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

D. M. Jonas, Organizer, Presiding

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


9:50 - 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


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


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


10:20 - Intermission.

11:00 - 12. Rotationally resolved infrared spectroscopy of the hydroxymethyl radical (CH2OH). L. Feng, J. Wei, H. Reisler


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


10:20 - Intermission.

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


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


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

10:20 - Intermission.


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


10:20 - Intermission.

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


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

N. Halas, Presiding

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.


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


3:20 - Intermission.


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

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


3:20 - Intermission.


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


3:20 - Intermission.


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


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

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


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.


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


3:20 - Intermission.

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


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 - Intermission.


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


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


10:20 - Intermission.

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

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


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

10:20 - Intermission.


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


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


10:20 - Intermission.


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**


10:00 - Intermission.


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


**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


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


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^2H exchange mass spectrometry. E. A. Komives


3:20 - Intermission.


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


3:20 - Intermission.


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

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

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

3:20 - Intermission.


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**


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.

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


**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**

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**

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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.


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**


10:20 - Intermission.

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_


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


10:20 - Intermission.


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**


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.


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


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.


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

L. Novotny, Organizer, Presiding

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

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**


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**


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

**Electronic-Vibronic Dynamics**

R. J. D. Miller, *Presiding*


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.

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**

Intermission.


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*


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

Intermission.


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

H. J. Kim, *Presiding*


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**


3:20 - Intermission.


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


Section E
Unknown Site -- Unknown Room
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


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**

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*


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.


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*


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.


**WEDNESDAY EVENING**

Section A
Unknown Site -- Unknown Room

Poster Session

D. J. Nesbitt, Organizer, Presiding
7:30 - 9:30


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


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


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 cyanoferriates 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


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 O2-N2O complex. W. M. Fawzy

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

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


267. H₂S dissociation on Fe(110) from first principles. E. A. Carter, D. E. Chang


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


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


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


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


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**


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


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


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


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


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


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**


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**


312. ZEKE spectra of Ar$_n$I (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**


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


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


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


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**


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


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


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

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


344. Rate constants and products of the reactions of PO$_x$Cl$_y^-$ 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$_5$H$_5$Mo(CO)$_3$H and C$_5$H$_5$W(CO)$_3$H complexes. C. Tanjaroon, K. Keck, M. Sebonia, C. Karunatilaka, S. G. Kukolich


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


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


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


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


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

365. Study of the reaction of CH3CHO + 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 O2(B, Triplet Sigma) + N2 -> NO + NO (or N + NO2) 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


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


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


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


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. 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-trichothece-9-ene nucleus. S. J. Gudowski, F. Tao


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


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


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


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

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


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


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**


425. Chemical dynamics of high energy molecules: The role of state density 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


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


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


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


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

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


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


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$_3$O$_2^-$ and H$_5$O$_2^+$: 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$_2$H$_2$ 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


469. IR/UV double resonance studies of the CH$_2$OH radical: Vibrational levels in the 3p$_z$ Rydberg state. J. Wei, L. Feng, H. Reisler

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 O₂ and NO. J. Park, C. Jongsma, R. Zhang, S. North


477. Laboratory studies of CO₂(ν₂)-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


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.


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


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


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+) [2P1, v] + (H2, D2): 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


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

10:20 - Intermission.


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


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


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.


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


3:20 - Intermission.


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**


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

3:05 - Intermission.


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*


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**


4:40 - 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*


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.


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*


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**


3:20 - Intermission.
