for applications in glycobiology. **C. E. Costello**, P. B. O'Connor, J. Zaia

4:20 - 54. Mass spectrometric approaches for assessing carbohydrate structure and function in bacterial pathogenesis. **B. Gibson**

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Condensed Phase Dynamics: Fluids

C. C. Martens, *Presiding*
1:20 - 55. Quantum time-correlation functions from classical mechanics: Applications to vibrational energy relaxation and diffusion in liquids. **J. L. Skinner**

2:00 - 56. Simulations of vibrational relaxation. **W. H. Thompson**, S. Li

2:40 - 57. Theoretical descriptions of vibrational relaxation in neat liquids of polar and nonpolar molecules. T. S. Gulmen, **E. L. Sibert III**, R. Rey

3:20 - Intermission.

3:40 - 58. Solvation in supercritical water. J. Duan, **H. J. Kim**

4:00 - 59. Simulation of quantum molecular dynamics in the condensed phase: Rate constants, correlation functions and nonequilibrium dynamics. **E. Geva**, Q. Shi

4:40 - 60. Molecular interpretation of 3-rd order Raman spectra in liquids: A case study. **R. M. Stratt**, A. Ma

Section E
Unknown Site -- Unknown Room
Nanocrystals and Nanotubes
Nanocrystals and Nanotubes

Cosponsored with PRES

P. McEuen and P. Collier, *Presiding*
1:20 - 61. Carbon Nanotube Electronics and Optoelectronics. **P. Avouris**

2:00 - 62. Tuning emission regimes in semiconductor nanocrystals: From solid-state lighting and LEDs to multicolor lasing. **V. I. Klimov**

2:40 - 63. Ultrafast carrier dynamics in single-walled carbon nanotubes probed by femtosecond spectroscopy. **Y. Ma**, J. Stenger, J. Zimmermann, S. M. Bachilo, R. E. Smalley, R. B. Weisman, G. R. Fleming

3:00 - 64. Single nanocrystal photoluminescence excitation spectroscopy: The first look into the structure of excited states not obscured by ensemble averaging. **P. J. Cox**, H. Htoon, J. A. Hollingsworth, V. I. Klimov

3:20 - Intermission.

3:40 - 65. Semiconductor quantum rods: synthesis, properties and optical gain. **U. Banin**

4:20 - 66. Fluorescence spectroscopy of single-walled carbon nanotubes: a new tool for basic and applied research. **R. B. Weisman**

5:00 - 67. Photoluminescence of individual single-walled carbon nanotubes. A. Hartschuh, H. N. Pedrosa, L. Novotny, **T. D. Krauss**

Section F
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

S. W. Hell, *Presiding*
1:20 - 68. Tip-scattering near-field microscopy in the infrared. **F. Keilmann**

2:00 - 69. Spectral self-interference fluorescence microscopy. **B. B. Goldberg**, A. K. Swan, L. Moiseev, M. Dogan, W. C. Karl, B. Davis, C. A. Cantor, M. B. Goldberg, M. S. Unlu

2:40 - 70. Virus-encapsulated optical probes. **B. Dragnea**, E. Kwak, C. Chen, D. Amarie, C. C. Kao, T. Onuta, P. Park, W. L. Schaich

3:20 - Intermission.

3:40 - 71. Single-molecule nano-optics. **B. Hecht**

4:20 - 72. Applications of near-field scanning optical microscopy to organic light-emitting electrochemical cell and field-effect transistor materials and devices. **M. A. Summers**, L. Edman, J. Swenson, A. J. Heeger, S. K. Buratto

4:40 - 73. Using two-photon standing wave microscopy to study motions on the 100 nm lengthscale. **S. K. Davis**, C. J. Bardeen

MONDAY MORNING

Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Nuclear Dynamics

N. Belabas, *Presiding*
8:20 - 74. Three-pulse femtosecond anisotropy technique for examining anomalous rotational diffusion and energy transfer. K. M. Gaab, **C. J. Bardeen**

8:50 - 75. Laser alignment of molecules with short laser pulses. **H. Stapelfeldt**

9:30 - 76. Switched wavepackets and field free molecular axis alignment. **J. G. Underwood**, B. J. Sussman, A. Stolow

10:00 - 77. Vibrational couplings and dynamics of transmembrane peptides studied with 2D IR spectroscopy. **M. T. Zanni**, P. Mukherjee, E. C. fulmer, A. T. Krummel, I. T. Arkin

10:20 - Intermission.

10:40 - 78. Hydrogen bond dynamics in water: Vibrational echoes and 2D IR spectroscopy. C. J. Fecko, J. J. Loparo, J. D. Eaves, P. L. Geissler, **A. Tokmakoff**

11:20 - 79. Vibrational climbing in carboxyhemoglobin by use of stretched infrared pulses. C. Ventalon, J. M. Fraser, M. H. Vos, A. Alexandrou, J. Martin, **M. Joffre**

Section B
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Ions and Radicals in the Condensed Phase

V. S. Batista, *Presiding*
8:20 - 80. Ab initio molecular dynamics investigations of anomalous charge transport mechanisms in solid and aqueous phases. **M. E. Tuckerman**

9:00 - 81. Isolation of biology-related molecules and their hydrated clusters from liquid beams. **T. Kondow**, J. Kohno, N. Toyama, F. Mafuné

9:40 - 82. Entrance channel complexes in helium nanodroplets: Infrared laser spectroscopy. **R. E. Miller**

10:20 - Intermission.

10:40 - 83. Infrared spectroscopy of radicals trapped in solid molecular hydrogen. **D. T. Anderson**

11:00 - 84. Photodissociation of ICN at the liquid/vapor interface of water. **N. D. Winter**, I. Benjamin

11:20 - 85. Dynamics of radicals in solution probed by femtosecond photodissociation and photodetachment. A. C. Moskun, X. Chen, **S. E. Bradforth**

Section C
Unknown Site -- Unknown Room
Mass Spectrometry of Biopolymers: From Model Systems to Ribosomes

Aggregates and Assemblies
Cosponsored with ANYL

M. L. Gross, *Presiding*
8:20 - 86. Two dimensional mass spectrometry of noncovalent complexes. **E. R. Williams**, S. Krishnaswamy, D. D. Garcia, J. C. Jurchen

9:00 - 87. The assembly of helical peptides into clusters and domains. **M. F. Jarrold**

9:40 - 88. Duplex formation and the onset of helicity in oligonucleotides. **J. Gidden**, E. Shammel Baker, A. Ferzoco, M. T. Bowers

10:20 - Intermission.

10:40 - 89. Tandem Mass Spectrometry of Supramolecular Assemblies. **C. V. Robinson**

11:20 - 90. Mass spectrometry view of the proteasome. **J. A. Loo**, B. Berhane, C. F. Silverio, K. M. Wooding, Y. Xie

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
The Interplay Between Electronic Structure and Dynamics

M. A. Ratner, *Presiding*
8:00 - 91. From electronic structure theory to electronic spectroscopy. **M. Nooijen**

8:40 - 92. Nonadiabatic dynamics on interpolated diabatic potentials. C. R. Evenhuis, **M. A. Collins**, X. Lin, D. H. Zhang

9:20 - 93. Dynamics Density Functional Theory: A tool for studies of coalescence of nanoparticles. **L. Wang**

10:00 - 94. A new efficient and accurate reaction path following algorithm. **H. P. Hratchian**, H. B. Schlegel

10:20 - Intermission.

10:40 - 95. Electron-proton correlation in the nuclear-electronic orbital method: Applications to hydrogen tunneling systems. **S. Hammes-Schiffer**

11:20 - 96. Semiclassical methods for electron dynamics. **T. Van Voorhis**

Section E
Unknown Site -- Unknown Room
Nanocrystals and Nanotubes
Nanocrystals and Nanotubes
Cosponsored with PRES

U. Woggon and M. Fuhrer, *Presiding*
8:00 - 97. Self-Assembly of Mesoscopic "Amphiphiles". **C. A. Mirkin**, S. Park, J. Lim, S. Chung

8:40 - 98. Manipulating Carbon Nanotubes with Nucleic Acids. **M. Zheng**

9:20 - 99. pH-dependent fluorescence of single-walled carbon nanotubes in aqueous suspension. **D. Tsyboulski**, S. M. Bachilo, R. B. Weisman

9:40 - 100. In situ growth of quantum dots on nanotube surfaces. S. Banerjee, **S. S. Wong**

10:00 - 101. Investigations on the effect of colloidal catalysis on the size and shape of transition metal nanocrystals. **R. Narayanan**, M. A. El-Sayed

10:20 - Intermission.

10:40 - 102. Electron transport in short macromolecular carbon nanotubes. **A. Javey**, H. Dai

11:20 - 103. Metallic nanorods and nanowires: synthesis, physical properties, and their use as templates for making hollow nanotubes. **C. J. Murphy**

Section F
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

B. B. Goldberg, *Presiding*
8:00 - 104. Single molecule charge transfer probed by cyclic voltammetry-single molecule spectroscopy. **A. J. Gesquiere**, S. Park, P. F. Barbara

8:40 - 105. Live Cell Imaging with Near-Field Optics. L. Kapkiai, D. Moore-Nichols, J. Carnell, **R. C. Dunn**

9:20 - 106. Probing energy transfer in molecular semiconductor thin films on a nanometer scale using NSOM. **S. K. Buratto**

9:40 - 107. Single molecule orientations determined by direct emission pattern imaging. **M. A. Lieb**, J. M. Z. Zavislan, L. Novotny

10:00 - Intermission.

10:20 - 108. Liquid Crystal and Charge Carrier Dynamics in Photorefractive Organic Thin Films. **D. A. Higgins**, J. E. Hall, A. Xie

11:00 - 109. Tailoring the near field for enhanced spectroscopies below the diffraction limit. **N. Halas**

11:40 - 110. Near field studies of RNA folding kinetics by single molecule FRET. **D. J. Nesbitt**, J. H. Hodak, A. Pardi, C. Downey

MONDAY AFTERNOON
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Electronic-Vibronic Dynamics

J. G. Underwood, *Presiding*

1:20 - 111. Towards imaging molecular dynamics with attosecond precision. **P. B. Corkum**

2:00 - 112. Four-wave mixing techniques applied to the investigation of non-adiabatic dynamics in polyatomic molecules. **M. Schmitt**, T. Siebert, R. Maksimenka, B. Dietzek

2:30 - 113. Two color photon echo peakshift: Probing electronic coupling in phthalocyanine dimers. **B. S. Prall**, D. Y. Parkinson, M. Yang, G. R. Fleming, N. Ishikawa

3:00 - 114. Femtosecond time-resolved photofragment translational spectroscopy: Applications to complex photodissociation reactions. **P. Cheng**, W. Chen, J. Ho

3:20 - Intermission.

