10:00 20. Preparation and selective adsorption desulfurization activity of Ti-Ce-Al-Ag-O adsorbent. **F. Sun**, X. Ma, C. Song
10:25 Intermission.
10:35 21. Ultraclean fuels via modified ultrasound assisted oxidative desulfurization process. S. S. Cheng, **T. F. Yen**
11:00 22. Recent advances in biodesulphurization of fuels. **R. C. Nwokoma**

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Catalysis and Reaction Mechanisms
Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

TUESDAY AFTERNOON

Section A

Hilton
Salon III

Chemistry of Petroleum and Emerging Technologies

K. Fjare, *Organizer*

2:00 Introductory Remarks.
2:10 23. Removal of carboxylic acids in Fischer-Tropsch hydrocarbon product. **F. H. A. Bolder**
2:35 24. The challenges for processing Canadian bitumen-derived crudes. **Z. Fan**, P. Rahimi, T. Alem
3:00 Intermission.
3:10 25. Total acid number determination in vacuum and atmospheric residue of petroleum using attenuated total reflectance Fourier transform infrared spectroscopy and different partial least squares algorithms. **E. I. Muller**, G. Parizotto, A. L. Hermes, M. F. P. dos Santos, R. C. L. Guimarães, M. F. Ferrão, É. M. M. Flores
3:35 26. Demulsification of heavy crude oils for salt extraction using closed vessels microwave heating and further chlorine determination by ion selective electrode or titration. É. M. Flores, **J. S. Pereira**, F. G. Antes, D. P. Moraes, L. O. Diehl, J. N. Paniz, V. L. Dressler, M. F. P. Santos, R. C. Guimarães

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Surface Chemistry of Oxides Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

WEDNESDAY MORNING

Section A

Hilton
Grand Ballroom C

Poster Session

K. Fjare, *Organizer*

9:00–11:00
27. Total acid number distribution in a Brazilian refinery oil sample after exposure to different levels of heating in the process units. **A. D. O. Gomes**, R. C. L. Guimarães, I. P. Batista
28. Biosynthesis of the acid by a new technology and bioreactors. **F. Abniki**, E. Bakhshi
29. How comb-type poly(maleic acid alkylamide -co-alfa-olefin) assembles in waxy oils and improves cold flowing ability. X. Zhang, J. Xu, J. Sun, L. Li, **X. Guo**
30. Hydro processing rape seed oil with gas oil for diesel fuel. **B. Gevert**, J. Claesson, K. Holmgren, U. Kuylenstierna, B. Lundin, L. Nilsson, A. Sherif
31. Investigation of safe operation of exothermic reactions in chemical industries: Presenting procedure. **E. Bakhshi**, F. Abniki, M. Mosalla
32. Investigation of water quality with changing the method of microorganisms control. **E. Bakhshi**, F. Abniki
33. On the lumped parameter called efficiency in vapor distillation problems. **S. R. Kal**
34. Pilot test study of an ex-situ presulfided NiMo/Al2O3 catalyst. **Y. Li**, D. Liu
35. Solid base and their performance in synthesis of dipropylene glycol. **L. Lu**, Y. Xiang, D. Xia, Y. Zhou
36. Storing sensible heat by supporting phase change material, PCM. **F. Abniki**, E. Bakhshi
37. Synthesis of mesoporous ZSM-5 by inverse self-assembly of secondary unit. **L. Dai**, Z. Yan
38. Thermal cracking studies by design of a pilot plant. **F. Abniki**, E. Bakhshi, M. Mosalla, A. Bakhshi

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Bimetallics and Electrocatalysis Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

WEDNESDAY AFTERNOON

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Surface Characterization and Chemistry Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

‡ **Cooperative Cosponsorship**

PHYS

Division of Physical Chemistry

M. Head-Gordon, *Program Chair*

SUNDAY MORNING

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Advances at the Interface of Electronic Structure and Dynamics

C. D. Sherrill and G. Galli, *Organizers, Presiding*

8:00 Introductory Remarks.
8:10 1. Photochemistry and mechanochemistry from first principles dynamics. **T. J. Martinez**
8:50 2. Predictive electronic structure methods for charge transfer systems. **A. I. Krylov**
9:30 3. Ab initio based potentials and dynamics using them. **J. M. Bowman**, B. J. Braams
10:10 Intermission.
10:30 4. Exploring electron transfer and bond breaking with constrained DFT. **T. Van Voorhis**
11:10 5. Developments in coupled-cluster molecular dynamics. **A. G. Taube**

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer, Presiding*

8:00 Introductory Remarks.
8:10 6. Reactivity trends in cooxidation from uhv to elevated pressures. S. M. Mcclure, M. Lundwall, F. Yang, Z. Zhou, **D. W. Goodman**
8:50 7. Which transition states and intermediates control catalyst activity, and how well do we know their energies? **C. T. Campbell**
9:30 8. What can we learn from empirically determined kinetic parameters? **K. Reuter**
10:10 9. Award Address (Gabor A. Somorjai Award for Creative Research in Catalysis, sponsored by Gabor A. and Judith K. Somorjai Endowment Fund). Structural and electronic effects in the reactivity of metal surfaces. **J. K. Norskov**
10:50 10. Theoretical and experimental studies using model systems for the design of selective catalysts with well-defined shapes. I. Lee, F. Delbecq, **F. Zaera**
11:10 11. Olefins at oxide surfaces studied by vibrational sum frequency generation. **F. M. Geiger**, A. M. Buchbinder, G. Y. Stokes
11:30 12. Pathways and intermediates of formic acid decomposition on the CeO2(111) surface. **Y. Xu**, W. O. Gordon, S. D. Senanayake, D. R. Mullins, S. H. Overbury
11:50 13. DFT modeling of the interaction of noble metals with ceria and zirconia surfaces. **R. Grau-Crespo**, N. C. Hernandez, J. F. Sanz, N. H. de Leeuw

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen, *Organizer*

A. Warshel, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 14. A dynamic duo where rate constants, or selectivity are determined by tuning dynamic trajectories. **R. Stroud**, J. Finer-Moore, S. Hur, Z. Newby
9:15 15. What X-ray diffraction can—and can't—tell us about functional motions. **G. A. Petsko**
9:55 Intermission.
10:10 16. The missing atom in functional motion: Reliable determination of hydrogen positions. **D. Ringe**
10:50 17. Elucidating functional motions in a single protein crystal. **E. N. Brown**, S. Ramaswamy, B. V. Plapp
11:30 18. Insight into RNA catalysis by hammerhead ribozyme from QM/MM free-energy profile simulations. **K-Y. Wong**, T-S. Lee, D. M. York

Please refrain from using cellular telephones and cameras during technical sessions.

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Accurate Calculation of Interactions of Dihydrogen with Nanoporous Materials
Cosponsored by NANO

M. D. Ward, *Organizer*

Z. Bacic, *Organizer, Presiding*

8:00 Introductory Remarks.
8:10 19. Accurate quantum chemical calculation of the interaction of dihydrogen with hydrogen-storage materials. **W. Klopper**, A. Mavrandonakis
8:50 20. Electronic structure methods for hydrogen storage calculations. **M. Head-Gordon**
9:30 21. Simulation of free energies of hydrogen adsorption in nanoporous systems with quantized molecular-fluid DFT. **S. Patchkovskii**, T. Heine
10:10 Intermission.
10:30 22. H2 generation and storage on nanoporous materials: Theoretical studies and new development. **S. Meng**
11:10 23. The physics of hydrogen clusters: Structure, superfluidity and quantum melting. **M. Boninsegni**

Section E

Salt Palace Convention Center
251 B

Chemical Methods of Nanofabrication
Cosponsored by NANO‡

Y. H. Wang and S-J. Park, *Organizers*

C. A. Mirkin, *Presiding*

8:30 24. Crystals as molecules. **O. M. Yaghi**
9:05 25. New nanofabrication strategies: Inspired by biomineralization. **J. Aizenberg**, B. Pokroy, S. H. Kang, A. Epstein
9:40 26. Cooperative self-assembly of nanoparticles and amphiphilic block-copolymers in selective solvents. **S-J. Park**, B. L. Sánchez-Gaytán, R. Hicky, A. Kamps
10:15 Intermission.
10:25 27. Controlling the synthesis and assembly of nanoscale building blocks. **Y. Xia**
11:00 28. Directing nanoparticle nucleation and assembly using self-assembled peptide conjugates. **N. L. Rosi**, C. Chen, P. Zhang

Section F

Salt Palace Convention Center
251 C

Progress in Polarizable Force Fields and Simulation
Large Scale Polarizable Force Field Development

T. Head-Gordon, *Organizer*

V. S. Pande, *Organizer, Presiding*

8:00 29. Fluctuating charge force fields for protein simulations. **C. L. Brooks III**
8:40 30. Calibration and validation of the AMOEBA polarizable force field. **J. W. Ponder**
9:20 31. Classical force field development: What can we learn from carbohydrates? **R. J. Woods**
10:00 Intermission.
10:20 32. Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules. **A. D. MacKerell Jr.**
11:00 33. Polarizable modeling of proteins: Force fields and empirical corrections. **R. A. Friesner**

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Scaling Molecular Dynamics Applications Sponsored by COMP, Cosponsored by PHYS

Frontiers in Imaging Biological Nanostructures Sponsored by BIOL, Cosponsored by ANYL, COLL, PHYS, POLY, and NANO‡

Polymers and Carbon Nanotubes
Tutorial on Carbon Nanotubes Sponsored by POLY, Cosponsored by COLL, I&EC, PHYS, PMSE, and NANO

SUNDAY AFTERNOON

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Electronic Structure Methods Appropriate for Bond-Breaking Reactions

C. D. Sherrill and G. Galli, *Organizers*

P. Piecuch, *Presiding*

1:30 34. Methodological advances in state-specific multireference coupled cluster theory: Connected triples, excited electronic states, and focal point extrapolations. **W. D. Allen**, F. A. Evangelista, A. C. Simmonett
2:10 35. Antisymmetrized geminal product with Jastrow factor: An accurate and efficient ansatz for quantum Monte Carlo calculations. **M. Casula**
2:50 36. Two-electron reduced-density-matrix mechanics with application to many-electron atoms and molecules. **D. A. Mazziotti**
3:30 Intermission.
3:50 37. Calculation of highly accurate potential energy curves by the CEEIS method. L. Bytautas, **K. Ruedenberg**, T. Nagata, M. S. Gordon, N. Matsunaga
4:30 38. Linear scaling multireference singles and doubles configuration interaction. **T. S. Chwee**, E. A. Carter

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

D. W. Goodman, *Presiding*

1:30 39. The effect of surface defects in oxygen bonding and hydrocarbon oxidation on gold(111). **C. M. Friend**, T. A. Baker, E. Kaxiras, B. Xu
2:10 40. Computational search for alloys as selective hydrogenation catalysts. **T. Bligaard**
2:50 41. Theoretical investigations of the adsorption and activation properties of CO on iron and iron carbide surfaces. **D. C. Sorescu**
3:30 42. From adsorbed atoms to supported clusters: Experiment vs. theory. **H-J. Freund**
4:10 43. Time resolved density functional theory for lifetimes of excited adsorbate states at metal surfaces. **X. Li**, C. Moss
4:30 44. Photocatalysis over TiO2: Insights from theory and experiment. **N. A. Deskins**, Y. Du, Z. Zhang, R. Zehr, M. Henderson, Z. Dohnálek, I. Lyubinetsky, M. Dupuis
4:50 45. Theoretical study on the stability of molecular platinum catalysts upon irradiation. **L. E. Roy**, E. R. Batista
5:10 46. Using STM to identify chemical species via a novel contrast mechanism. **N. Guo**, D. J. Doren

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen and A. Warshel, *Organizers*

K-Y. Wong, *Presiding*

1:30 47. Biomolecular simulations of enzymatic reactions. **A. J. Mulholland**
2:10 48. Toward quantitative understanding of enzyme reactions: Electrostatically embedded multiconfiguration molecular mechanics. **M. Higashi**, D. G. Truhlar
2:50 Intermission.
3:10 49. Computational studies of how enzymes break C-H bonds. **M. J. Sutcliffe**
3:50 50. Theoretical design of new biological catalysis. **V. Moliner**
4:30 51. Folding and chemical landscapes in enzyme catalysis. **M. Roca**, B. M. Messer, D. Hilvert, A. Warshel

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Metal-organic Frameworks Cosponsored by NANO