3:40 - 115. Femtosecond time-resolved photoelectron/photoion coincidence imaging. **C. C. Hayden**

4:20 - 116. Using COLTRIMS to probe the dynamics of small molecules on a fs time scale. **C. L. Cocke**

Section B
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Spectroscopy and Potentials of Open-Shell Systems

M. A. Collins, *Presiding*
1:20 - 117. Infrared spectroscopy of intracluster reactions and solvation in metal ion complexes. **M. A. Duncan**

2:00 - 118. Threshold Photoionization and Photoion-Pair Production: Dynamics and Spectroscopy. **J. W. Hepburn**, Q. Hu

2:40 - 119. Intermolecular potentials and non-adiabatic effects in complexes of open-shell molecules. **A. van der Avoird**, G. C. Groenenboom, J. A. Klos, V. F. Lotrich

3:20 - Intermission.

3:40 - 120. Diffusion Monte Carlo studies of the structure, spectroscopy and dynamics of radials. **A. B. McCoy**

4:20 - 121. Role of the electron spin in non-bonding interactions of group 14 atoms with rare gases. **P. J. Dagdigian**

5:00 - 122. Bound states of open-shell complexes: Coupling of unquenched angular momentum to rotation in OH-acetylene complexes. **M. D. Marshall**, M. I. Lester

Section C
Unknown Site -- Unknown Room
Mass Spectrometry of Biopolymers: From Model Systems to Ribosomes
Structural Aspects
Cosponsored with ANYL

E. R. Williams, *Presiding*
1:20 - 123. Protein-protein interaction dynamics by amide H/^{2}H exchange mass spectrometry. **E. A. Komives**

2:00 - 124. Kinetics and equilibria of protein-ligand interactions by mass spectrometry and H/D amide exchange. **M. L. Gross**, M. M. Zhu, D. L. Rempel, R. Chitta

2:40 - 125. Mapping protein energy landscapes using H/D exchange. **I. A. Kaltashov**

3:20 - Intermission.

3:40 - 126. Measuring Gas Phase Structures of LHRH Variants: Is it Relevant to Biologists? **P. Barran**, N. Polfer, T. Wyttenbach, M. T. Bowers, R. P. Millar

4:20 - 127. Mass Spectrometry and Structural Biology of Ion Channels. **M. Cadene**, B. T. Chait

4:40 - 128. Data mining of 30,000 peptide dissociation spectra: how cleavage varies with charge. **Y. Huang**, V. H. Wysocki, L. Ji, J. M. Triscari, R. D. Smith, L. Pasa-Tolic, G. A. Anderson, M. S. Lipton

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Semiclassical Dynamics

F. J. Aoiz, *Presiding*
1:20 - 129. Using the semiclassical initial value representation to add quantum effects to classical molecular dynamics simulations. **W. H. Miller**

2:00 - 130. Semiclassical IVR and experimental NMR; how to use signal processing to improve performance. S. D. Kunikeev, **H. S. Taylor**

2:40 - 131. Matching-Pursuit for simulations of quantum processes. **V. S. Batista**

3:20 - Intermission.

3:40 - 132. Novel quasiclassical approaches for non-adiabatic molecular dynamics. **O. V. Prezhdo**

4:20 - 133. On the dynamics of coupled Bohmian and phase-space variables: A new hybrid quantum-classical approach. I. Burghardt, **G. Parlant**

4:40 - 134. Forward-backward semiclassical dynamics: Theory and application to quantum fluids. **N. Makri**

Section E
Unknown Site -- Unknown Room
Nanocrystals and Nanotubes
Nanocrystals and Nanotubes
Cosponsored with PRES

S. S. Wong and M. Zheng, *Presiding*
1:20 - 135. Charged colloid quantum dots. Photophysics and transport. **P. Guyot-Sionnest**, C. Wang, B. Wehrenberg, D. Yu

2:00 - 136. Functionalization of Carbon Nanotubes. **J. M. Tour**

2:40 - 137. Electrochemical gating and redox processes in carbon nanotube transistors. **M. Shim**

3:00 - 138. Langmuir monolayers of ferrite nanocrystals: Preparation, magnetic and magneto-electronic properties. **G. Markovich**, T. Meron, T. Fried, P. Poddar, T. Telem-Shafir, G. Shemer

3:20 - Intermission.

3:40 - 139. High mobility semiconducting nanotubes for nanoelectronics. **M. S. Fuhrer**, B. M. Kim, T. Durkop, T. Brintlinger, E. Cobas

4:20 - 140. Nanocrystals for controlling photons in single and coupled microspheres. **U. Woggon**, B. Möller, M. Artemyev

5:00 - 141. Extinction spectra of nanoparticle arrays: The influence of size, shape, and interparticle spacing. **S. Zou**, L. Zhao, N. Janel, G. C. Schatz

Section F
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

F. Keilmann, *Presiding*
1:20 - 142. Far-field fluorescence nanoscopy. **S. W. Hell**, M. Dyba, V. Westphal, L. Kastrup

2:00 - 143. Zero-mode waveguides for single molecule spectroscopy and DNA sequencing. **M. J. Levene**

2:40 - 144. Nanometer-scale imaging of self-organized protein patterns at lipid bilayer junctions. **R. Parthasarathy**, J. T. Groves

3:00 - 145. Localized photoconductivity measurements of conjugated polymer materials using near-field scanning optical microscopy. **J. M. Imhof**, G. A. Brasher, D. A. Vanden Bout

3:20 - Intermission.

3:40 - 146. Plasmon-enhanced near-field Raman spectroscopy of molecules and nano-crystals. **S. Kawata**

4:20 - 147. Electronic properties of nanowires and their effect on catalysis. **H. Metiu**

Section G
Unknown Site -- Unknown Room
Protein Structure Prediction and Folding: Where Physical Chemistry Meets Genomics

Z. Schulten, *Organizer, Presiding*
1:10 - Introductory Remarks.

1:20 - 148. CASP: Progress, bottlenecks and prognosis. **J. Moult**

2:00 - 149. The emerging science of protein structure prediction. **P. G. Wolynes**

2:40 - 150. The rough energy landscape of folded and unfolded proteins. **M. Gruebele**

3:20 - Intermission.

3:40 - 151. Molecular anatomy: Building complexes and cell networks from. **R. B. Russell**

4:20 - 152. T-jump infrared absorption detected protein folding kinetics. **H. Ma**, M. Gruebele

MONDAY EVENING
Section A
Unknown Site -- Unknown Room
Sci-Mix

D. J. Nesbitt, *Organizer*
8:00 - 10:00
249-256, 298, 317, 319-321, 323, 327, 333-334, 336, 344, 368, 379, 384, 389, 392, 394, 396-399, 425, 430, 435, 439, 445, 447, 452, 456, 458, 462, 466, 468-469. See subsequent listings.

TUESDAY MORNING
Section A
Unknown Site -- Unknown Room
PChem Award Symposium
Cosponsored with WCC

D. J. Nesbitt, *Organizer, Presiding*
8:20 - 153. Anion photochemistry: Free radicals, clusters, and time evolving states. **W. C. Lineberger**

9:00 - 154. Indeterminacies in molecular spectroscopy. **J. K. G. Watson**

9:40 - 155. Some interesting problems in atmospheric chemistry: Old perspectives and new challenges. **B. J. Finlayson-Pitts**

10:20 - Intermission.

10:35 - 156. Imaging and kinetics of surface reactions: Fundamental phenomena with applications to important problems. **J. C. Hemminger**

11:15 - 157. Chemical dynamics at metal surfaces. **J. C. Tully**

TUESDAY AFTERNOON
Section A
Unknown Site -- Unknown Room
PChem Award Symposium
Cosponsored with WCC

D. J. Nesbitt, *Organizer, Presiding*
1:15 - 158. Nanowires and nanoscale science: Building towards future technologies. **C. M. Lieber**

1:55 - 159. Progress in Organic Light Emitting Diodes. **C. W. Tang**, **S. A. Van Slyke**

2:35 - 160. Solid-state NMR investigations of the structure and dynamics of disordered and membrane-bound proteins. **M. Hong**

3:15 - Intermission.

3:30 - 161. Liquids near the glassy bottom of the liquid state: What is going on? **C. A. Angell**

4:10 - 162. The wonders of poly(ethylene oxide) in solution. **S. C. Greer**

4:50 - 163. Electron Transfer - Molecules, Junctions and Between. **M. A. Ratner**

WEDNESDAY MORNING
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Nuclear Dynamics

P. B. Corkum, *Presiding*
8:20 - 164. Ultrafast X-ray studies of material dynamics. **R. Falcone**

9:00 - 165. Femtosecond electron diffraction studies of barrier crossing dynamics: Towards "making the molecular movie". **R. J. D. Miller**

9:40 - 166. Ultrafast coherent control in x-ray scattering. **P. H. Bucksbaum**, D. A. Reis

10:20 - Intermission.

10:40 - 167. Coherent control for vibrational microspectroscopy applications. **D. Oron**, N. Dudovich, Y. Silberberg

11:20 - 168. Femtosecond pulse shaping for biological imaging. **W. S. Warren**

Section B
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Reactive Scattering

M. H. Alexander, *Organizer, Presiding*
8:00 - 169. Reaction dynamics of highly vibrationally excited molecules and chlorine radicals. **A. S. Mullin**

8:20 - 170. Crossed beam reactive scattering of open shell species using "soft" electron impact ionization for product detection: Primary products, branching ratios, and reaction dynamics. **P. Casavecchia**

9:00 - 171. Dynamics of abstraction reactions of polyatomic molecules. **A. J. Orr-Ewing**, C. Murray, S. Rudic, J. N. Harvey

9:40 - 172. From pair correlation to reactive resonance in a six-atom reaction. **K. Liu**, J. J. Lin, W. Shiu, J. Zhou

10:20 - Intermission.

10:40 - 173. Real wave packet reactive scattering of open shell species in combustion, atmospheric, and astrophysical processes. **C. Petrongolo**, P. Gamallo, M. González, P. Defazio

11:00 - 174. VTST for radical reactions: from low temperatures to combustion. **Y. Georgievskii**, S. J. Klippenstein, L. B. Harding

11:20 - 175. Stereodynamics of simple reactions: How does the direction of the initial rotation control the reactivity. **F. J. Aoiz**, L. Banares, M. P. Miranda

Section C
Unknown Site -- Unknown Room
Mass Spectrometry of Biopolymers: From Model Systems to Ribosomes
Methods
Cosponsored with ANYL

M. T. Rodgers, *Presiding*
8:20 - 176. Noncovalent enzyme-ligand complexes: gas and solution phase studies. **J. A. Leary**

9:00 - 177. Integrating surface-induced dissociation into simple TOF mass spectrometers. **V. H. Wysocki**, C. Gamage, Z. Qi, F. Fernandez

9:40 - 178. Ion soft land as a preparative method: Protein microarrays generated by mass spectrometry. **R. G. Cooks**, Z. Ouyang, Z. Takats, B. Gologan, T. M. Blake, V. J. Davisson

10:20 - Intermission.

10:40 - 179. Field induced droplet ionization: A new window on the world of biomolecules in the gas phase. **J. L. Beauchamp**, R. L. Grimm

11:20 - 180. Profiling intact proteins from cells by MALDI-MS. **R. R. Ogorzalek Loo**, F. Hung, R. Hayes, J. A. Loo

11:40 - 181. The curved field reflectron: PSD and CID without scanning, stepping or lifting. **R. J. Cotter**, B. D. Gardner, S. Iltchenko, D. Wang, R. Gundry

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Mixed Quantum/Classical Dynamics

J. M. Bowman, *Presiding*
8:00 - 182. Mixed quantum-classical dynamics. **J. C. Tully**

8:40 - 183. Mixed quantum and classical nonadiabatic dynamics and relaxation of the aqueous dielectron. **R. E. Larsen**, B. J. Schwartz

9:00 - 184. Trajectory surface hopping studies of intersystem crossing. B. Maiti, **G. C. Schatz**

9:40 - 185. Applications of QM, QM+MM, and QM/MM direct dynamics simulations. **W. L. Hase**

10:20 - Intermission.

10:40 - 186. Approximate simulations of quantum dynamics for systems of many stoms: Separable methods and extensions. **R. B. Gerber**, E. Fredj, P. Jungwirth

11:20 - 187. Time propagation of the quantum-classical density matrix for electronically excited molecular systems. **D. A. Micha**, A. Reyes, A. Pacheco, B. Thorndyke

Section E
Unknown Site -- Unknown Room
Nanocrystals and Nanotubes
Nanocrystals and Nanotubes
Cosponsored with PRES

Y. Xia and M. Maillard, *Presiding*
8:00 - 188. Growth of Ultralong and Aligned Single Walled Carbon Nanotubes Using a "Fast Heating" Chemical Vapor Deposition Method. **J. Liu**

8:40 - 189. Strategy and Design in Transition Metal Oxide Nanocrystal Synthesis. **S. O'Brien**, M. Yin

9:20 - 190. Temperature dependence of optical transitions in single-walled carbon nanotubes. **S. M. Bachilo**, R. B. Weisman

9:40 - 191. Colloidal nanocrystal heterostructures with core/shell, linear, and branched topology. **D. J. Milliron**, S. Hughes, A. P. Alivisatos

10:00 - 192. Crystallographic alignment of high density gallium nitride nanowire arrays. **P. J. Pauzauskie**, T. Kuykendall, D. J. Sirbuly, J. D. Denlinger, P. Yang

10:20 - Intermission.

10:40 - 193. Controlling the structure of single-walled carbon nanotube with purposely designed heterogeneous catalysts. **D. E. Resasco**, J. E. Herrera, L. Balzano

11:20 - 194. Applications of Quantum Dots with Near-Unity Quantum Efficiencies. **C. Z. Hotz**, J. A. Treadway, D. A. Zehnder

Section F
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

L. Novotny, *Organizer, Presiding*
8:20 - 195. Playing with Lightning: Fluorescence Apertureless Near Field Microscopy. **S. R. Quake**

9:00 - 196. Spectral focusing: High resolution CARS microscopy with broad-band pulses. **A. Zumbusch**, T. Hellerer, A. Enejder, O. Burkacky

9:40 - 197. Correlated topographic and spectroscopic imaging beyond diffraction limit by metallic tip-enhanced near-field fluorescence lifetime microscopy. **D. Hu**, M. Micic, N. Klymyshyn, Y. D. Suh, H. P. Lu

10:00 - 198. Slow diffusion of single molecules in solution near periodic nano-structured templates. **E. Mei**, A. Sharonov, F. Gao, R. M. Hochstrasser

10:20 - Intermission.

10:40 - 199. New tools for nanoscale analyses. **P. S. Weiss**

11:20 - 200. Near-field scanning optical microscopy studies of interchain species in MEH-PPV films. **R. D. Schaller**, L. F. Lee, J. C. Johnson, R. J. Saykally, T. Nguyen, B. J. Schwartz, J. S. Vieceli, I. Benjamin

Section G
Unknown Site -- Unknown Room
Protein Structure Prediction and Folding: Where Physical Chemistry Meets Genomics

M. Gruebele, *Presiding*
8:20 - 201. Proteome Scale Protein Fold and Function Prediction. **J. Skolnick**

9:00 - 202. Comparative analysis of protein thermal adaptation. **G. J. Olsen**

9:40 - 203. The TIM barrel motif: alternative solutions to a common folding problem. **R. C. Matthews**

10:20 - Intermission.

10:40 - 204. Protein folding in cages. **D. Thirumalai**

11:20 - 205. Evolution of Structure in the Aminoacyl-tRNA Synthetases. **P. M. O'Donoghue**, Z. Luthey-Schulten

WEDNESDAY AFTERNOON
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Electronic-Vibronic Dynamics

R. J. D. Miller, *Presiding*
1:20 - 206. Multiphoton EUV photonics and applications in ultrafast chemical spectroscopies. H. C. Kapteyn, **M. M. Murnane**

2:00 - 207. Tunable two-dimensional femtosecond spectroscopy. **T. Brixner**, I. Stiopkin, M. Yang, G. R. Fleming

2:30 - 208. Relaxation dynamics in Hg(n)- : one and two electron dynamics in clusters. **J. R. R. Verlet**, A. E. Bragg, A. Kammrath, O. Cheshnovky, D. M. Neumark

3:00 - 209. Laser-induced ultrafast dynamics in C_{60} and electron correlation effects. **G. Zhang**, T. F. George, D. A. Jelski

3:20 - Intermission.

3:40 - 210. Ultrafast control of simple solution phase reactions. **R. J. Sension**, P. H. Bucksbaum, B. Pearson, E. Carroll, A. Florean, A. Prociuk

4:20 - 211. Strongly driven electrons - from slow photoelectron imaging to attosecond laser pulses and cluster explosions. **M. J. J. Vrakking**

Section B
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Frontiers in Photoelectron Spectroscopy

W. C. Lineberger, *Presiding*
1:20 - 212. Probing the reactivity of metal oxide clusters using mass spectrometry and anion photoelectron spectroscopy. **C. C. Jarrold**

2:00 - 213. Visualisation of photodetachment dynamics in reactive cluster anions. **A. Sanov**, R. Mabbs, E. Surber

2:40 - 214. Photodetachment of multiply charged anions. **L. Wang**

3:20 - Intermission.

3:40 - 215. Photoelectron spectroscopy of gas phase fullerene dianions. **J. M. Weber**, O. T. Ehrler, F. Furche, M. Kappes

4:20 - 216. Time-resolved dynamics in mercury and carbon cluster anions. **D. M. Neumark**, O. Cheshnovksy, A. E. Bragg, J. Verlet, A. Kammrath

5:00 - 217. DC slice imaging as a probe of vector correlations in open-shell systems. **D. Townsend**, S. K. Lee, M. P. Minitti, A. G. Suits

Section C
Unknown Site -- Unknown Room
Mass Spectrometry of Biopolymers: From Model Systems to Ribosomes
Model Systems
Cosponsored with ANYL

V. H. Wysocki, *Organizer, Presiding*
1:20 - 218. Hydration energetics of metallated amino acids. **P. B. Armentrout**, R. M. Moision, S. Ye

2:00 - 219. Hydration of small peptides. **T. Wyttenbach**, D. Liu, M. T. Bowers

2:40 - 220. High pressure mass spectrometric investigations of clustering reactions of protonated amino acids and amino acid esters. **T. B. McMahon**, A. Simon, S. Raspopov

3:20 - Intermission.

3:40 - 221. Nucleic acid reactivity: model studies. **J. K. Lee**

4:20 - 222. Structures and energetics of metal ion – nucleobase complexes. **M. T. Rodgers**, Z. Yang

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Novel Optical Probes: A Challenge to Theory

H. J. Kim, *Presiding*
1:20 - 223. Femtosecond and 2D Fourier transform experiments on Jahn-Teller dynamics. **D. M. Jonas**, D. A. Farrow, W. Qian, E. R. Smith, A. A. Ferro

2:00 - 224. Amide I vibrational dynamics of polypeptides: MD simulation studies and applications to coherent multidimensional vibrational spectroscopies. **M. Cho**

2:40 - 225. Reinterpreting the molecular origins of optical nonlinearity. **G. J. Simpson**

3:00 - 226. Classical and semiclassical vibrational echos. **W. G. Noid**, G. S. Ezra, R. F. Loring

3:20 - Intermission.

3:40 - 227. Ultrafast pulse shaping for control and automated learning in quantum systems. **H. C. Kapteyn**, M. M. Murnane

4:20 - 228. Quantum propagation on trajectory guided random grids of Coupled Coherent States. **D. Shalashilin**, M. Child

4:40 - 229. Structure, dynamics, and hydrogen bonding fluctuations of peptides probed by coherent infrared multidimensional spectra. **S. Mukamel**, D. Abramavicius, T. Hayashi, W. Zhuang, A. M. Moran, T. I. Jansen, R. Venkatramani

Section E
Unknown Site -- Unknown Room
Nanocrystals and Nanotubes
Nanocrystals and Nanotubes
Cosponsored with PRES

J. Liu and D. E. Resasco, *Presiding*
1:20 - 230. Shape-controlled synthesis of nanostructured materials. **Y. Xia**

2:00 - 231. Single molecule Raman spectroscopy and shape-controlled nanocrystal growth related to plasmon excitation. **M. Maillard**, P. Huang, J. Jiang, K. Bosnick, L. Brus

2:40 - 232. Growth of gold nanorods on surfaces. **G. Markovich**, N. Taub, O. Krichevski, T. Fried

3:00 - 233. Synthesis and characterization of single crystal metallic nanowires. **Y. Wu**, J. Xiang, C. M. Lieber

3:20 - Intermission.