M. D. Ward, *Organizer, Presiding*

1:30 52. Hydrogen storage in open framework materials. **O. M. Yaghi**, H. Furukawa, C. J. Doonan
2:10 53. Combined first-principles and inelastic neutron scattering study of quantum dynamics of hydrogen molecule in metal organic frameworks: A direct probe of the guest-host interaction potential surface. **T. Yildirim**
2:50 54. Hydrogen storage in microporous metal-organic frameworks with exposed metal sites. M. Dinca, S. S. Kaye, H. J. Choi, A. Demessence, S. Horike, L. J. Murray, **J. R. Long**
3:30 Intermission.
4:10 55. Cation-doped metal-organic framework materials for hydrogen storage. K. L. Mulfort, O. K. Farha, **J. T. Hupp**
4:50 56. Some aspects of the role of surface chemistry and framework flexibility on hydrogen and deuterium adsorption on metal-organic framework materials. **K. M. Thomas**

Section E

Salt Palace Convention Center
251 B

Chemical Methods of Nanofabrication
Cosponsored by NANO‡

Y. H. Wang and S-J. Park, *Organizers*

C. A. Mirkin, *Organizer, Presiding*

1:30 57. Nanoimprint lithography, self-perfection by liquefaction, and beyond. **S. Y. Chou**
2:05 58. Exploring the role of size and shape in engineered drug therapies using a top-down manufacturing technology. **J. M. DeSimone**
2:40 59. On-wire lithography. **C. A. Mirkin**
3:15 Intermission.
3:25 60. Multiphoton absorption polymerization: 3-D fabrication from the nanoscale to the macroscale. L. Li, R. Gattass, G. Kumi, E. Gershgoren, **J. Fourkas**
4:00 61. SAMDI Mass spectrometry and biological applications of monolayers. **M. Mrksich**

Section F

Salt Palace Convention Center
251 C

Progress in Polarizable Force Fields and Simulation
Ions in Bulk and at Interfaces

T. Head-Gordon and V. S. Pande, *Organizers*

C. D. Wick, *Presiding*

1:30 62. On the role of explicit electronic polarization in simulation studies of ions in interfacial settings. **D. J. Tobias**
2:10 63. Polarizable force fields for simulations of ionic liquids. **O. Borodin**
2:30 64. Computational studies of liquid interfaces. **L. X. Dang**
3:10 65. Charge screening and solvent polarization in models of ionic liquids. **R. M. Lynden-Bell**, T. G. A. Youngs
3:50 Intermission.
4:10 66. Importance of polarizability for understanding aqueous interfaces and bulk ion solvation. **C. D. Wick**
4:30 67. Ab initio studies of ion-ligand interactions: Evidence for polarizability. S. Varma, **S. B. Rempe**
5:10 68. Accurate force fields and model potential approaches for characterizing excess electrons and protons in water. **K. D. Jordan**, R. Kumar, T. Sommerfeld, A. A. DeFusco III

Section G

Salt Palace Convention Center
250 F

New Developments in Energy Conversion and Light-Harvesting
Organic Photovoltaics

D. V. Talapin, J. M. Lupton, and D. S. Ginger Jr., *Organizers*

Y. Yang, *Presiding*

1:30 69. Electrical detection of coherent spin motion in semiconductors and what it tells us about efficiency limiting processes in materials for photovoltaic and lighting applications. **C. M. Boehme**
2:10 70. Charge and energy transfer at PbSe quantum dot/conjugated polymer interfaces. **D. S. Ginger Jr.**, K. Noone, N. Anderson
2:30 71. Aggregation effects on the properties of individual conjugated oligomers and polymers as probed by Stark spectroscopy and fluorescence microscopy. **L. A. Peteanu**, G. A. Sherwood, J. Wildeman
2:50 Intermission.
3:10 72. Excited state dynamics in thiophene oligomers, dendrimers, and polymers. **D. A. Blank**, A. S. Huss, N. P. Wells
3:50 73. Synthetic, spectroscopic, and computational investigation of perylene diimide cyclophanes as models for charge transfer through π stacks. **J. Vura-Weis**, T. M. Wilson, M. Ratner, M. R. Wasielewski
4:10 74. Light-harvesting action spectroscopy of single conjugated polymer chains. **M. J. Walter**, N. J. Borys, J. M. Lupton
4:30 75. Studying charge transport properties of organic photovoltaics at metal surfaces using two photon photoemission. **J. E. Johns**, E. Muller, C. B. Harris

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Scaling Molecular Dynamics Developments Sponsored by COMP, Cosponsored by PHYS

Frontiers in Imaging Biological Nanostructures Sponsored by BIOL, Cosponsored by ANYL, COLL, PHYS, POLY, and NANO‡

Polymers and Carbon Nanotubes
Dispersion and Functionalization
Sponsored by POLY, Cosponsored by COLL, I&EC, PHYS, PMSE, and NANO

MONDAY MORNING

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Excited Electronic States

C. D. Sherrill and G. Galli, *Organizers*

W. D. Allen, *Presiding*

8:30 76. Electron transfer dissociation of peptides: An adventure in excited state dynamics. **J. Simons**
9:10 77. Electronic excitations in the condensed phase. **L. V. Slipchenko**
9:50 78. Excited electronic states of nonisolated nucleobases. **S. Matsika**
10:30 Intermission.
10:50 79. Balanced description of ground-state properties, valence excitations, and charge transfer excitations with long-range corrected density functionals. **M. A. Rohrdanz**, A. W. Lange, J. M. Herbert
11:10 80. Modeling the doubly-excited state with time-dependent Hartree-Fock and density functional theories. **X. Li**, C. M. Isborn
11:30 81. 2-D-IR spectroscopy of excited state proton transfer compounds. **P. B. Petersen**, S. T. Roberts, K. Ramasesha, R. A. Nicodemus, D. G. Nocera, A. Tokmakoff

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

S. Linic, *Presiding*

8:00 82. Major successes of combined theoretical and experimental studies in surface chemistry and heterogeneous catalysis from the perspective of an experimental scientist. **G. A. Somorjai**
8:40 83. DFT vs. the "real world" (or, Waiting for Godft). **P. J. Feibelman**
9:20 84. Rational design of bimetallic catalysts for hydrogenation and reforming reactions. **J. G. Chen**
10:00 85. Catalyst activation by molecular-sized centers. **H. Metiu**
10:40 86. Deposition and STM characterization of mass-selected vanadia clusters on TiO_2(110). **S. P. Price**, X. Tong, V. Shapovalov, H. Metiu, S. K. Buratto
11:00 87. The chemistry of hot electrons revealed in CO oxidation at metal surfaces. S. N. Maximoff, **M. Head-Gordon**
11:20 88. Reactivity relationships in hydrated oxides extracted from DFT studies. **S. E. Mason**, C. R. Iceman, T. P. Trainor, A. M. Chaka
11:40 89. Surface chemistry of alcohols on WO3 and MoO3 model oxide catalysts. **Y. K. Kim**, R. Rousseau, B. D. Kay, Z. Dohnálek

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen and A. Warshel, *Organizers*

M. Roca, *Presiding*

9:00 90. Proton-coupled electron transfer in soybean lipoxygenase: Impact of mutation on enzyme motions coupled to catalysis. **S. Hammes-Schiffer**
9:35 91. Functional dynamics of DNA repair in photolyase. **D. Zhong**
10:15 Intermission.
10:35 92. Calculations of activation entropies of biomolecular reactions. **J. Aqvist**
11:15 93. Dynamical coupling between conformational and chemical coordinates does not contribute significantly to enzyme catalysis. **A. Warshel**
11:35 94. A quantum wavepacket ab initio dynamical perspective to hydrogen tunneling in an enzyme active site. **S. S. Iyengar**

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Metal-organic Frameworks Cosponsored by NANO

Z. Bacic and M. D. Ward, *Organizers*

T. Yildirim, *Presiding*

8:00 95. Molecular hydrogen adsorbed in porous hosts: MOF-5, MIL-53, and the THF sII type clathrate. **F. M. Mulder**
8:40 96. Adsorption and diffusion of hydrogen in nanoporous materials. **J. K. Johnson**, R. B. Rankin, J-C. Liu
9:20 97. Simulating the adsorption of hydrogen in metal organic frameworks. **B. Smit**, D. Cao, W. Wang
10:00 Intermission.
10:20 98. Studying quantum dynamics of adsorbed hydrogen using infrared spectroscopy. **S. A. FitzGerald**
11:00 99. Theoretical modeling of hydrogen sorption in MOMs. **B. Space**

Section E

Salt Palace Convention Center
250 F

Attosecond Science: The Next Frontier Intense Fields

A. D. Bandrauk and S. Leone, *Organizers*

D. M. Neumark, *Presiding*

8:00 Introductory Remarks.
8:05 100. Molecules and attosecond science. **P. B. Corkum**
8:45 101. Tomographic imaging of molecular orbitals from harmonic spectra: Challenges in theory. **A. M. Maquet**, R. Taïeb, J. Caillat
9:25 102. Ab initio nonperturbative approaches for the treatment of atomic and molecular multiphoton processes in intense ultrashort laser pulses. **S-I. Chu**
10:05 Intermission.
10:25 103. Simulation of attosecond electron dynamics in CO2. **R. J. Levis**
11:05 104. Theory for laser induced nuclear and electronic ring currents and circulations: From femtosecond to attosecond time scales. **J. Manz**
11:45 105. Ultrafast molecular electronic dynamics studied using attosecond streaking. **M. J. Abel**, T. Pfeifer, P. M. Nagel, W. F. Boutu, D. M. Neumark, S. R. Leone

‡ **Cooperative Cosponsorship**

Section F

Salt Palace Convention Center
251 C

Chemical Methods of Nanofabrication
Cosponsored by NANO‡

Y. H. Wang and S-J. Park, *Organizers*

C. A. Mirkin, *Organizer, Presiding*

8:30 106. Techniques for molecular scale and 3-D nanofabrication. **J. A. Rogers**
9:05 107. Nanoscale chemical patterning. **P. S. Weiss**, A. M. Andrews
9:40 108. Pattern formation in molecular semiconductor films. **J. E. Reutt-Robey**
10:15 Intermission.
10:25 109. Chemically tailored carbon-based nanoelectronic materials. **M. C. Hersam**
11:00 110. "Cloning" and manipulation of carbon nanotubes. **Y. Wang**

Section G

Salt Palace Convention Center
251 B

Progress in Polarizable Force Fields and Simulation
Polarizability in Biological Systems

V. S. Pande, *Organizer*

T. Head-Gordon, *Organizer, Presiding*

8:30 111. Ion selectivity in proteins, a local cluster decomposition. **B. Roux**, H. Yu, S. Noskov
9:10 112. Molecular simulation of trypsin-ligand binding with a polarizable potential. **P. Ren**, D. Jiao
9:50 Intermission.
10:10 113. Diffusion-collision guided folding pathways of an α/β protein from ab initio folding simulations. **Y. Duan**
10:50 114. Polarizable force fields based on charge equilibration models: From water to complex biological systems. **S. Patel**
11:10 115. Effects of polarizability on peptide conformational changes and the development of coarse-grained force fields. **J-W. Chu**

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Quantum Chemistry Developments
Sponsored by COMP, Cosponsored by PHYS

Molecular Rotors and Motors Sponsored by COLL, Cosponsored by PHYS and NANO‡

Polymers and Carbon Nanotubes Processing of Composites Sponsored by POLY, Cosponsored by COLL, I&EC, PHYS, PMSE, and NANO

MONDAY AFTERNOON

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics Nanomaterials

C. D. Sherrill and G. Galli, *Organizers*

D. Alfe, *Presiding*

1:30 116. Understanding the conductance of single-molecule junctions from first principles. **J. B. Neaton**
2:10 117. Stability, chemical structure, and Clar's aromatic sextets of hydrogen-terminated graphene ribbons. T. Wassmann, A. P. Seitsonen, A. M. Saitta, M. Lazzeri, **F. Mauri**
2:50 118. An electronic structure study on the manipulation and control of the structure, morphology and properties of carbon nanotubes and heterostructures. **B. G. Sumpter**, V. Meunier
3:30 Intermission.
3:50 119. Water in nanoscale confinement: Insights into structure, dynamics, and 1H-NMR chemical shifts from first-principles theory. **P. Huang**, E. Schwegler, G. Galli
4:30 120. Ligand-protected gold cluster superatoms. **H. Häkkinen**

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

B. Hammer, *Presiding*

1:30 121. Connecting small molecule reaction dynamics to catalysis. **I. Harrison**
2:10 122. Energy descriptor to quantify the methane selectivity in Fischer-Tropsch synthesis: A density functional theory study. **P. Hu**
2:50 123. The relationships between theory and experiments in catalysis. **A. T. Bell**
3:30 124. Heterogeneous catalysis for hydrogen production and purification: First-principles, experiments, and microkinetic modeling. **M. Mavrikakis**
4:10 125. Probing reaction pathways on model catalyst surfaces: Vinyl acetate synthesis. **W. T. Tysoe**
4:30 126. The structure and reaction barriers of ethoxy groups on Cu surfaces. **A. J. Gellman**, D. S. Sholl, X. Li
4:50 127. Structure-dependence of the mechanism of CO activation on Hägg iron carbide (χ-Fe_5C_2) surfaces. **M. A. Petersen**, P. J. Steynberg, J-A. van den Berg, W. Janse van Rensburg
5:10 128. Catalyzing the catalyst: Novel pathways to hydrogen dissociation and spillover on palladium alloys. **H. L. Tierney**, A. E. Baber, J. R. Kitchin, E. C. H. Sykes

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen and A. Warshel, *Organizers*

S. S. Iyengar, *Presiding*

1:30 129. Enzyme fluctuations during a reaction cycle. **D. Thirumalai**
2:10 130. Instrinsic dynamics of proteins: Insights from network models. **I. Bahar**
2:50 Intermission.
3:10 131. Conformational diversity and catalysis. **D. Hilvert**
3:50 132. Role of enzyme's conformational fluctuations in catalytic reactions. W. Min, X. S. Xie, **B. Bagchi**
4:30 133. Intermolecular electron-transfers in protein/nanoparticle hybrids. **M. J. Knapp**, A. Carver

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Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Ahmed Zewail Prize in Molecular Sciences Advances in Nanoscience and Nonlinear Spectroscopy
Financially supported by Elsevier

S. S. Hall and K. Nederveen, *Organizers*

M. Okumura, *Presiding*

1:00 Introductory Remarks.
1:05 Award Presentation.
1:15 137. Award Address (Ahmed Zewail Prize in Molecular Sciences, sponsored by Elsevier). Metallic gold is more noble on the nanoscale because of the many more new acquired properties and their many useful applications in material science, in biology and in potential cancer therapy. **M. A. El-Sayed**
2:15 134. Anisotropic noble metal nanostructures. **C. A. Mirkin**
3:10 135. Dynamics of ions and polar molecules in water by 2-D IR. **R. M. Hochstrasser**, C-H. Kuo, D. Y. Vorobyev, D. Kuroda
4:05 136. Electrogenerated chemiluminescence of single conjugated polymer nanoparticles and thin films. **P. F. Barbara**
5:00 Concluding Remarks.

Section E

Salt Palace Convention Center
250 F

Attosecond Science: The Next Frontier Spatio-Temporal Attosecond Dynamics

A. D. Bandrauk and S. Leone, *Organizers*

K. Ohmori, *Presiding*

1:30 138. Award Address (Ahmed Zewail Award in Ultrafast Science and Technology, sponsored by the Ahmed Zewail Endowment Fund established by Newport Corporation). Probing coupled electron and nuclear dynamics in polyatomic molecules using ultrafast X-rays. **M. M. Murnane**, H. C. Kapteyn
2:10 139. Ultrafast hydrogen migration in hydrocarbon molecules: New frontiers in attosecond intense laser science. **K. Yamanouchi**
2:50 140. Ultrafast electronic dynamics in helium nanodroplets studied by femtosecond time-resolved EUV photoelectron imaging. **O. Gessner**, O. A. Kornilov, C. C. Wang, M. Leonard, A. Healy, S. R. Leone, D. M. Neumark
3:30 Intermission.
3:50 141. Attosecond time-resolved electron dynamics. **M. Vrakking**
4:30 142. Simultaneous description of electron and nuclear dynamics: A quantum approach for multielectron systems. P. von den Hoff, D. Geppert, I. Znakovskaya, M. F. Kling, **R. de Vivie-Riedle**
5:10 143. Attosecond imaging of CEWP's: Coherent electron wave packets. **S. Chelkowski**, A. D. Bandrauk

Section F

Salt Palace Convention Center
251 C

Chemical Methods of Nanofabrication
Cosponsored by NANO‡

Y. H. Wang and S-J. Park, *Organizers*

C. A. Mirkin, *Organizer, Presiding*

1:00 144. Scanning probe nanolithography in surface chemistry. M. Liu, N. A. Amro, Z. Deng, Y. H. Tan, **G-Y. Liu**
1:35 145. Constructive lithography goes from serial to parallel: Contact electrochemical pattern generation and transfer. **J. Sagiv**, A. Zeira, D. Chowdhury, J. Berson

2:10 146. Desktop nanofabrication with DPN-generated large-area nanoscale templates. **J. R. Haaheim**, O. A. Nafday, J-W. Jang, P. Stiles, T. Levesque
2:45 Intermission.
2:55 147. Metabolically and optically defined lithography using living cells. **C. J. Brinker**, E. C. Carnes
3:30 148. Dip pen nanolithography on tissue surfaces. **A. Ivanisevic**

Section G

Salt Palace Convention Center
251 B

New Developments in Energy Conversion and Light-Harvesting
Fundamental Aspects of Energy Conversion

D. V. Talapin and D. S. Ginger Jr., *Organizers*

J. M. Lupton, *Organizer, Presiding*

1:30 149. Interfacial exciton dissociation in inorganic quantum dot or organic semiconductor based solar cells. **X. Zhu**
2:10 150. Photothermal photonplasmon excitation to enhance energy conversion. **D. K. Roper**, W. Ahn, B. Taylor, A. G. Russell
2:30 151. Multielectron transfer from multiexciton states. **D. Balamurugan**, S. S. Skourtis, D. N. Beratan
2:50 152. Bioinspired macromolecular electrets. M. K. Ashraf, D. Bao, B. Millare, A. Ferreira, A. A. Gerasimenko, R. R. Pandey, R. K. Lake, **V. I. Vullev**
3:10 Intermission.
3:30 153. On 1-D nanostructure-guided chain reactions. **N. Nair**, M. S. Strano
3:50 154. Effects of a water environment on the structure and H_2 production of the $[FeFe]_H$ cluster of di-iron hydrogenase. **F. Zipoli**, R. Car, M. H. Cohen, G. C. Dismukes, A. Selloni
4:10 155. Light harvesting and coherence in multichromophoric systems: From Nature to nanoscale. **G. D. Scholes**, E. Collini, C. Curutchet

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Scaling Quantum Chemistry Applications Sponsored by COMP, Cosponsored by PHYS

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Nontraditional Density Functional Methods Sponsored by COMP, Cosponsored by PHYS

Frontiers in Imaging Biological Nanostructures Sponsored by BIOL, Cosponsored by ANYL, COLL, PHYS, POLY, and NANO‡

Molecular Rotors and Motors Sponsored by COLL, Cosponsored by PHYS and NANO‡

Polymers and Carbon Nanotubes
Properties of Composites Sponsored by POLY, Cosponsored by COLL, I&EC, PHYS, PMSE, and NANO

Undergraduate Research Poster Session: Physical Chemistry Sponsored by CHED, Cosponsored by PHYS and SOCED

MONDAY EVENING

Section A

Salt Palace Convention Center
Hall 5

Sci-Mix

M. Head-Gordon, *Organizer*

8:00–10:00
267-268, 285, 291, 316, 321-322, 357, 369, 379, 390, 393. See subsequent listings.

TUESDAY MORNING

Section A

Salt Palace Convention Center
Combo Rooms 250 A-F

Physical Chemistry Awards Symposium

M. Head-Gordon, *Organizer, Presiding*

8:30 156. Award Address (Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry, sponsored by Waters Corporation). Energetics and mechanisms for the decomposition of metallated and protonated amino acids. **P. B. Armentrout**
9:15 157. Award Address (ACS Award in Pure Chemistry, sponsored by Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation). Strongly interacting electrons in chemistry. **G. K. Chan**
10:00 Intermission.
10:20 158. Award Address (Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry, sponsored by the American Chemical Society). Chemisorption and heterogeneous catalysis: Creative tension between the real world and the DFT world. **D. A. King**
11:05 159. Award Address (ACS Award in Theoretical Chemistry, sponsored by the American Chemical Society). Chemical density functional theory: A language for unifying chemical concepts. **R. G. Parr**

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Quantum Monte-Carlo Sponsored by COMP, Cosponsored by PHYS

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Catalysis and Reaction Mechanisms Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Molecular Rotors and Motors Sponsored by COLL, Cosponsored by PHYS and NANO‡

Polymers and Carbon Nanotubes
Applications Sponsored by POLY, Cosponsored by COLL, I&EC, PHYS, PMSE, and NANO

TUESDAY AFTERNOON

Section A

Salt Palace Convention Center
Combo Rooms 250 A-F

Physical Chemistry Awards Symposium

L. J. Butler, *Presiding*

M. Head-Gordon, *Organizer, Presiding*

1:30 160. Award Address (Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids, sponsored by ExxonMobil Research and Engineering Company). Liquid dynamics and the dynamics of polar solvation. **G. R. Fleming**
2:15 161. Award Address (E. Bright Wilson Award in Spectroscopy, sponsored by the American Chemical Society). A spectroscopic view of condensed phase chemical dynamics. **P. F. Barbara**
3:00 Intermission.
3:20 162. Award Address (Ahmed Zewail Award in Ultrafast Science and Technology, sponsored by the Ahmed Zewail Endowment Fund established by Newport Corporation). Harnessing attosecond science for molecular dynamics. **H. C. Kapteyn**, M. M. Murnane
4:05 163. Award Address (Peter Debye Award in Physical Chemistry, sponsored by E. I. du Pont de Nemours & Company). X-ray absorption spectroscopy of liquid microjets: A new probe of ion hydration. **R. J. Saykally**

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of Mark S. Gordon Sponsored by COMP, Cosponsored by PHYS

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Looking Toward the Future Sponsored by COMP, Cosponsored by PHYS

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Surface Chemistry of Oxides Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

TUESDAY EVENING

Polymers and Carbon Nanotubes Sponsored by POLY, Cosponsored by NANO, COLL, I&EC, PHYS, and PMSE

WEDNESDAY MORNING

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Accurate Methods for Condensed Phase Simulations

C. D. Sherrill and G. Galli, *Organizers*

L. V. Slipchenko, *Presiding*

8:30 164. QM/QM electronic embedding models for materials chemistry. **K. Raghavachari**, H. P. Hratchian, P. V. Parandekar
9:10 165. Ultrafast QM/MM calculations with electronic charge embedding. **P. Pulay**, M. Dupuis
9:50 166. The fragment molecular orbital method: Water clusters and ionic liquids. **M. S. Gordon**, S. R. Pruitt, J. M. Mullin
10:30 Intermission.
10:50 167. The dynamics of radical+alkane reactions: From gas-phase to gas/surface reactions. **D. Troya**, J. P. Layfield
11:30 168. New algorithms and potentials for three-body interactions in molecular dynamics simulations: Application to argon simulations. **A. L. Ringer**, J. T. Waters, W. March, M. S. Marshall, C. D. Sherrill, A. Gray

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

A. J. Gellman, *Presiding*

8:00 169. Successes and pitfalls in design of silver catalysts for ethylene epoxidation. **M. A. Barteau**, J. Dellamorte, A. B. Mhadeshwar, J. Lauterbach
8:40 170. Convergence of theory and experiment in hydrotreating catalysis. **B. Hinnemann**, P. G. Moses, J. V. Lauritsen, F. Besenbacher, J. K. Nørskov, N-Y. Topsøe, H. Topsøe
9:20 171. Impact of theory on developments in industrial catalysis. **H. Topsøe**, B. S. Clausen, J. Sehested, S. Helveg, N-Y. Topsøe, C. H. Christensen, B. Hinnemann, A. Molenbroek, C. V. Ovesen, S. Dahl, E. Törnqvist, J. R. Rostrup-Nielsen, K. G. Knudsen
10:00 172. Measuring and relating the electronic structure of nonmodel supported catalytic materials to their performance. **S. Linic**
10:40 173. Simulating surface science experiments from first principles: Part I—temperature programmed desorption. V. Viswanathan, **H. A. Hansen**, J. Rossmeisl, T. F. Jaramillo, H. Pitsch, J. K. Norskov
11:00 174. Simulating surface science experiments from first principles: Part II—cyclic voltammetry. **V. Viswanathan**, H. A. Hansen, J. Rossmeisl, T. F. Jaramillo, H. Pitsch, J. K. Norskov
11:20 175. Electronic structure of intermediates in oxygen reduction reaction on Pt electrode. **L. Qi**, X. Qian, J. Li
11:40 176. Finding simplicity in complexity: Similarities in the coverage dependence of atomic adsorption energies on late transition metals. **J. R. Kitchin**