3:40 - 234. Plasmonic nanoparticles by rational design. **N. Halas**

4:20 - 235. Electronic structure of single-walled carbon nanotubes and interaction with atoms and molecules: synchrotron radiation photoelectron spectroscopy investigations. **A. Goldoni**, R. Larciprete, L. Petaccia, S. Lizzit

5:00 - 236. High-performance nanowire electronics and photonics on glass and plastic substrates. **M. C. McAlpine**, C. M. Lieber

Section F
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

R. C. Dunn, *Presiding*
1:20 - 237. Single molecule detection: femtosecond dynamics on the nanometer scale. E. M. H. P. van Dijk, J. Hernando, M. F. García-Parajó, **N. F. van Hulst**

2:00 - 238. Nano-optics for infrared chemical imaging and heat assisted magnetic recording. **G. C. Walker**, B. B. Akhremitchev, L. Stebounova, T. E. Schlesinger, J. Bain, F. Chen

2:40 - 239. Coherent anti-Stokes Raman nano-imaging with metal-tip field enhancement. N. Hayazawa, T. Ichimura, M. Hashimoto, Y. Inouye, **S. Kawata**

3:00 - 240. Computed imaging and tomography for near-field optics. **P. S. Carney**

3:20 - Intermission.

3:40 - 241. Probing single molecules by surface enhanced Raman spectroscopy. **A. J. Meixner**, T. Vosgröne, A. Hartschuh, H. Kneppe, W. Plieth

4:20 - 242. Plasmon optics to localize and enhance chemical interaction. **O. J. F. Martin**

Section G
Unknown Site -- Unknown Room
Protein Structure Prediction and Folding: Where Physical Chemistry Meets Genomics

C. R. Matthews, *Organizer, Presiding*
1:20 - 243. Evolution of proteins from peptides. **A. Lupas**

2:00 - 244. Exploring the protein funnel energy landscape for folding and function. **J. N. Onuchic**

2:40 - 245. Evolutionary optimized protein folding reactions. **T. Kiefhaber**

3:20 - Intermission.

3:40 - 246. Fold recognition without folds. **K. K. Koretke**, A. Lupas, R. B. Russell

4:20 - 247. Gatekeepers and protein folding: insights from the theoretical investigation of minimalist models. **A. D. Stoycheva**, J. N. Onuchic, C. L. Brooks III

WEDNESDAY EVENING
Section A

Unknown Site -- Unknown Room
Poster Session

D. J. Nesbitt, *Organizer, Presiding*
7:30 - 9:30
248. Coherent excitations in a two dimensional multi-chromophore macromolecule using ultra-fast nonlinear optical spectroscopy. **S. A. Lahankar**, T. Goodson III

249. Experimental and Theoretical Considerations of SO2 Adsorption on VOx Cluster Anions. **R. B. Wyrwas Jr.**, J. A. Bradshaw, A. J. Leavitt, R. L. Whetten

250. Infrared signature of structural changes associated with the "magic" H3O+(H2O)20 cluster. J. Shin, **N. I. Hammer**, E. G. Diken, J. M. Headrick, M. A. Johnson, R. S. Walters, T. D. Jaeger, M. A. Duncan, R. A. Christie, K. D. Jordan

251. Near ultraviolet photodissociation of vinoxy radical via the B^2A'' state: the H-atom product channel. K. Xu, G. Amaral, **J. Zhang**

252. Spectroscopy and photodissociation dynamics of microsolvated multiply-charged transition metal ions. **R. B. Metz**

253. Structure and dynamics of dipole-bound cluster anions. **P. Jungwirth**, M. Sindelka, S. Ronen, B. Schmidt, D. Nachtigallova, V. Spirko

254. Toward ab initio cavities in dielectric continuum models of solvation: Application to radicals and ions in water. **M. Dupuis**, D. M. Camaioni

255. Ultrafast infrared studies of orientational dynamics of cyanoferrates in solution and reverse micelles. **G. M. Sando**, Q. Zhong, J. C. Owrutsky

256. Vibrational spectroscopy of ions and radicals present in the interstellar medium and in planetary atmospheres: A theoretical study. **G. M. Chaban**

257. Ultrafast Selected Energy X-ray Absorption Spectroscopy (USEXAS) for Chemical Dynamics Studies. **T. Guo**, F. Shan, C. Houchines, J. E. Carter

258. Ultrafast spectroscopic studies on energy transfer processes in application of cationic conjugated polymer as DNA sensors. **Q. Xu**, B. J. Gaylord, S. Wang, G. C. Bazan, D. Moses, A. J. Heeger

259. Vibrational dynamics in five-coordinate, high-spin hemes. **M. C. Simpson**, J. R. Challa, T. Gunaratne

260. Ab initio characterization of van der Waals excited states of ClOO. **K. K. Irikura**

261. Ab initio study of the O_2-N_2O complex. **W. M. Fawzy**

262. Dynamics of charge-transfer-to-solvent relaxation in small iodide-solvent clusters. Q. K. Timerghazin, **G. Peslherbe**

263. Experimental approaches to measure the enthalpies of formation of organic radicals in solution. **T. Autrey**, J. Franz, D. M. Camaioni

264. Large-scale assembly of carbon nanotube-based circuit structures. **S. Hong**, S. Rao, L. Huang

265. Fluorescence from aromatic radical cations in sulfuric acid. **J. F. Kauffman**, J. Turner, M. W. Karl

266. Fabrication and Applications of Porous Silicon Structures Patterned by Dry-Removal Soft Lithography. **D. J. Gargas**, D. J. Sirbuly, G. M. Lowman, B. J. Scott, G. D. Stucky, S. K. Buratto

267. H_2S dissociation on Fe(110) from first principles. E. A. Carter, **D. E. Chang**

268. Investigation of a two-state mechanism for reactions involving nitric oxide: Nonadiabatic quantum dynamics of FO + NO. **J. M. Herbert**, A. B. McCoy, J. F. Stanton

269. Potential for Single Walled Carbon Nanotube Purification via Polymer-Assisted Dispersion in Alcohols. **J. H. Rouse**, E. J. Siochi

270. Synthesis and characterization of uniform diameter single walled carbon nanotubes in Co-MCM-41. **D. Ciuparu**, Y. Chen, S. Lim, G. L. Haller, L. Pfefferle

271. Ion-surface scattering trajectories from first principles electronic structure and dynamics calculations of charge transfer lifetimes. E. A. Carter, **K. Niedfeldt**, P. Nordlander

272. Low-temperature emission spectra of individual single-wall carbon nanotubes: Multiplicity of subspecies within "single-species" nanotube ensembles. **H. Htoon**, M. J. O'Connell, P. J. Cox, S. K. Doorn, V. I. Klimov

273. Measurement of the elastic properties of metal nanorods by ultrafast spectroscopy. **G. V. Hartland**, M. Hu, X. Wang, P. Mulvaney, J. Sader

274. Photoinduced charge separation and charge transfer in CdSe quantum dots. **P. V. Kamat**, S. Sharma, V. Subramanian

275. Jet Spectroscopy and Excited State Dynamics of Diphenylmethyl Radical and its Derivatives. **M. Tsuge**, S. Hamatani, A. Kawai, K. Tsuji, **K. Shibuya**

276. KINETICS OF OXIDATION OF ADENOSINE BY t-BUTOXYL RADICAL -. **A. Mundra**

277. Mixed-state kinetics in the collision-induced intersystem crossing of methylene*. **G. E. Hall**, A. Komissarov, A. Lin, T. J. Sears

278. Lanthanide(III)-based luminescent processable nanoparticles and their applications. **F. C. van Veggel**, J. W. Stouwdam, G. A. Hebbink, J. Huskens

279. Photophysics of quantum dots bound to amino acids, polypeptides and genetically engineered proteins. **G. Rumbles**, M. Jones, M. E. Himmel, S. Ding

280. Luminescence from PbS nanoparticles and their quenching with water. **S. W. Buckner**, P. A. Jelliss, R. Konold

281. Molecular Mechanism of the Reactions of Nitrous Oxide with Metal Atoms: A Theoretical Study. **M. T. Nguyen**, O. Tishchenko

282. New Spectroscopic Detection of Acetylene in the Highly-Excited Gerade Rydberg States. **K. Misawa**, K. Tsuji, A. Kawai, **K. Shibuya**

283. Self-assembled nanoporous origami silica crystals. **I. Sokolov**, Y. Kievsky

284. Melting of unsupported clusters and nanocrystals. **G. A. Breaux**, **M. Jarrold**

285. Nonadiabatic quantum dynamics using derivative propagation along quantum trajectories. G. Parlant, **J. Julien**

286. Nonequilibrium projection operator formulation of path integral centroid dynamics. **S. Jang**

287. Novel quasi-classical approach to complex autocorrelation function. **P. R. Zdanska**

288. Photonic nanowires investigated by simgle molecule fluorescence and atomic force microscopy. **J. Hernando**, P. A. J. de Witte, E. M. H. P. van Dijk, R. J. M. Nolte, A. E. Rowan, M. F. Garcia-Parajo, N. F. van Hulst

289. Slow structuring kinetics of the dense liquid precursor determines the rate of crystal nucleation. **P. G. Vekilov**, O. Galkin, L. F. Filobelo

290. Novel methods for producing transition metal doped nanoparticles. **G. P. Glaspell II**, A. Manivannan

291. Probing the interactions ion-molecule bimolecular reactions. **M. R. Salazar**

292. Surface chemistry of quantum dots. K. M. Gattás-Asfura, C. A. Constantine, G. Sui, J. Orbulescu, **R. M. Leblanc**

293. Probing the Intrinsic Electronic Structure of the Cubane [4Fe-4S] Cluster. X. Wang, S. Niu, **X. Yang**, S. K. Ibrahim, C. J. Pickett, T. Ichiye, L. Wang