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis Cosponsored by BIOL

A. Kohen and A. Warshel, *Organizers*

M. J. Knapp, *Presiding*

8:30 177. Dynamic excursions and enzymatic transition state properties. **V. L. Schramm**
9:10 178. Functional protein motions during activation of a matrix metalloproteinase zymogen. **I. Sagi**, G. Rosenblum, S. O. Meroueh, M. Toth, J. F. Fisher, R. Fridman, S. Mobashery
9:50 Intermission.
10:10 179. Linking enzymatic C-H activation to protein flexibility: Properties of a series of active site mutants within the thermophilic alcohol dehydrogenase from B. stearothermophilus (ht-ADH). **J. P. Klinman**, Z. Nagel
10:50 180. Using hydrostatic pressure to search for promoting motions in enzyme catalysis. **N. Scrutton**
11:30 181. Enzyme motion from kinetic measurements. **A. Kohen**

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Chemical Methods of Nanofabrication Cosponsored by NANO‡

Y. H. Wang and S-J. Park, *Organizers*

C. A. Mirkin, *Organizer, Presiding*

8:30 182. Functionalized nanoparticles and surfaces for bioanalysis using SERRS. **D. Graham**, D. Thompson, R. Stokes, F. McKenzie, C. Dalton, R. Stevenson, E. Irvine, K. Faulds
9:05 183. Templated nanoassembly for mass-production of nanostructure-based integrated devices. **S. Hong**
9:40 184. Surface-templated assembly for organic solar cell and nanophotonic applications. **D. S. Ginger Jr.**, L. Y. Park, J. H. Wei, D. C. Coffey, A. Munro, Y. Chen, K. Munechika
10:15 Intermission.
10:25 185. Controlled growth of bio- and nano-arrays on basis of dip pen nanolithography. **H. Zhang**
11:00 186. Polymer self assembly in nanostructured electronic devices. **C. T. Black**
11:35 187. A biomimetic approach to template-driven fabrication of nanostructures. **J. J. De Yoreo**

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

Section E

Salt Palace Convention Center
250 F

Attosecond Science: The Next Frontier
Spatio-Temporal Attosecond Dynamics

A. D. Bandrauk and S. Leone, *Organizers*

J. Manz, *Presiding*

8:00 188. Spatiotemporal coherent control with picometer and attosecond precision. **K. Ohmori**
8:40 189. Controlling charge flow with vibronic pathways in a molecular interferometer. D. Xiao, S. S. Skourtis, I. V. Rubtsov, **D. N. Beratan**
9:20 190. Pump and probe ultrafast purely electronic reorganization. **R. D. Levine**
10:00 Intermission.
10:20 191. Ultrafast hole migration modular molecules from small peptides to hydrogen bonded clusters. **F. Remacle**, R. D. Levine
11:00 192. Intermolecular coulombic decay and ultrafast energy transfer. **L. Cederbaum**

Section F

Salt Palace Convention Center
251 C

Progress in Polarizable Force Fields and Simulation
Polarizability in Biological Systems

T. Head-Gordon and V. S. Pande, *Organizers*

S. Patel, *Presiding*

8:00 193. Does polarization help? Tests of next generation polarizable force fields. **V. S. Pande**
8:20 194. Comparison of the computed folding thermodynamics of Trp-cage miniprotein under various force fields and water models. **A. E. Garcia**, R. Day, N. Sgourakis, D. Paschek
9:00 195. Comparison of popular force fields for use by pharmaceutical industry by computation of hydration free energies of drug-like molecules. **W. C. Swope**, J. E. Rice, J. W. Pitera, H. W. Horn, G. Srinivas, D. Price, M. S. Head, J. D. Madura
9:40 196. Polarizable models: Hydration water dynamics near biological interfaces. M. E. Johnson, C. Malardier-Jugroot, R. K. Murarka, **T. Head-Gordon**
10:00 Intermission.
10:20 197. Are current molecular dynamics force fields too helical? R. B. Best, **G. Hummer**
11:00 198. Advances in using free-energy calculations for molecular design. **W. L. Jorgensen**

Section G

Salt Palace Convention Center
251 B

New Developments in Energy Conversion and Light-Harvesting
Materials for Inorganic and Nanostructured Photovoltaics

J. M. Lupton and D. S. Ginger Jr., *Organizers*

D. V. Talapin, *Organizer, Presiding*

8:00 Introductory Remarks.
8:20 199. Multicomponent nanocrystals for solar photovoltaics and photoctalysts. **A. P. Alivisatos**
9:00 200. Semiconductor nanowires for solar energy harvesting. **P. Yang**
9:40 201. Solution based semiconductor nanowires for possible photovoltaic applications. **M. Kuno**
10:20 Intermission.
10:40 202. How to improve electronic communication in nanocrystal solids? **D. V. Talapin**, M. Kovalenko
11:00 203. New aspects of carrier multiplication in semiconductor nanocrystals. **V. I. Klimov**
11:40 204. Functionalized quantum dots and conjugated polymers for light harvesting applications: Theoretical insights. **S. Tretiak**

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Bimetallics and Electrocatalysis Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Hydrogen Storage in Clathrate Materials
Sponsored by FUEL, Cosponsored by PHYS‡

WEDNESDAY AFTERNOON

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Fundamental Theoretical Advances

C. D. Sherrill and G. Galli, *Organizers*

W. E. Pickett, *Presiding*

1:30 205. Recent progress in ab initio dielectric response theory: Applications to ground state and excited state problems. **D. Lu**
2:10 206. Semiclassical origins of density functional theory. **K. Burke**, P. Elliott, D. Lee, A. Cangi
2:50 207. Toward exact numerical solutions of polyatomic Schrödinger equations. T. Shiozaki, E. F. Valeev, **S. Hirata**, M. Kamiya
3:30 Intermission.
3:50 208. Electron-proton correlation in the nuclear-electronic orbital approach: Explicit correlation and multicomponent density functional theory. **S. Hammes-Schiffer**
4:30 209. Stretched hydrogen molecule from a constrained-search density functional perspective. S. M. Valone, **M. Levy**

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

D. Sorescu, *Presiding*

1:30 210. Catalytic model systems and surface reactivity studied by high-resolution, fast-scanning STM. **F. Besenbacher**
2:10 211. Insights into the mechanisms and kinetics that control methane conversion processes. **M. Neurock**, E. Iglesia, C. Chin, C. Buda
2:50 212. Complementary structure sensitive and insensitive catalytic relationships. **R. A. van Santen**
3:30 213. Synergy between theory and experiments: Enhanced insight through working together. **J. K. Johnson**
4:10 214. Theoretical explanation of the nature of free and surface bound cerium endohedral fullerenes. **M. Kaliappan**, J. A. Larsson, S. Anna, V. Bert

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4:30 215. On the mechanism of the diruthenium-substituted polyoxotungstate $[\gamma\text{-}Ru^{III}_2(H_2O)_2H_2SiW_{10}O_{38}]^{4-}$ catalyzed O-O bond activation. **A. E. Kuznetsov**, Y. V. Geletii, G. L. Hill, K. Morokuma, D. G. Musaev
4:50 216. Modeling Si(100) reactivity using ONIOM calculations: Does bigger mean better for cluster size? **S. M. Casey**, N. Aldis
5:10 217. Convergence between theory and experiment for catalytic NO oxidation. **W. F. Schneider**, R. B. Getman

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Warshel, *Organizer*

A. Kohen, *Organizer, Presiding*

1:30 218. Probing the dynamics of dihydrofolate reductase using small molecule inhibitors. **A. L. Lee**
2:10 219. Dynamic energy landscape of DHFR catalysis. **P. E. Wright**, D. D. Boehr, D. J. McElheny, H. J. Dyson
2:50 Intermission.
3:10 220. Validation of the dynamical proxy for conformational entropy of proteins. **A. J. Wand**
3:50 221. Probing single-molecule protein function: Conformational dynamics under enzymatic reactions. Y. He, S. Mukherjee, **H. P. Lu**
4:10 222. A peroxidase-linked conformational switch in cytochrome c, with implications for apoptosis. **T. G. Spiro**, G. Balakrishnan, J. Su, J. T. Groves

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Nanostructured Carbon Materials
Cosponsored by NANO

Z. Bacic and M. D. Ward, *Organizers*

K. Kaneko, *Presiding*

1:30 223. Adsorptive storage of hydrogen in nanoporous materials. **S. K. Bhatia**
2:10 224. Hydrogen storage in carbon nanostructures. **G. Seifert Sr.**, A. M. Mesa, S. Yurchenko, L. Zhechkov Jr., T. Heine, S. Patchkovski
2:50 225. Cryogenic investigation of molecular hydrogen in fullerenes by means of NMR, IR and INS. **M. Carravetta**
3:30 Intermission.
4:10 226. Interactions of hydrogen in porous materials probed by rotational tunneling spectroscopy. **J. Eckert**
4:50 227. Hydrogen storage via hydrogen spillover to nanoporous materials. **A. D. Lueking**, Q. Li

Section E

Salt Palace Convention Center
250 F

Attosecond Science: The Next Frontier
Spatio-Temporal Attosecond Dynamics

A. D. Bandrauk and S. Leone, *Organizers*

M. Vrakking, *Presiding*

1:30 228. Attosecond interferometry. **K. Midorikawa**, Y. Nabekawa
2:10 229. Attosecond spectroscopy in condensed matter. **A. L. Cavalieri**
2:50 230. Attosecond science at ALLS. **J-C. Kieffer**
3:30 Intermission.
3:50 231. Attosecond dynamics in molecules and clusters. **D. M. Neumark**
4:30 232. Multidimensional attosecond X-ray spectroscopy of molecules. **S. Mukamel**, I. V. Schweigert
5:10 233. Charge-separation reaction in a donor-bridge-acceptor complex modulated by excitation of high-frequency modes at the bridge: UV-VIS/mid-IR/VIS study. R. V. Shapovalov, C. M. Lawrence, D. Xiao, S. S. Skourtis, J. L. Sessler, D. N. Beratan, **I. V. Rubtsov**

Section F

Salt Palace Convention Center
251 C

Progress in Polarizable Force Fields and Simulation
New Polarizable Models and Methods

T. Head-Gordon and V. S. Pande, *Organizers*

F. Paesani, *Presiding*

1:30 234. New approaches to including charge polarization in simulations. **D. G. Truhlar**, E. E. Dahlke, M. Higashi, Y. Kim, H. Leverentz, A. Sorkin, O. Tishchenko, B. Wang
2:10 235. Effective potentials for protein simulations: The AGBNP 2.0 implicit solvent model and hydrogen bonding to solvent. **R. M. Levy**, E. Gallicchio
2:50 236. Treating many-body polarization and many-body dispersion in complex systems: The quantum Drude oscillator formalism. **G. J. Martyna**
3:30 237. Hydrogen-bond dynamics in liquid water from an ab initio-based polarizable force field. **F. Paesani**, S. S. Xantheas, G. A. Voth
3:50 Intermission.
4:10 238. Monte Carlo simulations using polarizable force fields: From atmospheric nucleation to aqueous solvation. **J. I. Siepmann**, B. Chen, B. L. Eggimann, K. A. Maerzke
4:50 239. Systematic mapping of electrostatic and many-body electronic polarization effects into simpler short-ranged interactions. **G. A. Voth**

Section G

Salt Palace Convention Center
251 B

New Developments in Energy Conversion and Light-Harvesting
Organic Photovoltaics

D. V. Talapin and J. M. Lupton, *Organizers*

D. S. Ginger Jr., *Organizer, Presiding*

1:30 240. Bimolecular crystals and intercalated molecular structures of polymer/fullerene in bulk heterojunction solar cells. **M. D. McGehee**, A. C. Mayer, M. F. Toney, S. R. Scully, J. Rivnay, N. C. Cates, R. Gysel, M. Heeney, I. McCulloch
2:10 241. Optical probes of P3HT/bis-PCBM blends for organic photovoltaic applications. **G. Hukic**, T. Drori, Z. Vardeny
2:30 242. Spectroscopic imaging of charge transfer in donor/acceptor photovoltaic materials. **J. K. Grey**, Y. Gao
2:50 243. Ultrafast photoexcitation dynamics in blends of RR-P3HT/fullerene derivatives. **S. Singh**, J. Holt, Z. V. Vardeny
3:10 Intermission.
3:30 244. Modification of nanomorphology in polymer/fullerene blends-route toward high efficiency polymer solar cells. **Y. Yang**, G. Li, V. Shrotriya, Y. Yao, H-Y. Chen, S. Sista
4:10 245. Ultrafast studies of charge generation in P3HT/fullerene blends by mid-IR femtosecond transient absorption spectroscopy. **J. M. Holt**, S. Singh, Z. V. Vardeny
4:30 246. Charge transfer states in conjugated polymer/fullerene blends. **E. Da Como**

‡ Cooperative Cosponsorship

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Surface Characterization and Chemistry
Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

WEDNESDAY EVENING

Section A

Salt Palace Convention Center
Hall 5

Advances in Electronic Structure Theory and First Principles Dynamics

M. Head-Gordon, *Organizer*

7:30–9:30
247. A noniterative perturbative triples correction for spin-flipping and spin-conserving equation-of-motion coupled-cluster methods with single and double substitutions. **P. U. Manohar**, A. I. Krylov
248. Ab initio molecular dynamics study on the solute-solvent cross-effects in nucleic acid bases solutions. **A. Furmanchuk**, O. Isayev, L. Gorb, J. Leszczynski
249. Ab initio study of alternative genetic systems. **A. Vazquez-Mayagoitia**, M. Fuentes-Cabrera, B. G. Sumpter, J. E. Sponer
250. Coupled-cluster based effective fragment potential method. **S. Sok**, L. V. Slipchenko, M. S. Gordon
251. Details of proton dynamics and water transport in a polymer electrolyte membrane, Nafion. **Y-K. Choe**, E. Tsuchida, T. Ikeshoji, S. Yamakawa, S-A. Hyodo
252. Dramatic rate enhancements in pyridine catalyzed oxidation of some á- amino acids by lead tetra acetate: Kinetics, mechanism and structure-reactivity correlation analysis. **K. C. Rajanna**, **U. Umesh Kumar**, P. K. Saiprakash
253. Dynamics of the H^+ + HCl (E_{lab} = 10 eV), H^+ + HF, H^+ + CO_2, and H^+ + N_2O (E_{lab} = 30 eV) reactions: A complete electron nuclear dynamics investigation. **P. M. McLaurin**, J. A. Morales
254. Efficient computation of the dispersion interaction with density functional theory. **J. Kong**, E. Proynov, Z. Gan, M. Freindorf, T. R. Furlani
255. Efficient exploration of QM:MM potential energy surfaces. **H. P. Hratchian**
256. Electron dynamics from ab initio calculations and the reduced density matrix: Photovoltages and electron transfer at nanostructured semiconductor surfaces. **D. S. Kilin**, D. A. Micha, A. S. Leathers
257. Electronic structure of self-assembled amorphous polyfluorenes. **S. V. Kilina**, E. R. Batista, P. Yang, S. Tretiak, A. B. Saxena, R. L. Martin, D. L. Smith
258. Formation of dioxouranium(VI) glycine complexes in solution: Ab initio implication for bioremediation of radionuclides. **Y. Kholod**, J. Leszczynski, M. S. Gordon
259. Hybrid many-body interaction model for molecular condensed-phase systems. **G. J. O. Beran**
260. Implementation of analytical energy gradient for the time-dependent density-functional theory/effective fragment potential method: Application to the excited-state molecular dynamics in the solution phase. **N. Minezawa**, F. Zahariev, M. S. Gordon
261. Investigation of electron-induced disulfide bond cleavage using ab initio electronic structure calculations. **D. L. Neff**, J. Simons
262. Kinetic simulation of gas-phase experiments on nucleobases. **D. Kosenkov**, L. Gorb, J. Leszczynski
263. Linear and nonlinear response TDDFT/EFP. **F. Zahariev**, M. S. Gordon
264. Quantum mechanical study of solvent effects on vertical excitations of amides. **N. De Silva**, S. Yoo, M. S. Gordon
265. Self-consistent polarization density functional theory: Applications to Argon and water. **G. Murdachaew**, C. J. Mundy, G. K. Schenter, K. A. Maerzke, J. I. Siepmann
266. Spin-orbit generalized van Vleck perturbation theory. **W. Jiang**, M. R. Hoffmann
267. Three-state conical intersections in cytosine and pyrimidinone bases. **K. Kistler**, S. Matsika
268. Tractable spin-pure method for bond breaking: The CC-VB model. **D. W. Small**
269. Ultrafast dynamics of hexabromoplatinate complex in aqueous environment. **I. L. Zheldakov**, M. Ryasantsev, A. N. Tarnovsky
270. Ultrafast photochemistry of small polyatomic molecules in solution. **P. Z. El-Khoury**, A. N. Tarnovsky
271. Water-mediated midrange attractive interaction of antiparallel β-sheets. **S. Yoo**, S. S. Xantheas
272. Weizmann-5 (w-5) method: Combining the completely renormalized coupled cluster doubles and noniterative triples theory and polarizable continuum model theory in a composite method. **S. A. Nedd**, M. S. Gordon

Section B

Salt Palace Convention Center
Hall 5

General Computational and Theoretical Physical Chemistry

M. Head-Gordon, *Organizer*

7:30–9:30
273. A hybrid coarse-graining approach for lipid bilayers at large length and time scales. **G. S. Ayton**, G. A. Voth
274. Ab initio study of OH . . . X (X=CO, ethylene) prereactive complexes. **C. Lowe**, B. Chambers, R. Burcl
275. Ab initio study of OH . . . X (X=methane, acetylene) van der Waals complexes. **B. Chambers**, C. Lowe, R. Burcl
276. Ab inito investigation of naphto and benzo homologated DNA bases and the effects of substituents. **A. Vazquez-Mayagoitia**, M. Fuentes-Cabrera, B. G. Sumpter, O. Huertas, F. J. Luque, M. Orozco, R. Di Felice
277. Adsorption of sarin and dimethylmethylphosphonate on ZnO (1010). **M. J. Dorko**, J. P. Olson
278. Coarse-grained modeling of domain motions in bacteriophage T4 lysozyme. **Z. Zhang**, L. Lu, G. A. Voth
279. Computational modeling of atmospheric reactions of carbonyl oxides. **K. T. Kuwata**, E. J. Guinn, M. R. Hermes
280. DFT study on the reaction of V with SO2. **R. E. McClean**
281. Dispersion and induction forces in serotonin synthesis: DFT and ab initio results. **C. Lee**, M. Cafiero
282. Effects of double excited configurations in spiropyran-merocyanine conversion reaction. **J. E. Mendez**, C. W. Dirk
283. Electronic excited states of branched oligosilanes. **M. K. MacLeod**, C. Krempner, J. Michl
284. Evaluating potential interaction energies of synthetic peptides with natural peptides using computer simulations. **F. N. Ngassa**, E. M. Nkabyo, E. Lindsey, B. E. Haines, K. A. Thomasson
285. First principles prediction of fluorescence quenching in proteins. **P. R. Callis**, A. Petrenko, J. R. Tusell, P. L. Muiño, R. Hutcheson, C. Fahlstrom
286. Folding oligomers of 3,4'-difluoro-2,2'-X, with X = bifuran, bithiophene, or thienylfuran: A DFT study. **R. D. Parra**
287. Functional group based design of novel cholesterol moderating drugs using ab initio and DFT methods. **H. E. Utkov**, M. Cafiero
288. Gas-liquid nucleation in a 2-D system. **S. Chakrabarty**, M. Santra, B. Bagchi

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

289. Intermolecular photoinduced electron transfer between suspect molecules: Development of a systematic methodology to investigate using MO theory calculations. **N. J. Westfall**, C. W. Dirk
290. Ion pair structure as a key to understanding enormous substituent effects on pK_a of the CH vertex of $CB_{11}H_{12}^-$ in DMSO. **J. Chocholoušová**, J. Vacek, J. Michl
291. IR-controlled tunneling pathways. A molecular analog of the double-slit experiment. **D. Xiao**, S. S. Skourtis, I. V. Rubtsov, D. N. Beratan
292. Localized orbital corrections for the calculation of barrier heights in density functional theory. **M. L. Hall**, A. Bochevarov, R. A. Friesner
293. Models of PCNA-monoubiquitin interaction complexes. **A. W. Van Wynsberghe**, I. Ivanov, J. A. McCammon
294. Molecular dynamics study of gatekeeper-residue switch in hybrid globin-peroxidase, DHP. **D. C. Chatfield**, A. Pardillo
295. Multiple ice phases in hydrophobic confinement. **N. Kastelowitz**, V. Molinero
296. Mutations can increase proton conductance in aquaporin-1. H. Li, **H. Chen**, G. A. Voth
297. Nonaromatic cation-π interactions: A computational investigation. **T. P. Hanusa**, S. C. Chmely, R. M. Meier
298. Optical properties of complex nanorod architectures. **K. L. Shuford**, S. H. Park
299. Predicting the adsorption trends of hydrocarbons onto activated carbon using docking algorithms and semiempirical calculations. **J. DePalma**, E. Alkhatib, P. Snetsinger, J. Audie
300. Predictions of protein circular dichroism calculated by the dipole interaction model and compared to synchrotron radiation circular dichroism experiments. **N. Y. Forlemu**, K. A. Thomasson
301. Protein-DNA interactions: A Monte Carlo simulation study of facilitated diffusion. **R. K. Das**, A. B. Kolomeisky
302. Quantum control of ultrafast electron dynamics: A time-dependent multiconfiguration computational study. **F. Remacle**, M. Nest, R. D. Levine
303. Quantum solvation of molecules and small molecular dimers in superfluid He^4 clusters. **J. Ramilowski**, D. Farrelly
304. Quasiclassical surface-hopping trajectory calculations of the C(3P)+C2H2. **C. Chen**, B. J. Braams, J. M. Bowman
305. Withdrawn.
306. Relay of structural perturbations in GlpG rhomboid protease. **A. N. Bondar**, S. H. White
307. Small-molecule sequestration and transport in a nonporous crystal. A. J. Schmitz, J. R. Cox, M. D. Breite, D. J. Shaughnessy, C. A. Deakyne, **J. E. Adams**
308. Spectroscopic and structural signature of the CH--O H-bond. **S. Scheiner**, T. Kar
309. Structural microheterogeneity in binary mixtures of nitrotoluene isomers with *n*-decane. **K. A. Maerzke**, J. I. Siepmann
310. Theoretical investigation of the formation of [nCH3SO3 + H]$^-$ clusters (n=2-4): Implications to the formation of fine aerosol particles. **H. Hernandez-Soto**
311. Theoretical studies on the purpose of the surface binding site of avian influenza neuraminidase. **J. C. Sung**, A. W. Van Wynsberghe, R. E. Amaro, J. A. McCammon
312. Theoretical study of structure and spectra of phthalocyanine derivatives. **J. Fahrmann**, R. Burcl
313. Theoretical study on mechanisms of epoxy – phenol curing reaction. **M-P. Pham**, M. J. Marks, H. Pham, T. N. Truong
314. Theoretical study on mechanisms of epoxy-carboxylic acid and anhydride cure reactions. **M-P. Pham**, M. J. Marks, H. Pham, T. N. Truong
315. Theoretical study on mechanisms of the epoxy-amine cure reaction: The role of primary and secondary amines. **M-P. Pham**, M. J. Marks, H. Pham, T. N. Truong
316. Theoretical study on the nature of on- and off-states of reversibly photoswitching fluorescent protein Dronpa. **X. Li**, L. W. Chung, K. Morokuma, A. Miyawaki
317. Visualization of molecular orbitals and the related electron densities. **M. Haranczyk**, M. S. J. Gutowski
318. What is the reaction mechanism between formaldehyde and water? T. Cours, S. Canneaux, **F. Louis**, B. Hanoune
319. What is there in formaldehyde aqueous solutions? P. Delcroix, S. Canneaux, **F. Louis**, B. Hanoune
320. Zinc-coordinated pyrogallol[4]arene assemblies: Host vs. guest protonation. **C. A. Deakyne**, T. Szabo, C. M. Mayhan, S. A. Nussbaum, N. P. Power, S. J. Dalgarno, J. L. Atwood
321. Photo-induced conductivity of DNA-templated composite nanowire. **D. S. Kilin**, K. Tsemekhman, S. V. Kilina, O. V. Prezhdo