294. PbSe nanocrystals: Auger processes, optical gain, and amplified spontaneous emission. **R. D. Schaller**, M. A. Petruska, V. I. Klimov

295. Pulsed-field-ionization ZEKE spectroscopy of metal complexes with multidentate ligands. **D. Yang**, X. Wang, S. Li, J. Fuller, B. Sohnlein, P. Bhowmik

296. Quantification of photoacid generation in photolithography at 157, 193 and 248 nm using a novel method. **M. G. Ivan**, J. C. Scaiano

297. Synthesis, microstructural characterization, and spectroscopic studies of "inverted" core/shell ZnSe/CdSe nanocrystals. **S. A. Ivanov**, J. Nanda, M. Achermann, V. I. Klimov

298. Quantum origin of anomalous isotope effect in ozone formation. **D. Babikov**, B. K. Kendrick, R. B. Walker, R. T. Pack

299. Reactions of atmospherically important nitrogen ion species at high temperatures: experiment and theory. **A. Midey Jr.**, S. Popovic, A. Fernandez, S. Williams, A. A. Viggiano, P. Zhang, S. Irle, K. Morokuma

300. Protein structural information using FTIR, CD and Raman. **A. L. Jenkins**, R. A. Larsen, K. Akao, T. Williams

301. Reliable prediction of reaction rates in spin-forbidden reactions: Rational design of paramagnetic chromium catalysts. **D. J. Doren**, D. R. Fitzgerald, J. S. Hess, K. H. Theopold

302. Semiclassical dynamics based on linearized quantum force. **V. A. Rassolov**, S. Garashchuk

303. Superexcited state dynamics probed with an extreme-ultraviolet free electron laser. **W. Li**, R. R. Lucchese, A. G. Suits

304. The bond strength of water in water; solvent effects on the thermochemistry of hydroxyl radical in aqueous solvents. **T. Autrey**, D. M. Camaioni

305. Theory of open-shell metal atoms in cryogenic clusters. J. A. Boatz, R. J. Hinde, J. A. Sheehy, **P. W. Langhoff**

306. Thermochemistry, Kinetics and Kinetic Modeling on Atmospheric Reactions of the Benzene-OH - Adduct with O2. **J. W. Bozzelli**, C. Chen

307. Toward a unifying approach to coherent state theory: from nuclei to electrons. **J. A. Morales**

308. Ultraviolet photodissociation dynamics of n-propyl and iso-propyl radicals. **W. Zhou**, Y. Yuan, **J. Zhang**

309. Vertical Franck-Condon model: A general adiabatic approach for calculating electronic absorption spectra. **A. Hazra**, M. Nooijen

310. Vibrational dynamics from the molecule's perspective. **J. D. Eaves**, C. J. Fecko, J. J. Loparo, A. Tokmakoff, P. L. Geissler

311. Vibrational relaxation dynamics of cyanoferrates in solution. **J. C. Owrutsky**, G. M. Sando, Q. Zhong

312. ZEKE spectra of Ar_nI^- (n=2-7) by quasi-classical calculation. **P. R. Zdanska**, N. Moiseyev, B. Schmidt, P. Jungwirth

313. A completely general method for utilizing highly accurate ab initio potentials in dynamical calculations. **M. R. Salazar**

314. A semiclassical study of decoherence of an anharmonic oscillator in a thermal bath. **Y. Elran**, P. Brumer

315. Canonical representations and efficient propagations schemes for Quantum-Gaussian-Classical dynamical models. **P. Grochowski**, B. Lesyng

316. Computational analysis and simulation of hydrogen chemisorption to carbon nanotubes: Energetics as a function of nanotube size and geometry. **R. C. Brown**, J. J. Vadnal, L. Karapuda

317. Dielectric properties of liquid water from first principles. **M. Sharma**, R. Car

318. Mixed quantum and classical dynamics with many electron wavefunctions: Efficient real-space configuration-interaction method for nonadiabatic dynamics. **R. E. Larsen**, B. J. Schwartz

319. Mixed quantum-classical dynamics of hydrated electrons in fluctuating-charge water. **J. E. Aremu-Cole**, G. Goodyear, S. J. Stuart

320. Mixed quantum/classical simulations of electron photodetachment in charge-transfer-to-solvent (CTTS) reactions. **C. J. Smallwood**, M. J. Bedard, W. B. Bosma, R. E. Larsen, B. J. Schwartz

321. Low temperature IR spectroscopy of water and ammonia ices. **J. N. Stone**, R. F. Ferrante, M. H. Moore

322. Menshutkin reaction in quadrupolar solvents. **S. Dorairaj**, H. J. Kim

323. Microsolvation and Acidity : Implications towards heterogeneous chemistry. **M. Sharma**, W. I. -. Kuo, R. Car, C. J. Mundy

324. Monte Carlo simulations of 1,2-dichloroethane in nanoconfined systems. **A. K. Phillips**, T. D. Shepherd, W. H. Thompson

325. Multi-walled carbon nanotube coatings for improved thermal contact. **J. L. Sample**, R. Osiander, K. Rebello, H. Saffarian

326. Non-Born-Oppenheimer quantum chemistry of atoms and molecules. **M. L. Cafiero**

327. Novel structures of platinum and gold clusters predicted from Density Functional Theory calculations. **L. Xiao**, L. Wang

328. On the Dissolving Drop and Finite Speed Mass Diffusion and Relaxation. **K. R. Sharma**

329. On the planarity of small gold clusters: A photoelectron spectroscopy and density-functional study. **H. Zhai**, H. Hakkinen, B. Yoon, U. Landman, X. Li, L. Wang

330. One color femtosecond laser photochemistry of 2,4,6-Trinitrotoluene. **L. M. Gomez**, S. P. Hernandez, N. Mina, A. Santana, A. La Pointe, S. Grossman, **M. E. Castro**

331. Overall rotation and internal motions in molecular dynamics. **F. J. Lin**

332. Nanotubes with complex wall architectures by template wetting. **M. Steinhart**, P. Göring, Y. Luo, H. Hofmeister, A. Greiner, J. H. Wendorff, R. B. Wehrspohn, E. Pippel, U. Gösele

333. Overtone excitation of gas-phase hydroperoxides. S. Hsieh, **S. C. Homitsky**, L. A. Morrison

334. Photoelectron spectroscopic studies of complex anion solvation in the gas phase. **X. Wang**, X. Yang, Y. Fu, L. Wang

335. Potential dependant sum frequency generation study of 5-methylbenzotriazole on polycrystalline copper, platinum, gold, and Cu(111). **C. R. Romero**, S. Baldelli

336. Predicting shielding constants in solution using gauge invariant atomic orbital theory and the effective fragment potential method. **M. A. Freitag**, B. Hillman, A. Agrawal, M. S. Gordon

337. Prediction of the acidities of carboxylic acids, phenols, and related compounds using calculated molecular properties of their complexes with water and ammonia. **L. Tao**, F. Tao

338. Protein structure prediction using minimal NMR data and a simple residue-based force field. **B. L. Eggimann**, A. Mascioni, J. I. Siepmann, G. Veglia

339. Pyrrolidinone hydrogen-bonding in carbon tetrachloride: experiment and theory. **S. G. Lieb**

340. Quantitative characterization and theoretical analysis of silica tube growth in chemical gardens. **S. Thouvenel-Romans**, O. Steinbock

341. R2PI and UV-UV hole burning spectroscopy of small peptides. **A. G. Abo-Riziq**, B. Crews, L. Grace, M. DeVries

342. Radical anions of bis- tris- and tetrakis-cyclooctatetraeneoxyalkane systems: A unique interannular p-p communication. **S. J. Peters**, C. D. Stevenson, L. F. Szczepura, R. C. Reiter

343. Radius of curvature effect of Co-MCM-41 on the size of single-walled carbon nanotubes. **S. Lim**, D. Ciuparu, Y. Chen, L. Pfefferle, G. L. Haller

344. Rate constants and products of the reactions of $PO_xCl_y^-$ ions with O_2 and O_3. **A. Fernandez**, A. J. Midey, T. M. Miller, A. A. Viggiano

345. Ratio of Convection To Storage and Origin of Pulsations that is Subcritical Damped Oscillatory. **K. R. Sharma**

346. Reconstructing macromolecular assembly from individual subunits. **I. Y. Torshin**

347. Resonance Raman and computational study of resveratrol and related stilbene derivatives. **J. D. Scanlan**, D. Bernhardson, **J. M. Smith**

348. Rotational spectra and structures of the $C_5H_5Mo(CO)_3H$ and $C_5H_5W(CO)_3H$ complexes. **C. Tanjaroon**, K. Keck, M. Sebonia, C. Karunatilaka, S. G. Kukolich

349. Silver nanostructures from nanoparticles at the liquid-liquid interface. J. K. Sakata, A. Dwoskin, **E. M. Spain**

350. Simulation of environmental effects on coherent quantum dynamics in many-body systems. **J. M. Riga**, C. C. Martens

351. Simulation of molecular dynamics on coupled electronic states using the semiclassical Liouville approach with a single trajectory ensemble. **E. Roman**, C. C. Martens

352. Simulation of quantum effects in thermally activated chemical processes using entangled trajectory ensembles. **J. Goldsmith**, C. C. Martens

353. Synthesis and Acidity of Mesoporous Aluminosilicates MCM-41. **C. Song**, **Z. Yan**

354. Electron transfer in a dissipative environment: A modified Zusman equation. **Q. Shi**, **E. Geva**

355. Simulations of the large kinetic isotope effect and the temperature dependence of the hydrogen atom transfer in lipoxygenase. **M. H. M. Olsson**, A. Warshel

356. Synthesis and Optical Properties of Anisotropic Metal Nanoparticles. **E. Hao**, J. T. Hupp, G. C. Schatz

357. Solvent Effects on M(EDTA) Complexes in Determining the Metal Cation Concentrations and Their Intramolecular Dynamics. **S. Han**, Y. Ba

358. Synthesis of Size Quantized Arylthiol/Gold Nanocrystals. **R. C. Price**, T. G. Schaaff

359. Spatially resolved, high sensitivity Raman spectroscopy for probing polymer films and catalysts. **E. L. Orazem**, S. Cross, A. Ranasinghe, M. A. Summers, S. K. Buratto

360. Spectrally resolved vibrational coupling of two different modes of a small molecule through triply vibrationally enhanced four-wave mixing. **K. A. Meyer**, D. E. Thompson, J. C. Wright