Section C

Salt Palace Convention Center
Hall 5

General Experimental Physical Chemistry

M. Head-Gordon, *Organizer*

7:30–9:30
322. Absolute hydration energies of Zn2+ and Cd2+. **T. E. Cooper**, P. B. Armentrout
323. Aromatic electron acceptors change the chirality dependence of oxidation of single-walled carbon nanotubes. **F. J. Knorr**, W-C. Hung, C. M. Wai
324. Characterization of electrodeposited nickel, iron, and nickel-iron thin films. T. S. Boman, M. J. Ouma, **J. R. Hampton**
325. Chromophore synthesis and characterization for two-photon absorption vesicle photolysis. **T. R. Ewy**, P. A. Sullivan, B. C. Olbricht, K. A. Dendramis, J. A. Davies
326. Comparison of NO_2 reactivity with α- and γ-Fe_2O_3. **H. M. Bevsek**, B. C. Hixson
327. Conformational stability, r0 structural parameters, barriers to internal rotation, ab initio calculations and vibrational assignment for 2,2-difluoroethanol. **A. Ganguly**, S. Bell, G. A. Guirgis, J. R. Durig
328. Deliquescence of pharmaceutical and food ingredients: Phase transition of model systems and moisture sorption studies. **K. Kwok**, L. Mauer, L. S. Taylor
329. Deliquescence of pharmaceutical and food ingredients: The effect of relative humidity on the chemical stability of the sucrose-citric acid system. **K. Kwok**, L. Mauer, L. S. Taylor
330. Effect of dissociated oxygen on the infrared spectra of low-temperature water ice films. **S. R. Doering**, K. M. Strobush, J. E. Boulter
331. Effect of symmetry of the cation and alkyl chain length on the structure and intermolecular dynamics of 1,3-dialkylimidazolium bis(trifluoromethanesulfonyl)imide ionic liquids. D. Xiao, L. G. HInes Jr., R. A. Bartsch, **E. L. Quitevis**, O. Russina, A. Triolo
332. Electrochemical study of ferrocene in 1,4-bis(3-methylpyridinium)butane bromide ionic liquid. **X. Yang Sr.**, J. Wang Sr., G. Li Sr., Z. Zhang
333. Electronic spectrum of the all-benzenoid polycyclic aromatic hydrocarbon hexa-peri-hexabenzocoronene, $C_{42}H_{18}$. **T. D. Varberg**, D. L. Kokkin, T. P. Troy, M. Nakajima, K. Nauta, G. F. Metha, N. T. Lucas, T. W. Schmidt
334. Electronic structure and magnetization of diluted magnetic semiconductor nanowires. **K. H. Ji**
335. Experimental detection of dangling OH groups in the hydration-shell of water around hydrocarbon solutes. **K. R. Fega**, P. Perera, D. Ben-Amotz
336. Experimental observation of inelastic pathways in charge-transfer reaction in a donor-bridge-acceptor complex using UV-VIS/mid-IR/VIS spectroscopy. **R. V. Shapovalov**, C. M. Lawrence, D. Xiao, S. S. Skourtis, J. L. Sessler, D. N. Beratan, I. V. Rubtsov
337. Experimental strategies for determining the inner shell hydration energies of alkaline earth metal dications. **D. R. Carl**, P. B. Armentrout

338. Formation dynamics of secondary phase of poly(9,9-dioctylfluorene) in solution. **C. W. Cone**, D. A. Vanden Bout
339. Hydrogen detection by polyaniline nanofibers: Effect of the electrode metal. J. D. Fowler, S. Virji, R. B. Kaner, **B. H. Weiller**
340. Hydrogen-deuterium atom exchange in photolyzed methane-water ice mixtures. **A. S. Weber**, P. V. Johnson, R. Hodyss
341. Infrared spectra of $K^+(APE)(H_2O)_n$. **A. L. Nicely**, J. M. Lisy
342. Ion exclusion and acidity of ice films. **K. F. Searles**, R. R. H. Michelsen
343. IR Diode laser study of collision energy transfer between tetrafluorobenzene isomers and CO_2. **K. Kim**, A. M. Johnson, E. T. Sevy
344. Isothermal titration calorimetry studies of thrombin interaction with tetrapeptides reversible inhibitors. **C. C. Clement**, M. Philipp
345. Kinetic study of hydrolysis of ATP and GTP at 37 ^{o}C and a mechanistic study by theoretical calculations. **B. A. Dougan**, H. Liu, Y-D. Wu, Z-L. Xue
346. Kinetics study of the reaction of OH with xylenes at 1-9 Torr and 240-340K using the relative rate/discharge flow/mass spectrometry technique. **D. N. Mehta**, A. Nguyen, Z. Li
347. Lanthanide ion reduction by an intense femtosecond laser pulse. **N. Nakashima**, D. Nishida, M. Kusaba, T. Yatsuhashi
348. Laser assisted poling of binary chromophore organic glasses. **B. C. Olbricht**, P. A. Sullivan, J. A. Davies, T. R. Ewy, B. E. Eichinger, B. H. Robinson, P. J. Reid, L. R. Dalton
349. Methane activation by Os+. **L. G. Parke**, P. B. Armentrout
350. Morphology-controlled synthesis of lead chalcogenide nanocrystals using vapor transport and solvothermal methods. **S. Y. Jang**, J. Park, J. W. Cho, H. S. Kim, Y. J. Cho, C. H. Kim
351. Novel phenomena of crystallization and crystal growth by photon pressure of a focused cw laser beam. **H. Masuhara**, T. Sugiyama
352. Novel preparation and characterization of doped para-hydrogen solids. **B. B. Smith**, J. S. Winn
353. Phase transitions in Langmuir films of n-perfluorocarboxylic acids. **K. G. Nelson**, C. D. Vecitis, E. M. Spain, N. F. Dalleska
354. Probing molecular structures of silicone elastomer-silane interfaces. **A. V. Vázquez**, N. E. Shephard, S. Rhodes, Z. Chen
355. Raman spectra of 1,3-butadiene-d_0 and -d_6 and their torsional potential energy function. **P. Boopalachandran**, J. Laane, N. C. Craig
356. Reactive and nonreactive interactions of thiophene with WS2 and MoS2 fullerene-like nanoparticles. **A. Sand**, J. Goering, U. Burghaus, B. W. Arey, O. Eidelman, A. Zak, R. Rosentsveig, R. Tenne
357. Reduction of poly-2,7-(9,9-dihexylfluorene) molecular wires to form polyanions. **L. Zaikowski**, C. Gelfond, E. D. Selvaggio, S. Asaoka, N. Takeda, A. Yang, J. Miller
358. Refractive index effects on molecular electronic oscillator strengths and radiative decay rates in supercritical fluids. **B. J. Hrnjez**, J. A. Saperia, J. J. Hefter
359. Relaxation of highly vibrationally excited trifluorobenzene by collisions with CO_2. **A. M. Johnson**, K. Kim, E. T. Sevy
360. Solid-state NMR and quantum chemistry of melamine-cyanuric acid. **G. S. Harbison**, M. Kinde-Carson
361. Solvent effects in extraction of carboxylic acids. **M. Prezhdo**, L. P. Loginova, V. V. Prezhdo
362. Studies of hydrocarbon evaporation. **R. S. Booth**, A. N. VanTilburg, C. Pursell, P. Kelly-Zion
363. Suggestion for rationalization of anomalous dispersion of excitability waves in the ferroin-catalyzed Belousov-Zhabotinsky (BZ) reaction with 1,4-cyclohexanedione as the organic substrate. R. M. Boger, **R. J. Field**
364. Synthesis and characterization of silver nanorods and nanotriangles. **A. Roth**, H. McBride, A. M. Brun, I. Gryczynski, T. Shtoyko
365. The gas-phase reaction of atomic chlorine with ethylene: Experiments and computations. **I. M. Alecu**, K. E. Kerr, K. Thompson, N. Wallace, Y. Gao, **P. Marshall**
366. The photocatalytic activity of nanoparticles–carbon nanotube and -TiO2 hybrid nanostructures toward decomposition of 1,4-dioxane and methylene blue. **D. M. Jang**, J. Park
367. The protonation of 1-pentanol and tert-butanol in sulfuric acid solutions at cold temperatures. **A. V. Maclauchlan**, R. R. H. Michelsen
368. Thermal stability and decomposition kinetics of *N,N*-diethyl-*N'*-(4-chloro)benzoylthiourea and its copper(II) and nickel(II) complexes. **H. Arslan**, G. Binzet, N. Külcü, U. Flörke
369. Time-resolved dynamics of photoelectrons in He droplets: VUV-IR study with femtosecond resolution. **O. A. Kornilov**, C. C. Wang, A. Healy, M. Leonard, S. Peng, S. R. Leone, O. Gessner, D. M. Neumark
370. Toward bulk materials with a negative index of refraction in the visible. **S. Roy**, T. F. Magnera, J. Michl
371. Vibrational spectroscopic studies of host/guest interactions in cyclophane/anthracene complexes. **T. Buthelezi**
372. Water bonding and structure in the presence of ions at the fluorite/water interface. **A. J. Hopkins**, G. L. Richmond
373. Crystallization kinetics of an induced crystallization studied in nanocolloidal octylecyanobiphenyl liquid crystal gels. **D. Sharma**
374. Architectural complexity and charge transfer in metal--organic coordination networks at surfaces. **S. L. Tait**, A. Langner, T-C. Tseng, N. Lin, K. Kern
375. Factors that determine molecular structure of polystyrene surfaces. **A. D. Curtis**, B. J. Nielson, S. B. Moxley, A. D. Quast, J. E. Patterson
376. Carbon-silica composite mesoporous films: Impact of silica content on conductivity and modulus. **L. Song**, D. Feng, C. G. Campbell, A. M. Forster, D. Zhao, B. D. Vogt
377. Catalytic nanocutting of graphene sheets. **L. Ci**, L. Song, W. Gao, D. Jariwala, P. M. Ajayan, A. Elías
378. Effects of carbon source geometry and reactivity on the CVD growth of single-walled carbon nanotubes. **C. Beasley**, B. M. Clemens, H-S. P. Wong
379. Fast nonlinear ion transport via field-induced hydrodynamic slip in sub-20nm hydrophilic nanofluidic channels. **U. Vermesh**, J. W. Choi, O. Vermesh, R. Fan, J. Nagarah, J. R. Heath
380. Gold nanorods with tunable size evenly distributed in the channels of mesoporous silica. **Z. Li**, R. M. Richards, C. Kuebel
381. Individually-wired nanoelectrodes for a 3-D nanostructured battery systems. **D. Teeters**, P. L. Johnson
382. UHV-STM investigations on DNA bases. **W. Xu**, R. Otero, M. Lukas, R. Kelly, E. Laegsgaard, L. Kantorovich, F. Besenbacher

Section D

Salt Palace Convention Center
Hall 5

New Developments in Energy Conversion and Light-Harvesting

M. Head-Gordon, *Organizer*

7:30–9:30
383. Chemical mapping of donor/acceptor polymer thin film morphologies: Effect of processing conditions. **Y. Gao**, J. K. Grey
384. Degradation of organic compounds by photocatalytically active MoS_2 and WS_2 particles. **D. James**, T. Zubkov
385. Effect of surface active agents on the photoluminescence of titanium dioxide nanocrystals. **C. C. Rich**, J. L. McHale
386. Long lived charge separation in perylene-quinone dyad using proton coupled electron transfer. **P. Kucheryavy**, G. Li, K. D. Glusac
387. Molecular triads comprised of boron dipyrrin-C60 dyad connected to either an energy or electron donating entity to probe sequential energy/electron transfer events. **C. A. Wijesinghe**, F. D'Souza
388. Nanoscale insights into the internal structure of porphyrin nanorods. **B. A. Friesen**, U. Mazur, J. L. McHale, K. Nishida
389. Near-field scanning optical microscopy for high resolution photocurrent and time correlated single photon counting lifetime measurements in organic photovoltaics. **M. S. Glaz**, D. A. Vanden Bout
390. Noncovalent aggregates of 1,3 diphenylisobenzofuran for singlet fission studies. **M. B. Smith**, J. C. Johnson, J. Michl
391. On 1-D nanostructure-guided chain reactions: Harmonic interactions. **N. Nair**, M. S. Strano
392. Solvent effects on dye structure and electron transport properties of sensitized nanocrystalline titanium dioxide. **J. A. Downing**, J. L. McHale
393. Spectroscopy of betanin and its application as a sensitizer for TiO_2 based dye-sensitized solar cells. **C. S. Sandquist**, J. L. McHale
394. Charge delocalization and separation in type II tunneling structures of CdTe and CdSe nanocrystals by surface photovoltage spectroscopy. **D. Gross**, I. Mora Seró, T. Dittrich, A. S. Susha, A. L. Rogach, E. Da Como, J. Feldmann
395. Withdrawn.
396. Excitonic and vibronic coupling in supramolecular light harvesting porphyrin complexes probed by resonance Raman spectroscopy. **J. L. McHale**, U. Mazur, B. A. Friesen
397. Interfacial structure and dynamics at the electrode/organic interface. **M. L. Blumenfeld**, M. P. Steele, O. L. A. Monti
398. Photoluminescence and Raman spectroscopy of titanium dioxide nanotubes. **C. C. Mercado**, J. L. McHale
399. Rate of glucose equivalent production in C4 plants and the effect of pressure and temperature. **A. Panda**, S. N. Datta
400. The effect of surface ligands on optical and electronic spectra of semiconductor nanoclusters. **S. V. Kilina**, S. A. Ivanov, S. Tretiak
401. Ultrafast exciton dynamics in a DNA duplex helix and its application to nonlinear spectroscopy. **H-D. Kim**, Y. Tanimura, M. Cho