361. Stopped flow kinetics of Phycocyanin subunit refolding. **K. L. Thoren**, Y. M. Gindt

362. Tribochemical effects in linear sliding of carbon nanotubes. **S. J. Stuart**, P. L. Piotrowski, M. H. Müser

363. Structure and Energetics of [B, C, F, H_2]: Quantum chemistry shows multiple minima. **C. A. Deakyne**, A. K. Corum, J. F. Liebman

364. Structure of protonated water clusters: Finite temperature behavior. **J. Kuo**, M. L. Klein

365. Study of the reaction of CH_3CHO + Cl using TR-FTIR spectroscopy. **Y. Gong**, V. I. Makarov, B. R. Weiner

366. Synthesize and application of higher alcohol acrylates. **L. Song**, C. Jiang, Z. Han

367. The intriguing O_2(B, Triplet Sigma) + N_2 -> NO + NO (or N + NO_2) reaction: Its pragmatic importance and physical chemistry challenges. **S. Prasad**

368. The Reaction of NH2 with O2 in the Presence of H2O. **R. D. Johnson III**, R. E. Huie

369. Theoretical Investigation of the Two-Photon Absorption Cross Sections of Anthocyanidin Compounds. **J. N. Woodford**

370. Theoretical studies on atmospheric Criegee reactions with water: transition state and rate constant calculations. **C. Wu**, F. Tao

371. Theoretical study of adsorption of water dimer on the perfect MgO (100) surface: Molecular adsorption versus dissociative chemisorption. **Y. Wang**, T. N. Truong

372. Theoretical study of the rates and branching ratios for the reaction of acrolein with hydroxyl radical. **J. K. Merle**, C. M. Hadad

373. Time-resolved absorption studies of the radical-radical reaction: NCO+ CH3. **R. G. Macdonald**, Y. Gao

374. Time-resolved resonance Raman and density functional theory study of intermediates produced upon photolysis of p-hydroxyphenacyl acetate. C. Ma, **P. Zuo**, W. M. Kwok, W. S. Chan, D. L. Phillips

375. Two and three-body dissociative charge exchange dynamics of H3-+. **C. M. Laperle**, J. E. Mann, R. E. Continetti

376. Two methods for relating MO theory to structural formulas applied to cyclopropenyl cation and cyclobutadiene. **J. D. Alia**, M. C. Nupen

377. Ultrafast infrared absorption and dynamic ellipsometry of shock-compressed energetic materials. **D. S. Moore**, S. D. McGrane, D. J. Funk

378. Ultrafast ionization-induced charge transfer in 2-phenylethyl-N,N-dimethylamine. **W. Cheng**, N. Kuthirummal, J. L. Gosselin, W. Nie, P. M. Weber, R. Weinkauf

379. Using Cavity Ringdown Spectroscopy to Measure Equilibrium Constants: NO2 - N2O4 at 260-280K. **M. F. Tuchler**, **K. Schmidt**

380. Vibrational Micro-Raman measurements of 2,4-DNT and 2,6-DNT and their interactions with sand particles. **A. Blanco**, J. Castillo, N. Mina, M. E. Castro, S. Hernández-Rivera

381. Water-catalyzed dehalogenation reactions of isobromoform and its reaction products. **Y. L. Li**, W. M. Kwok, C. Zhao, X. Guan, D. L. Phillips

382. Surface Enhanced Resonance Raman Scattering of an azo dye on silver colloid at 632, 514 and 488 nm. **B. D. Gilbert**, H. Olejnik

383. Theory of FRET Distributions from Single-Molecule Experiments. **I. Gopich**, A. Szabo

384. Microwave measurements of the molecular structure of o-benzyne. **S. G. Kukolich**, C. Tanjaroon, M. C. McCarthy, P. Thaddeus

385. NH radical reactions studied in a pulsed supersonic laval nozzle flow reactor between 50 – 200 K. **C. Mullen**, M. A. Smith

386. Nonadiabatic MD simulations of IBr^- photodissociation. **M. A. Thompson**, R. Parson

387. OH-stretch relaxation of methanol in solution. **T. S. Gulmen**, E. L. Sibert III

388. Our ab initio calculations and kinetics study on unimolecular reactions of ethoxy radical. **Y. Zhang**, S. Zhang, Q. S. Li

389. Photodissociation dynamics of BrCN and ICN in solution. **A. C. Moskun**, S. E. Bradforth

390. Photodissociation dynamics of the ethoxy free radical. **A. E. Faulhaber**, **K. E. Kautzman**, D. M. Neumark

391. Photodissociation of Ozone embedded in water clusters. D. M. M. Philip, **S. D. Dalosto**, **V. S. Batista**

392. Near IR cavity ringdown spectroscopy of chloro-alkyl peroxyl radicals. **A. Deev**, D. N. Powers, J. Sommar, M. Okumura

393. Solvent effects in molecular or metal cation recognition. T. Buthelezi, **M. O'Brien**, **R. Smalley**

394. Spectroscopic studies of aqueous alkali halide solution surfaces. **E. A. Raymond**, G. L. Richmond

395. Time correlation functions for quantum fluids using forward-backward semiclassical dynamics. **A. Nakayama**, N. Makri

396. Ultrasensitive spectroscopy and kinetics studies using NICE-OHMS. **J. Bood**, D. L. Osborn, A. McIlroy

397. What really prevents proton transport through aquaporin? Charge self-energy versus proton wire proposals. **A. Burykin**, A. Warshel

398. A fluctuating charge force field for methanol: liquid-vapor interfacial properties. **S. Patel**, C. L. Brooks

399. Time dependent dynamics of $Ne^{79}Br_2$. **J. A. Cabrera**, C. Bieler, W. Van der Veer, K. Janda

400. REMPI Spectroscopy of actinide oxides . M. C. Heaven, **V. Goncharov**, J. Han, L. Kaledin

401. *Ab Initio* density functional study of the IR spectra and conformers of fluorinated acyl pernitrate compounds. **J. E. Stevens**

402. A comparison study of LiH and NaH. **B. K. Taylor**

403. A density functional study of relative stabilities of various conformations and substitutions of the 12,13 epoxy-trichothec-9-ene nucleus. **S. J. Gudowski**, F. Tao

404. A density functional theory study of explicit solvent effect on the conformational stability of the alpha-L-aspartate-containing dipeptide. **M. Moffitt**, F. Tao

405. A novel method for the detection of triacetone triperoxide (TATP) on surfaces using fiber optic coupled FT-IR. **O. M. Primera**, L. Pacheco, L. F. De la Torre, S. P. Hernandez, R. T. Chamberlain, R. T. Lareau

406. A Spectroscopic Study of the Electronic and Protein Structural Properties of Hemerythrin. **J. Hayes**, M. D. Edington

407. Ab initio QM/MM Simulation with Proper Sampling: a study of the reaction of Orotidine-5'-Monophosphate Decarboxylase. **E. Rosta**, A. Warshel

408. Ab initio study cis and trans cycloheptene isomerization. M. Squillacote, **Q. Shu**

409. Ab initio study of metallic species in the upper atmosphere. **G. Sánchez**, R. Berríos, R. Delgado, J. S. Friedman, Y. Ishikawa, B. R. Weiner

410. Ab initio study of the UV spectrum of the 1, 1', 5, 5' – tetramethyl – 6, 6' – dioxo – 3 – 3' – biverdazyl diradical. **C. J. Utter**, J. E. Stevens

411. Additivity of the basis set superposition error in noble gas clusters, noble gas cluster ions, and water clusters. **L. M. Visco**, F. Tao

412. Alcohol-induced conformational changes of Cytochrome c on fused silica surfaces. **M. Su**, H. Chang, K. M. Gligorich, G. C. Hoops, T. A. Hopkins, S. A. Hocker, S. Lin, S. Mistry, Y. Cheng

413. Alkaline-earth cations enhance ascorbate oxidation rates in the presence of orto-quinones, but not para-quinones: role of metal chelation by semiquinones. **A. E. Alegria**, P. Sanchez-Cruz, L. Rivas

414. An Analysis of the Most Probable Location in Excited States of the Hydrogen Atom. **J. J. Diamond Jr.**

415. Analysis of energetic profiles allows 99%-accurate prediction of the transmembrane regions. **I. Y. Torshin**

416. Analysis of IR chemiluminescent products from gas-phase ethene - O-atom interactions. **J. A. Dodd**, K. J. Castle, E. S. Hwang, G. D. DeBoer

417. Anion photoelectron spectroscopy of MnCu and $NbC_n(H/D)_n$ (n=2,4,6). **D. G. Leopold**, T. P. Marcy, E. L. Millam, S. R. Miller

418. Application of Gibbs Ensemble Monte Carlo simulation to phase diagram of 2-butoxyethanol-H2O. **D. K. Phelps**, N. J. Scocozzo

419. Anomalous photoinduced emission of highly constrained [Ar]-P=P-[Ar] diphosphenes. **H. Peng**, T. Copeland, T. Gunaratne, M. C. Simpson

420. Binding kinetics of damaged DNA to DNA Photolyase. **M. Ramsey**, J. Schelvis, Y. M. Gindt

421. Breakdown of the equipartition theorem in molecular dynamics simulations using periodic boundary conditions. **R. B. Shirts**, S. R. Burt, A. M. Johnson

422. Calculations of binding free energies for chorismate mutase inhibitors. **M. Kato**, A. Warshel

423. Changes in Proton NMR Spectra of 1,1'-Diethyl-2,2'-Cyanine Iodide during the Formation of the J-band in its Absorption Spectrum. **I. A. Struganova**

424. Charge transfer in conformationally selected small peptides. **B. Crews**, A. G. Abo-Riziq, L. Grace, M. DeVries

425. Chemical dynamics of high energy molecules: The role of state denstiy in collisional relaxation. **E. M. Miller**, A. S. Mullin

426. Chemical reactivity of (0001) Cr2O3 surface in the presence of an aqueous solution. **A. A. Rigos**, S. Petrosyan, T. A. Arias

427. Classical trajectory studies of OH (v) quenching by O atoms. **M. R. Dolgos**, R. J. Hinde

428. Clustering and activation in reactions of CoCp+ with hydrogen and methane. **J. K. Perry**, C. J. Carpenter, P. A. M. van Koppen, P. R. Kemper, J. E. Bushnell, P. Weis, M. T. Bowers

429. Comparison of electron transfer dynamics from sensitizers to different metal oxide nanoparticle thin films. **X. Ai**, J. Guo, D. Stockwell, N. A. Anderson, T. Kitamura, S. Yanagida, T. Lian

430. Computational methods for protein design and protein sequence variability: Biased Monte Carlo Methods and Replica Exchange. **X. Yang**, J. G. Saven

431. Controlled Hydrogen Abstraction from Substituted Aromatic Thiols on Cu(111). L. Bartels, **V. R. Bommisetty**, K. Kwon, J. Zhang, A. Liu

432. Corrections to microcanonical hard-sphere virial coefficients for small numbers of particles and for small enclosures. **R. B. Shirts**, A. M. Johnson, S. R. Burt

433. Dependence of the structure of diols on wetting-penetration characteristics onto the papers. **Y. Jung**, S. Ryu, J. Jang, S. Lee, J. Shin

434. Computed energetics of macromolecules: identification of the functional residues in proteins and functional nucleotides in RNA. **I. Y. Torshin**

435. Deviations from the Boltzmann distribution for small, isolated classical systems. R. B. Shirts, **S. R. Burt**, A. M. Johnson

436. DFT Calculations of Dinitrotoluenes and their Interactions with Soil. **C. M. Ramos**, L. F. Alzate, A. Santana, Y. Colon, J. Castillo, M. E. Castro, S. P. Hernandez, **N. Mina**

437. DFT Calculations of the Interactions of TNT with the Siloxane Surface of Kaolinite. **L. F. Alzate**, C. M. Ramos, A. Santana, J. Castillo, S. P. Hernandez, M. E. Castro, Y. Colon, N. Mina

438. Difference FT-IR study of protein structural changes in the inositol 5-phosphatase, OCRL. R. N. Burnette, M. V. Kisseleva, P. W. Majerus, G. E. Gillaspy, **S. Kim**

439. Direct observation of the ultrafast solvent response in condensed phase chemical dynamics. **D. F. Underwood**, S. J. Schmidtke, D. A. Blank

440. Dissociation Pathway of H2O on the Oxygen Vacancy of the TiO2(110) Surface: An Embedded Cluster Study. **H. Nguyen**, T. N. Truong

441. Dramatic Rate Accelerations in Ultrasonically Assisted Mn(III) Oxidation of Alcohols, Aldo and Keto Sugars in aqueous Acid Media - A Kinetic Study. **K. C. Rajanna**, K. Zaheeruddin, P. K. Saiprakash

442. Effects of explicit water molecules on the structure and stability of alanine dipeptide conformers: A density functional study. **P. Y. Ting**, F. Tao

443. Effects of hydrogen bonding ability in DNA binding using ruthenium pteridinyl-phenanthroline complexes. **S. Glazier**, S. J. N. Burgmayer, S. R. Dalton

444. Electric fields at protein active sites as determined by hole-burning Stark spectroscopy. **P. Geissinger**, J. C. Woehl, B. J. Prince

445. Electronic structure transformation through negative ion photoelectron angular distributions. **R. Mabbs**, E. Surber, A. Sanov

446. Energy transfer at a gas-surface interface in a Lennard-Jones system. **A. Siavosh-Haghighi**, T. Szabo, J. E. Adams

447. Energy transfer at a liquid nitromethane interface: A molecular dynamics study. **T. Szabo**, A. Siavosh-Haghighi, J. E. Adams

448. Energy transfer in hyperthermal collisions of Ar and O_2 with ethane. **A. L. Brunsvold**, D. J. Garton, T. K. Minton, D. Troya, G. C. Schatz

449. Equilibrium constants of hydrated H2SO4, NH3?H2SO4, and SO3?NH3 clusters from density functional theory calculations. **R. H. Moy**, P. M. Pawlowski, F. Tao

450. Equivalent Wannier-like functions for molecular calculations. **T. Baruah**, M. R. Pederson

451. Erosion of Kapton polyimide and FEP Teflon by hyperthermal atomic oxygen. **D. M. Buczala**, T. K. Minton, K. L. Kelly, J. C. Tully

452. Evaulating the configurational entropy in the binding of hydrogen-bonded complexes with varying numbers of single bonds. **K. L. Mardis**

453. Evolution of electronic structure as a function of size in indium phosphide semiconductor clusters. G. Meloni, **S. M. Sheehan**, M. J. Ferguson, D. M. Neumark

454. Exact hard sphere equation of state in arbitrary dimensions in terms of the mean free path. **R. B. Shirts**

455. Experimental and computational studies of benzene-cyclohexane clusters. **D. C. Easter**

456. Experiments and predictions for BOOMERANG force-detected NMR. **M. C. Butler**, R. A. Elgammal, V. A. Norton, D. P. Weitekamp

457. Fragmentation and Reactions of gas phase neutral metal oxide clusters. Y. Matsuda, D. N. Shin, **E. R. Bernstein**

458. Femtosecond study of vibrational relaxation of thiocyanate, ferri- and ferrocyanide anions in polar solvents and on SnO_2 and TiO_2 semiconductor nanoparticles. **V. A. Lenchenkov**, C. She, T. Lian

459. FTIR spectroscopy and Partial Least Squares regression studies of conformational changes of Myelin Basic Protein. **R. M. Simmons**, L. M. Ng, D. L. Sulton, T. Mckay

460. Group VI hydrides: from the lightest to the heaviest. **J. S. Underwood**, S. Lee, L. Smith, D. Chastaing, C. Wittig

461. $H_3O_2^-$ and $H_5O_2^+$: New potential energy surfaces and full-dimensional quantum calculations. **X. Huang**, S. Carter, B. J. Braams, J. M. Bowman

462. High-flux, tunable-velocity supersonic atomic oxygen beam source. **S. D. Chambreau**, E. S. Hwang, J. A. Dodd

463. IceIh - IceXI phase transition: A quantum mechanical study. **J. Kuo**, M. L. Klein, S. J. Singer, L. Ojamäe

464. Imaging studies of the electronic states of NO dimer. **A. B. Potter**, V. Dribinski, H. Reisler

465. Influence of bound-water molecules in the hydroxylation and epoxidation reactions in cytochromes P450cam wild-type and T252A mutant. **S. D. Dalosto**, **V. S. Batista**

466. Infrared spectra of neutral and ionic SO_2H_2 species trapped in solid neon. **M. E. Jacox**, W. E. Thompson

467. Intermediate state spectroscopy and dynamics of 1,3-cyclohexadiene. **N. Kuthirummal**, P. M. Weber

468. Intra- and interband relaxation dynamics of anionic mercury clusters via time-resolved photoelectron imaging and phofragmentation studies. **A. E. Bragg**, **A. Kammrath**, J. R. R. Verlet, O. Cheshnovsky, D. M. Neumark

469. IR/UV double resonance studies of the CH_2OH radical: Vibrational levels in the $3p_z$ Rydberg state. **J. Wei**, **L. Feng**, **H. Reisler**

470. In silico design of neutralizing antibodies to botulinum toxin type A. **J. M. Warfel**, T. Minh, S. R. Herron, K. A. Kantardjieff

471. Is the radical-radical reaction of methoxy with hydrogen atom yielding formaldehyde and hydrogen molecule barrierless? **Y. Zhang**

472. Isolation of discreet magnetite clusters in the 1-2nm range. **M. G. Arredondo**, R. L. Whetten

473. Isoprene oxidation initiated by OH in the presence of O_2 and NO. **J. Park**, C. Jongsma, R. Zhang, S. North

474. Kinetics of Chlorine Atom Reactions with Cyclic Ethers. **M. Quant**, **G. Nagasundaram**, R. Kelley, R. Aguilera, L. Gonzalez, S. Hewitt

475. Kinetics of Chlorine Atom Reactions with Naphthalene and Alkylnaphthalenes. **G. Aleman**, C. Quant, X. Peng, M. Luu, S. Hewitt

476. Kinetics of Immunoprecipitation Reactions. **J. S. Middleton**, S. Hewitt

477. Laboratory studies of $CO_2(\nu_2)$-O vibrational energy transfer. **K. J. Castle**, K. M. Kleissas, C. M. Gherghisan, J. A. Dodd

THURSDAY MORNING
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Nuclear Dynamics

P. H. Bucksbaum, *Presiding*
8:20 - 478. Watching proteins function with picosecond X-ray crystallography and MD simulations. **P. A. Anfinrud**, F. Schotte, G. Hummer, M. Wulff

9:00 - 479. Towards Ultrafast Excited State Molecular Structural Studies Using Pulsed X-rays. **L. X. Chen**, G. B. Shaw, G. Jennings, K. Attenkofer, D. M. Tiede

9:30 - 480. Hydrogen bonds in action. **E. Pines**, D. Pines, Y. Ma, G. R. Fleming

10:00 - 481. Using nonlinear IR spectroscopy to probe early events in the thermal unfolding of proteins. **H. S. Chung**, M. Khalil, A. Tokmakoff

10:20 - Intermission.

10:40 - 482. Transient 2D IR spectroscopy. **J. Bredenbeck**, J. Helbing, P. Hamm

11:20 - 483. Time-resolved structural dynamics in photoreceptors studied by X-ray crystallography. **K. Moffat**

Section B
Unknown Site -- Unknown Room
Industrial Applications of Theoretical Chemistry
Cosponsored with COMP

D. C. Spellmeyer, *Organizer, Presiding*
8:00 - 484. Design of materials for phosphorescent OLEDs. **D. J. Giesen**, J. Deaton, K. M. Vaeth

8:35 - 485. Electronic structure studies of semiconductor and optical materials. **K. Raghavachari**

9:10 - 486. Modeling of electronically conjugated materials. **D. S. Dudis**

9:45 - 487. Evolution of an academic/industrial collaboration. Synergies and potential pitfalls. **C. Breneman**

10:20 - Intermission.

10:40 - 488. Computational methods for combinatorial materials and catalyst discovery. **G. A. Landrum**, J. E. Penzotti, S. Putta

11:15 - 489. Applying molecular modeling in catalytic processes. **J. T. Golab**

Section C
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Reactive Scattering

W. L. Hase, *Presiding*
8:00 - 490. Chemical reactions within mass selected cluster ions. **J. Garvey**

8:20 - 491. Ab initio potential energy surfaces for the reactions of mercury with halogen radicals. **K. A. Peterson**, N. B. Balabanov, B. C. Shepler

9:00 - 492. Dynamics of elementary combustion reactions. **H. F. Davis**, M. F. Witinski, M. Ortiz-Suarez

9:40 - 493. Full dimensionalty quantum reactive scattering in O(3P)+HCl (3A', 3A") and H2O+H3O+ in reduced dimensionality. **J. M. Bowman**, T. Xie, J. Rheinecker

10:20 - Intermission.