Section E

Salt Palace Convention Center
Hall 5

Progress in Polarizable Force Fields and Simulation

M. Head-Gordon, *Organizer*

7:30–9:30
402. Applications of a novel QM/MM method incorporating a polarizable force field. **C. F. Williams**
403. Effects of sodium hydroxide on the solvation of dimethyl-succinate in water: A computational study. **X. Sun**, Y. Cao, S. Niwayama, W. L. Hase, L. X. Dang
404. Fluctuating-charge models in bond space and their exact reformulation in atomic space. **J. Chen**, D. Hundertmark, T. J. Martínez
405. Atomistic molecular dynamics simulations of poly (ethylene oxide) aqueous solutions as a function of concentration and temperature using polarizable force field. **O. N. Starovoytov**, O. Borodin, D. Bedrov, G. D. Smith

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406. Coarse-grained ions without charges: Improving computational efficiency by eliminating electrostatic interactions. **R. C. DeMille**, V. Molinero
407. Developing polarizable force fields from ab initio calculations: A critical analysis of methods. **J. R. Hammond**, S. S. Xantheas, K. Kowalski
408. Solvation of ions: Molecular dynamics simulation using combined quantum mechanical, effective fragment potential and continuum solvation model. **H. Li**, P. Su

Section F

Salt Palace Convention Center
Hall 5

Convergence between Theory and Experiment in Surface Chemistry and Catalysis

M. Head-Gordon, *Organizer*

7:30–9:30
409. Ab initio study of Au_3 cluster interactions with titanium dioxide. **Y. Kholod**, B. Njegic, M. S. Gordon
410. Catalysis of Henry reaction in mesoporous silica nanospheres. **S. A. Nedd**, M. S. Gordon
411. Chemical structure of CuO-NiO/chabazite oxygen carrier in chemical-looping combustion. **E. M. Eyring**, P-H. Liao, H. P. Wang
412. CO oxidation and ethylene hydrogenation over one nanometer bimetallic RhPt particles. **W. Huang**, Y. Li, J. N. Kuhn, C-K. Tsung, G. A. Somorjai
413. Measuring surface interactions using fluorescence correlation spectroscopy. **C. R. Daniels**, C. G. Reznik, C. F. Landes
414. Methanol oxidation on neutral iron oxide clusters in the gas phase. **Y. Xie**, F. Dong, E. R. Bernstein
415. Partitioning behavior of perchlorate vs. chloride ions in aqueous solutions: An electron spectroscopy and first principles MD simulations study. **S. Ghosal**
416. STM Study of adsorption sites of size-selected Au_1, V_x, and V_xO_y clusters on a TiO_2(110)-1x1 surface. **X. Tong**, S. P. Price, C. Ridge, L. B. Benz, P. Kemper, H. Metiu, M. T. Bowers, S. Buratto

THURSDAY MORNING

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics Challenging Applications

C. D. Sherrill and G. Galli, *Organizers*

B. G. Sumpter, *Presiding*

8:30 417. Ab initio molecular dynamics study of the density of liquid water: How reliable are DFT-based simulations of wet systems? **M. Fernandez-Serra**
9:10 418. Many-body corrections to density functional theory level alignment at organic-inorganic hybrid interfaces using quantum Monte Carlo calculations. **Y. Kanai**, Z. Wu, J. C. Grossman
9:50 419. Melting of iron at Earth's core conditions from quantum Monte Carlo free energy calculations. **D. Alfe'**
10:30 Intermission.
10:50 420. Reduced dimensional studies of roaming radicals. **L. B. Harding**, S. J. Klippenstein, Y. Georgievskii
11:30 421. Tackling thermal effects on molecular chiroptical properties. **F. Furche**

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Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

T. F. Jaramillo, *Presiding*

8:00 422. Designing new electrocatalysts for the hydrogen evolution reaction (HER): Combining theory and experiment. **T. F. Jaramillo**, K. P. Jorgensen, J. Bonde, J. P. Greeley, J. Zhang, B. L. Ooi, J. H. Nielsen, S. Horch, J. Ulstrup, J. K. Norskov, I. Chorkendorff
8:40 423. Water-gas shift on gold- and copper-oxide catalysts: Active phase and reaction mechanism. **J. A. Rodriguez**
9:20 424. Gamma alumina from first principles matches experiments and goes beyond. **H. Toulhoat**, M. Digne, P. Sautet, P. Raybaud, D. Guillaume
10:00 425. Toward predictive power in the discovery of heterogeneous catalysts. **C. H. Christensen**
10:40 426. Comparison of the adsorption of transition metals on α-alumina surfaces. **L. Briquet**, C. R. A. Catlow, S. A. French
11:00 427. Small tantalum species on amorphous silica: DFT calculations reveal a notable flexibility of the support. A. Genest, H. Aleksandrov, S. M. Parker, M. Metzner, A. M. Shor, V. A. Nasluzov, B. C. Gates, **N. Roesch**
11:20 428. Single-molecule dynamics of nanocatalysis. **P. Chen**
11:40 429. Continuous, quadrature-friendly potential energy surfaces for *polyatomic* molecule-surface interactions: N_2O/Cu. **S. Manzhos**, K. Yamashita

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen and A. Warshel, *Organizers*

H. P. Lu, *Presiding*

8:00 430. Enzyme dynamical changes upon substrate binding and structural interconversions measured with ultrafast 2-D IR vibrational echo spectroscopy. **M. D. Fayer**, H. Ishikawa, I. J. Finkelstein, J. K. Chung, K. Kwak, S. Kim
8:40 431. Femtosecond to picosecond dynamics of formate dehydrogenase. **C. M. Cheatum**, J. N. Bandaria, M. W. Nydegger, S. Dutta, A. Kohen
9:20 Intermission.
10:00 432. Quantum coherence in photosynthetic light harvesting. **G. R. Fleming**, T. Calhoun, G. Schlau-Cohen, H. Lee, N. S. Ginsberg, A. Ishizaki, Y-C. Cheng
10:40 433. Fate of photoexcited pyridoxal 5'-phosphate in solution and in the enzyme environment. **M. P. Hill**, E. C. Carroll, M. D. Toney, D. S. Larsen
11:00 434. Protein dynamics and catalysis: Recent results at a variety of timescales. **S. D. Schwartz**

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Nanostructured Carbon Materials
Cosponsored by NANO

Z. Bacic and M. D. Ward, *Organizers*

S. K. Bhatia, *Presiding*

8:00 435. Quantum effect in low temperature physical adsorption of H2 and D2 in nanopores. **K. Kaneko**, H. Tanaka, T. Ohba, H. Kagita, D. Noguchi, A. Kondo, K. Hata, M. Yudasaka, M. Yumura, S. Iijima, H. Kanoh
8:40 436. Designing nanoporous materials for hydrogen storage. **G. E. Froudakis**
9:20 437. Chemical reactivity within carbon nanotubes: Classical and quantum mechanical studies of the D + $H_2 \rightarrow$ HD + H reaction. **E. M. Goldfield**, T. Lu, S. K. Gray
10:00 Intermission.
10:20 438. Carbon nanostructures for molecular hydrogen confinement. A. K. Singh, F. Ding, R. S. Aga, **B. I. Yakobson**
11:00 439. Quantum mechanical studies of molecular hydrogen in nanoporous environments. **S. K. Gray**, P. Zapol, E. M. Goldfield

Section E

Salt Palace Convention Center
250 F

Attosecond Science: The Next Frontier Intense Fields

S. Leone, *Organizer*

A. D. Bandrauk, *Organizer, Presiding*

8:00 440. Theoretical investigation of the electronic and nuclear dynamics of molecules in intense laser fields: H_2 and C_{60}. **H. Kono**, N. Niitu, H. Ikeda, K. Nakai, T. Kato, R. Islam
8:40 441. Ab initio theoretical modeling of multiple ionization processes in intense laser fields. **T. T. Nguyen-Dang**
9:20 442. Attosecond nonadiabatic electron dynamics with and without intense optical field. **K. Takatsuka**, T. Yonehara
10:00 Intermission.
10:20 443. Multichannel coherence in strong-field ionization. **R. Santra**
11:00 444. Strong field double ionization: The phase space perspective. **T. Uzer**, F. Mauger, C. Chandre

Section F

Salt Palace Convention Center
251 C

Progress in Polarizable Force Fields and Simulation
New Polarizable Models and Methods

T. Head-Gordon and V. S. Pande, *Organizers*

J. M. Herbert, *Presiding*

8:00 445. On the nature of the water-water hydrogen bond. **M. Head-Gordon**
8:20 446. An ab initio based transferable interaction potential for water. **S. S. Xantheas**, G. S. Fanourgakis
9:00 447. Progress toward a multiscale SIBFA/GEM/QM integrated polarizable scheme using Hermite Gaussian densities. **J-P. Piquemal**, G. A. Cisneros, T. A. Darden, N. Gresh
9:40 448. Fourier grid QM/MM simulations of the hydrated electron using a polarizable model Hamiltonian. L. D. Jacobson, C. F. Williams, **J. M. Herbert**
10:00 449. Electrostatic interaction model for the calculation of the polarizability of large noble metal nanoclusters. **L. Jensen**
10:20 Intermission.
10:40 450. Phase separation in hydrocarbon-alcohol-water systems at the molecular level: A first-principles-based theoretical study. **L. V. Slipchenko**
11:00 451. Achieving reactive, polarizable force fields through bond charges. **S. J. Stuart**, B. Walder

Section G

Salt Palace Convention Center
251 B

New Developments in Energy Conversion and Light-Harvesting
Dye and Quantum Dot Sensitized Devices

D. V. Talapin, J. M. Lupton, and D. S. Ginger Jr., *Organizers*

M. Kuno, *Presiding*

8:30 452. Mechanistic insights of quantum dot sensitized solar cells. D. Baker, K. Tvrdy, **P. V. Kamat**
9:10 453. Narrowband-sensitized J-aggregate/quantum dot conjugates in solution. **B. J. Walker**, G. P. Nair, L. F. Marshall, J. R. Tischler, V. Bulovic, M. G. Bawendi
9:30 454. Femtosecond Raman structural studies of photoinduced electron transfer at a dye/semiconductor interface. **R. Frontiera**, J. Dasgupta, R. A. Mathies
9:50 455. New Ru-based dyes with significantly increased extinction coefficients and interesting electron and hole transfer properties relevant to solar energy conversion. **M. Abrahamsson**, W. B. Heuer, G. J. Meyer
10:10 Intermission.
10:30 456. Interfacial charge transfer at the single molecule level: Insights for dye-sensitized solar cells. **O. L. A. Monti**, L. K. Schirra, M. L. Blumenfeld, B. S. Tackett, J. M. Tyler
10:50 457. Assessing methods for energy transfer calculations: Lessons from 2-pyridone dimer. **E. Sagvolden**, F. Furche
11:10 458. Optical sensitization of anatase TiO_2 with 8-hydroxyquinoline aluminum (Alq) complexes. **L. G. C. Rego**, R. Silva, J. A. Freire, R. C. Snoeberger, V. S. Batista
11:30 459. Energy transfer between individual quantum dots and single-wall nanotubes. **J. M. Gerton**, C. Mu, E. Shafran, B. D. Mangum

THURSDAY AFTERNOON

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Fundamental Theoretical Advances

C. D. Sherrill and G. Galli, *Organizers*

S. Hirata, *Presiding*

1:30 460. Stable long-time semiclassical description of zero-point energy in high-dimensional molecular systems. **V. A. Rassolov**, S. Garashchuk
2:10 461. Full charge self-consistency in LDA+DMFT theory. **W. E. Pickett**
2:50 462. Extending electronic structure theory to complex molecular problems: Local correlation coupled-cluster and correlation energy scaling methodologies. **P. Piecuch**, W. Li, J. J. Lutz, J. R. Gour
3:30 Intermission.
3:50 463. New method for accelarating numerical integration in density functional theory. **J. Kong**, N. J. Russ, C. Chang
4:10 464. High-rank local cluster models for strong correlation. **J. A. Parkhill II**, M. Head-Gordon
4:30 465. Constructing diabatic states with Boys localization. **J. E. Subotnik**, S. Yeganeh, R. J. Cave, M. A. Ratner

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer*

I. Chorkendorff, *Presiding*

1:30 466. Identifying the rate limiting step and its reaction site: The key to new and improved catalysts. **I. Chorkendorff**
2:10 467. Elementary molecular reactions on rutile TiO2 surfaces. **B. Hammer**
2:50 468. Consequences of acid strength in isomerization and elimination catalysis on solid acids. J. Macht, R. Carr, M. J. Janik, M. Neurock, **E. Iglesia**
3:30 469. Resolving the electronic properties of catalytically important Pd/Au alloys at the subnanometer level. **A. E. Baber**, H. L. Tierney, E. C. H. Sykes
3:50 470. Unraveling of a new mechanism of atmospheric chemistry reactions: Formation of ClNO. **B. Njegic**, J. D. Raff, W. L. Chang, D. Dabdub, B. J. Finlayson-Pitts, M. S. Gordon, R. B. Gerber
4:10 471. Heterogeneous chlorine activation from NOx-HCl reactions on surfaces. **J. D. Raff**, B. Njegic, R. B. Gerber, B. J. Finlayson-Pitts
4:30 472. Acid dissolution at ice surfaces. **P. Ayotte**, R. Iftimie, P. Marchand, V. Thomas
4:50 473. Nitric acid on ice: Dissociation and photolysis. **P. Marchand**, P. Ayotte

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen and A. Warshel, *Organizers*

M. P. Hill, *Presiding*

1:30 474. Free energy excitation "spectra" and landscapes of folding and function. **P. G. Wolynes**
2:10 475. Coupling between protein and reaction dynamics for enzymatic processes. **J. T. Hynes**
2:50 Intermission.
3:10 476. Single molecule and other properties in enzyme catalysis. **R. A. Marcus**
3:50 Panel Discussion: **R. A. Marcus, V. L. Schramm, R. L. Schowen**.