10:40 - 494. Many open shell products result from the reaction of hyperthermal oxygen atoms with hydrocarbons. D. Troya, **G. C. Schatz**

11:00 - 495. State-specific low temperature reactions (HBr^+, DBr^+) [^2P_i , v] + (H_2, D_2): channels and rates. **M. Smith**, A. Belikov

11:20 - 496. IR/UV crossed beam studies of nonadiabatic dynamics: the road taken or not taken? **D. J. Nesbitt**, M. P. Deskevich, M. Wocjik, M. Ziemkiewicz, A. Zolot, E. Whitney

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Condensed Phase Dynamics

A. B. McCoy, *Organizer, Presiding*
8:00 - 497. Perturbed wavepacket approach to many body spectra. **E. J. Heller**

8:40 - 498. Semi-classical methods for quantum simulations. **J. Cao**

9:20 - 499. Mixed classical-quantum simulations using the semiclassical Liouville representation. **C. C. Martens**

9:40 - 500. Multidimensional variational Gaussian wave packets. **V. Buch**

10:20 - Intermission.

10:40 - 501. Mixed dynamical descriptions of proton transfer in a polar solvent. **B. C. Garrett**, G. K. Schenter, R. P. McRae, D. G. Truhlar

11:20 - 502. Exact solutions for quantum dissipative dynamics. **D. G. Evans**, R. D. Coalson

Section E
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

R. J. Saykally, *Presiding*
8:20 - 503. Non-linear optical microscopy, recent developments. **W. Denk**

9:00 - 504. Near-field Raman and fluorescence spectroscopy of single-walled carbon nanotubes. **A. Hartschuh**, A. J. Meixner, L. Novotny, T. D. Krauss

9:40 - 505. A nanoscale device for single-molecule sensing by force detection of electric fields. **B. M. Lambert**, V. A. Norton, D. P. Weitekamp

10:00 - 506. Polarization-based approaches to superresolution in far-field optical microscopy and fabrication. **J. T. Fourkas**

10:20 - Intermission.

10:40 - 507. On the relation between spatial photon localization and near-field optics. **O. Keller**

11:20 - 508. Near-field scanning optical microscopy studies of nanostructured SiN membranes. **J. W. P. Hsu**, A. L. Campillo, G. W. Bryant

Section F
Unknown Site -- Unknown Room
Protein Structure Prediction and Folding: Where Physical Chemistry Meets Genomics

C. R. Matthews, *Organizer, Presiding*
8:20 - 509. Protein universe in evolutionary prospective: from atoms to organisms and back. **E. I. Shakhnovich**

9:00 - 510. Using evolutionary information to study G-Protein coupled receptors. **R. A. Goldstein**

9:40 - 511. Cooperativity and the predictability of protein folding rates. **K. W. Plaxco**

10:20 - Intermission.

10:40 - 512. Folded to bind: side chain conformations in molecular recognition. **C. J. Camacho**, D. Rajamani, S. C. Thiel, S. Vajda

11:20 - 513. Free Energy Landscape of Protein Folding in Water: Explicit vs. Implicit Solvent. **R. Zhou**

11:40 - 514. Markov modelling of peptide folding with dynamical parameters. **W. Swope**

THURSDAY AFTERNOON
Section A
Unknown Site -- Unknown Room
Emerging Ultrafast Spectroscopies: From Chemistry to Biophysics
Electronic-Vibronic Dynamics

A. Stolow, *Organizer, Presiding*
1:20 - 515. Control and spectroscopy of electrons on an attosecond time scale. **F. Krausz**

2:00 - 516. Ultrashort deep ultraviolet pulses for reaction dynamics studies in solution. A. Jailaubekov, **S. E. Bradforth**

2:40 - 517. Time resolved experiment with a VUV pump pulse. **V. Blanchet**, S. Zamith, B. Girard, S. Sorensen, I. Hjelte, J. Norin, J. Mauritsson, A. L'Huillier

3:20 - Intermission.

3:40 - 518. Third- and fifth-order photon echo studies of colloidal CdSe quantum dots: Can many-body effects be resolved in disordered systems? **G. D. Scholes**, A. E. Colonna, M. W. Graham, V. M. Huxter, M. R. Salvador, X. Yang

4:20 - 519. Ultrafast charge- and energy-transfer dynamics in functionalized Ru(II) chromophores. **J. M. Papanikolas**

Section B
Unknown Site -- Unknown Room
Industrial Applications of Theoretical Chemistry
Cosponsored with COMP

D. C. Spellmeyer, *Organizer, Presiding*
1:20 - 520. Application of computational methods to agrochemical discovery. **J. M. Ruiz**

1:55 - 521. Computational characterization of metal binding groups for crop protection chemicals. K. D. Dobbs, A. M. Rinehart, M. H. Howard, Y. Zheng, **D. A. Kleier**

2:30 - 522. Improving accuracy and precision in molecular simulations. **W. Swope**

3:05 - Intermission.

3:25 - 523. Classical dynamics approach to modeling hydrocarbon pyrolysis. **S. J. Stuart**, O. Kum, B. M. Dickson, B. P. Uberuaga, A. F. Voter

4:00 - 524. Automatic construction of chemical mechanisms for challenging pyrolysis systems. **D. Matheu**, A. M. Dean, J. M. Grenda, W. H. Green Jr.

4:35 - 525. Multiscale modeling of high explosive detonations. **L. E. Fried**, M. R. Manaa, J. E. Reaugh, P. A. Vitello

Section C
Unknown Site -- Unknown Room
Intermolecular Interactions and Reactions Involving Ions and Open-Shell Systems
Ions and radicals in the atmosphere

M. I. Lester, *Organizer, Presiding*
1:20 - 526. Hyperthermal reactions of $O(^3P)$ with hydrogen and small alkanes. **T. K. Minton**, D. J. Garton, A. L. Brunsvold, D. Troya, B. Maiti, G. C. Schatz

2:00 - 527. Ion-molecule reactions at high temperature and pressure: Ionospheric and combustion related applications. **A. A. Viggiano**

2:40 - 528. Production of atmospherically important radicals via overtone chemistry. **D. J. Donaldson**, V. Vaida, A. F. Tuck

3:20 - Intermission.

3:40 - 529. Radical-radical reactions in the atmosphere: Role of adducts and chaperones. **M. Okumura**

4:20 - 530. Novel synthesis and characterization of HOONO by IR action spectroscopy. **I. M. Konen**, I. B. Pollack, E. X. J. Li, M. I. Lester

4:40 - 531. Ozonolysis of undecylenic and oleic acid films studied with infrared cavity-ring down spectroscopy. **S. Nizkorodov**, A. Gomez, A. Lin

Section D
Unknown Site -- Unknown Room
Mixed Quantum, Classical and Semiclassical Dynamics
Dynamics in Complex Environments

M. E. Tuckerman, *Presiding*
1:20 - 532. Nonadiabatic multiple spawning dynamics of Green Fluorescent and Photoactive Yellow Proteins. **T. J. Martinez**, C. Ko, A. Toniolo, S. Olsen

2:00 - 533. Energy transfer in dendrimers. **J. L. Krause**

2:40 - 534. Vibrational energy transfer in proteins. **D. M. Leitner**

3:00 - 535. Ab initio and polarizable force field base molecular dynamics simulations of anion solvation at aqueous interfaces. **D. J. Tobias**, P. Jungwirth, E. Brown, M. Mucha, I. W. Kuo, C. J. Mundy

3:20 - Intermission.

3:40 - 536. Multiple-timescale classical dissipative dynamics on stochastic surfaces. **R. Hernandez**, J. Moix

4:20 - 537. Application of mixed-quantum classical methods to non-equilibrium chemistry in the middle and upper atmosphere. **B. Naduvalath**, R. Sultanov, A. Varandas

4:40 - 538. From quantum chemistry to kinetics via trajectory simulations, transition state theory, and the master equation. **S. J. Klippenstein**, Y. Georgievskii, J. A. Miller, L. B. Harding, J. A. Nummela, B. K. Carpenter, P. R. Westmoreland

Section E
Unknown Site -- Unknown Room
Optical Microscopy Beyond the Diffraction Limit
Cosponsored with PRES

A. J. Meixner, *Presiding*
1:20 - 539. Fluorescence lifetime imaging near-field scanning optical microscopy (FLI-NSOM) of thin film materials. **D. A. Vanden Bout**, J. M. Imhof, E. Kwak

2:00 - 540. Ultrafast nano-optics: Controlling excitons in single quantum dots. **C. Lienau**, T. Unold, K. Mueller, T. Elsaesser

2:40 - 541. Quantum dot functionalized scanning probes for fluorescence energy transfer based microscopy. **Y. Ebenstein**, T. Mokari, U. Banin

3:00 - 542. Dielectrophoretic force imaging of nanostructured materials. **G. J. Simpson**

3:20 - Intermission.

3:40 - 543. Near-field optical microscopy of biological material in liquid. **A. Naber**

4:20 - 544. Detection and spectroscopy of single gold nanoparticles and their interactions with single emitters. **V. Sandoghdar**

Section F
Unknown Site -- Unknown Room
Protein Structure Prediction and Folding: Where Physical Chemistry Meets Genomics

Z. Schulten, *Organizer, Presiding*
1:20 - 545. Electron- and Energy-Transfer probes of protein conformation and dynamics. **J. R. Winkler**

2:00 - 546. Probing the phase diagram of protein folding in photoactive yellow protein. **G. A. Papadantonakis**, W. D. Hoff

2:20 - 547. Energy landscape and folding mechanisms of small proteins. **S. Takada**

3:00 - 548. Fast methods for protein structure prediction. **G. Martyna**, P. Minary, M. E. Tuckerman

3:20 - Intermission.

3:40 - 549. Ab initio prediction of protein structure with an off-lattice all-atom force field. **H. A. Scheraga**, J. A. Vila, D. R. Ripoll

4:20 - 550. Automated protein structure prediction for structural genomics. **D. Fischer**