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Various Nanostructured Materials
Cosponsored by NANO

Z. Bacic and M. D. Ward, *Organizers*

A. D. Lueking, *Presiding*

1:30 477. Complex borohydride and hydrogen interactions with Pt-loaded ZrO_2 frameworks. **S. M. Opalka**, X. Tang, T. H. Vanderspurt, D. A. Mosher, B. L. Laube
2:10 478. Enhanced H_2 adsorption in isostructural metal-organic frameworks with open metal sites: Strong dependence of the binding strength on metal ions. **W. Zhou**, H. Wu, T. Yildirim
2:50 479. Hierarchical storage of hydrogen in clathrates of ammonia borane. **M. S. J. Gutowski**, A. Abramov
3:30 Intermission.
4:10 480. Proton disorder in type II clathrate hydrates. **S. Rick**, D. L. Freeman

4:50 481. Quantum dynamics of hydrogen interacting exohedrally with single-walled carbon nanotubes. **B. Poirier**
5:30 Concluding Remarks.

Section E

Salt Palace Convention Center
250 F

Attosecond Science: The Next Frontier Intense Fields

S. Leone, *Organizer*

A. D. Bandrauk, *Organizer, Presiding*

1:30 482. Attosecond molecular science with IR pulses. **F. Legare**
2:10 483. Ultrafast measurements of plasmon-field accelerated electrons in metal nanostructures. **P. M. Nagel**, T. Pfeifer, M. J. Abel, M. J. Bell, D. M. Neumark, S. R. Leone
2:30 Concluding Remarks.

Section F

Salt Palace Convention Center
251 C

New Developments in Energy Conversion and Light-Harvesting
Materials for Inorganic and Nanostructured Photovoltaics

J. M. Lupton and D. S. Ginger Jr., *Organizers*

D. V. Talapin, *Organizer, Presiding*

1:30 484. New semiconductor materials for high efficiency solar cells. **W. Walukiewicz**
2:10 485. Solution processing of CIGS absorber layers using a hydrazine-based approach. **D. B. Mitzi**
2:50 486. Withdrawn.
3:10 Intermission.
3:30 487. Designing nanowires for energy storage and photovoltaics. **Y. Cui**
4:10 488. Phonon bottleneck effect in quantum dots. **A. Pandey**, P. Guyot-Sionnest
4:30 489. Charge separation in hybrid structures of semiconductor nanocrystals. **A. L. Rogach**

POLY

Division of Polymer Chemistry

J. G. Linhardt, G. N. Tew, and K. L. Kiick, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

ACS Award in Applied Polymer Science: Symposium in Honor of Benny D. Freeman (see *PMSE*, Sun, Mon)

Cooperative Research Award Symposium in Honor of Professor Robert Waymouth and Dr. James Hedrick (see *PMSE*, Sun)

Degradable Polymers: From Synthesis to Nanotechnology (see *PMSE*, Tue)

Functional Polymer Nanocomposites for Energy Storage and Conversion (see *PMSE*, Mon, Tue)

Multiphase Polymer Materials: From Fundamentals to Applications (see *PMSE*, Sun, Mon, Tue, Wed, Thu)

Nanostructured Block Copolymer Materials (see *PMSE*, Sun, Mon, Tue)

Novel Applications of Supramolecular Materials (see *PMSE*, Thu)

Polymers for Microencapsulation and Coating Technologies (see *PMSE*, Wed)

Detection and Monitoring of Engineered Nanoparticles in Environmental and Biological Systems (see *COLL*, Sun)

Frontier Applications of Nanotechnology in Engineering Extracellular Matrices (see *COLL*, Wed, Thu)

Frontiers in Nanoparticle and Nanoporous Materials (see *COLL*, Sun, Mon, Tue, Wed, Thu)

Lipid Assemblies: Preparation, Characterization and Applications (see *COLL*, Wed, Thu)

Polymeric Microcapsules: Theory, Experiment and Applications (see *COLL*, Sun, Mon, Tue)

Structure and Function of Membranes, Proteins, and Lipids (see *COLL*, Sun, Mon, Tue, Wed, Thu)

The Influence of Ions and Osmolytes on Aqueous Macromolecules (see *COLL*, Mon, Tue)

Biomedical Applications of Polysaccharide-based Materials (see *CELL*, Mon)

Protein Adhesives, Hydrogels, Films, Sponges, and Scaffolds (see *CELL*, Tue)

Water Soluble Polymers from Cellulose: Materials and Applications (see *CELL*, Thu)

Genetically Designed Molecular Materials (see *NANO*, Sun, Mon, Tue)

ACS Award for Creative Invention: Symposium in Honor of Robert H. Grubbs (see *ORGN*, Tue)

Material, Devices and Switches (see *ORGN*, Sun)

Molecular Recognition and Self-Assembly (see *ORGN*, Tue, Wed)

Peptides, Proteins and Amino Acids (see *ORGN*, Tue)

Physical Organic Chemistry, Molecular Recognition, Self-Assembly and Biomolecules (see *ORGN*, Tue)

Membranes for Fuel and Energy Applications (see *FUEL*, Mon)

SUNDAY MORNING

Section A

Sheraton
Granary Room

Ion-Containing Polymers for New Technologies
Fundamentals and Applications
Cosponsored by PMSE

R. B. Moore, T. E. Long, and R. Colby, *Organizers*

S. M. Ramirez, *Presiding*

8:30 1. Synthesis of ion-containing polymers: New strategies and structures. **A. Mueller**
9:10 2. Control of polymer properties via ionic interactions: An overview. **A. Eisenberg**
9:50 3. Unified morphological model for ionomers with ordered aggregate structures. **B. P. Grady**
10:15 4. Synthesis of functional ionenes for nonviral gene transfection. S. M. Ramirez, N. G. Moon, M. A. Lang, **T. E. Long**
10:40 5. Crystalline component in fuel cell membranes. J. K. Park, **R. B. Moore**
11:05 6. Efficient synthesis and properties of anion exchange membranes. **M. A. Hickner**, J. Yan

Section B

Sheraton
Seasons Ballroom South

Polymers and Carbon Nanotubes
Tutorial on Carbon Nanotubes
Cosponsored by COLL, I&EC, PHYS, PMSE, and NANO

B. P. Grady, P. M. Ajayan, and R. Krishnamoorti, *Organizers*

W. T. Ford, *Organizer, Presiding*

8:30 7. Tutorial on the purity of single-walled carbon nanotubes: Relationship to chemistry, properties and applications. **R. C. Haddon**
9:10 8. Organic functionalization of carbon nanoforms. **M. Prato**
9:50 9. Spectroscopic characterization of single-walled carbon nanotube samples. **R. B. Weisman**
10:30 Intermission.
10:45 10. Single walled carbon nanotube reference materials. **K. B. Migler**, J. A. Fagan
11:25 11. Commercial status of carbon nanotubes. **P. M. Ajayan**

Section C

Sheraton
Market Street Room

Undergraduate Research in Polymer Science

S. E. Morgan and S. Nazarenko, *Organizers*

8:30 12. Atomic force microscopy of high molecular weight thin film polymer blends compatibilized with triblock and graft copolymers. **E. M. Zimmerman**, D. A. Waldow
8:50 13. Hierarchical block copolymer microstructures as multiresponsive materials. **S. L. Young**, S. Chang, S. Singanameni, V. V. Tsukruk
9:10 14. Interactions between chitosan and selected anionic polymers for mucoadhesive drug delivery in the nasal cavity. **A. Cox**, R. Lochhead
9:30 15. Metal-organic biopolymers: Self-assembly and thermoplastic properties. **G. Escalera**, B. M. Porta, A. Metta, I. Rodriguez, D. Valles, J. C. Noveron
9:50 Intermission.
10:05 16. Polymer modified gold/gadolinium nanoparticles for targeted multimodal imaging and photothermal treatment. **C-C. G. Chang**, M. D. Rowe, S. G. Boyes
10:25 17. Proliferation of aortic adventitial fibroblasts on novel polyisobutylene-based thermoplastic elastomers. L. Munoz-Robledo, **S. Poroski**, M. Evancho-Chapman, S. Schmidt, J. E. Puskas
10:45 18. Protein resistant silicones prepared with branched PEO silanes. **B. M. Bailey**, R. Murthy, M. A. Grunlan
11:05 19. Nucleophilic aromatic substitution polymerization of 2,7-difluorothianthrene for the synthesis of novel poly(arylene sulfide)s. **M. J. Robb**, D. M. Knauss
11:25 20. The effects of pH on the polymerization of methylene green. **J. W. Breeden**, M. N. Germain, S. D. Minteer

‡ Cooperative Cosponsorship

Section D

Sheraton
Executive Room B

Off the Beaten Path: Alternative Career Options for a Degree in Polymer Science
Cosponsored by CEPA

E. H. Martin and K. O. Havelka, *Organizers*

8:30 21. Beating a path to patents: A practitioner's perspective. **J. K. Pike**
9:00 22. Career opportunities for chemists and chemical engineers in technical service and market development roles. **J. Gavenonis**
9:30 23. Catalyzing an alternative career path. **J. L. Petoff**
10:00 Intermission.
10:15 24. From polymer synthesis to open innovation transactions: A hybrid technical career. **C. Smith**
10:45 25. Publishing in polymer science. **S. Kalveram**
11:15 Panel Discussion: Career path experiences of polymer scientists.

Frontiers in Imaging Biological Nanostructures Sponsored by BIOL, Cosponsored by ANYL, COLL, PHYS, POLY, and NANO‡

Green Nanoscience Sponsored by INOR, Cosponsored by COLL, POLY, and NANO

SUNDAY AFTERNOON

Section A

Sheraton
Granary Room

Ion-Containing Polymers for New Technologies
Emerging Technologies Cosponsored by PMSE

R. B. Moore, T. E. Long, and R. Colby, *Organizers*

M. A. Hickner, *Presiding*

2:00 26. Tracking nucleic acid delivery with the help of lanthanide containing polymers. **J. M. Bryson**, K. M. Fichter, P. M. McLendon, T. M. Reineke
2:25 27. Ion-containing polyphosphazenes and their potential applications in life sciences. **A. K. Andrianov**
2:50 28. Synthesis of photocrosslinkable aliphatic based ammonium ionenes. **S. M. Ramirez**, M. A. Lang, S. R. Williams, T. E. Long
3:15 29. Ion-containing polymer-surfactant association for improved tissue compatibility. **R. M. Walters**, M. J. Fevola, H. Jerri, J. J. LiBrizzi, K. Martin
3:40 30. Control of morphology by counterion in fluorinated polymer/polyelectrolyte blends for fuel cell membranes. **S. Norvez**, C. M. Gibon, S. Tencé-Girault, J. T. Goldbach
4:05 31. Smooth high capacitance thin film dielectrics prepared from poly(styrene-b-ethylene oxide-b-styrene)/lithium perchlorate blends. **J. Chen**, C. D. Frisbie, F. S. Bates
4:30 32. Polyaniline nanofiber/silica aerogel composites with improved strength and sensor applications. **D. J. Boday**, D. A. Loy

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