Monday Afternoon

Section A
1:30
R. Kaiser, Y. Ba, and Nitrate on Molybdenum-modified Hematin Model System
2:05
A. Augspurger, J. Ha, Y. Gu, K. Marchuk, B. Kaehr, and Interference
2:30
M. A. Pasek, E. W. Castner Jr., and Interference
3:00
B. Kaehr, J. Ha, Y. Gu, K. Marchuk, B. Kaehr, and Interference
3:30
B. Kaehr, J. Ha, Y. Gu, K. Marchuk, B. Kaehr, and Interference
4:00
B. Kaehr, J. Ha, Y. Gu, K. Marchuk, B. Kaehr, and Interference
4:30
B. Kaehr, J. Ha, Y. Gu, K. Marchuk, B. Kaehr, and Interference

Section B
1:30
M. Johnston, B. Bzdek, J. DePalma, and Interference
2:00
R. Martinez, Y. Zhang, D. Hagan, I. Ulbrich, J. Jimenez, T. Hohaus, J. Jayne, D. Worsnop, and Interference
2:30
A. Holder, J. T. Hynes, X. Shan, and Interference
3:00
J. Jimenez, T. Hohaus, J. Jayne, D. Worsnop, and Interference
3:30
J. Jimenez, T. Hohaus, J. Jayne, D. Worsnop, and Interference

Section C
1:30
H. J. Kulik, D. I. Huppert, and Interference
2:00
D. I. Huppert, H. J. Kulik, and Interference
3:00
D. I. Huppert, H. J. Kulik, and Interference
4:00
D. I. Huppert, H. J. Kulik, and Interference

Section D
1:30
Photo-control of pH-driving Interference
2:00
Photo-control of pH-driving Interference
3:00
Photo-control of pH-driving Interference
4:00
Photo-control of pH-driving Interference

Section E
1:30
Between Theory and Experiment Interference
2:00
Between Theory and Experiment Interference
3:00
Between Theory and Experiment Interference
4:00
Between Theory and Experiment Interference

Section F
1:30
Exploring the interface of elec- Interference
2:00
Exploring the interface of elec- Interference
3:00
Exploring the interface of elec- Interference
4:00
Exploring the interface of elec- Interference

Section G
1:30
Small quantum dot probes for Interference
2:00
Small quantum dot probes for Interference
3:00
Small quantum dot probes for Interference
4:00
Small quantum dot probes for Interference

Technical program information known at press time.

The official technical program for the 248th ACS National Meeting is available at:
www.acs.org/sanfran/2014
Liquid State Theory: Symposium in Honor of Jay Rasek
Aqueous Solutions, Ions, Electrolytes
Sponsored by COLL, Co-sponsored by PHYS
 Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage
Battery Materials and Interfaces (Mostly Electrodes)
Sponsored by COMP, Co-sponsored by PHYS
 Molecular Mechanics: We improve the MoroFields, You asHannahah
About the Achievements. #WeAreModest
Sponsored by COMP, Co-sponsored by PHYS
 Quantum Chemical Calculation of Molecular Properties: Symposium in Honor of Professor Nicholas C. Handy
Sponsored by COMP, Co-sponsored by PHYS

TUESDAY AFTERNOON
Section A
Moscone Center, West Bldg. 2002
Physical Chemistry Awards Symposium
N. Levinger, Organizer, Presiding
1:30 Introductory Remarks.
J. F. Lieb
1:45 Poster Session I: Condensed Phase Spectroscopy
1:45 Poster Session II: Ab Initio Molecular Dynamics and Applications
2:00 Poster Session III: Nonlinear Spectroscopy
2:05 Poster Session IV: Computational Chemistry Applications
2:20 Poster Session V: Thermodynamics

Section B
Moscone Center, West Bldg. 2003
Physical Chemistry of Ionic Liquids
Ionic Liquids at Interfaces
Co-sponsored by ENFL and INOR
J. D. C. Jones, M. Cardona, T. H. Geballe, Organizers

Section C
Moscone Center, West Bldg. 2004
Photoinduced Proton Transfer in Chemistry and Biology
Co-sponsored by COMP
Financial support received by Excelent Material Tech Corporation, Ltd.
P. Chou, K. Solslev, Organizers

Section D
Moscone Center, West Bldg. 2005
Fundamental Processes of Atmospheric Chemistry
Aerosols: Climate Implications
D. Farmer, F. Keutsch, Organizers
C. Cappa, K. Barsanti, Presiding
8:00 Chapter 31. Combining field and laboratory studies of aerosol chemical composition to understand ice cloud formation.
D. G. J. Cziczo, D. Murphy, K. Froyd, S. Garmella, K. Arden-Otto
3:30 Toward a better understanding of the physical chemistry of surfactants in cloud activation: Laboratory results and field observations at the Pallas GAW station, Finland.
B. Nurmela, B. Edstrom, H. Hyvarinen, L. Lihavainen, V. Anttila, T. Raatkainen
2:30 Impact of aerosols on clouds and regional climate.
K. A. Prather
9:30 Intermission.

Wednesday Morning
Section A
Moscone Center, West Bldg. 2006
The Future of Computational Chemistry
Co-sponsored by COMP

Technical program information known at press time.

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3 Cooperative Co-sponsored

PHYS

TECHNICAL PROGRAM

T. Crawford, T. Winds, Organizers
K. Bravaya, Presiding
8:30 Poster 285. Methods and models for software and hardware simulation.
9:00 Poster 286. Scalable strategies for polarizable molecular dynamics simulations.
9:30 Poster 287. Present and future of QM/classical approaches to simulate the effect of the environment on molecular processes.
B. Mennucci
10:00 Poster 288. Evaluating force field accuracy of DNA dynamics using enhanced sampling methods.
C. Berrogeot, N. M. Henderson.
D. R. Roe, T. E. Chahattham III
10:30 Intermission.
10:40 Poster 289. Software for computational chemistry and materials modeling.
E. Deuens
11:10 Poster 290. Exploring computational frameworks for future computational chemistry.
M. Parashar
11:40 Poster 291. Barrier height problem needs a solution solution.
D. Tomlinson, M. S. Gordon

Catalytic growth of nanomaterials: A new look at an old concept.
to probe norharmane. S. Ghosh, S. Chakrabarty,
D. J. Tobias
281.

Dipole moment of the HOOO
1:35 Section A
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2002
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Catalytic growth of nanomaterials: A new look at an old concept.
to probe norharmane. S. Ghosh, S. Chakrabarty,
D. J. Tobias
281.
**Liquid State Theory: Symposium in Honor of Jay Rasaiha**

**Hydrophilicity and Water in Biology**
By T. Greaves, J. Wishart, E. Maginn, E. Castner, C. Margulis

**Physical Chemistry of Ionic Liquids**

- **Section C**
  - **Moscow Center, West Bldg.**
  - **2004**
  - **Photoinduced Proton Transfer in Chemistry and Biology**
    - Organized by COMP
    - Financially supported by Excess Material-Tech Corporation, Ltd
    - P. Chou, K. Shobart, Organizers
    - J. Walick, Presiding
    - **1:30 pm** [**352**] Intramolecular excited state proton transfer. The key to photon induced dynamics in protonated aminoacids. C. Josset, C. Dedonder, F. Geraud, G. Gregoire, M. Broquier, S. Soorkia
    - **2:05 pm** [**353**] Hydrogen-bond assisted non-adiabatic decay in solutions and liquid/liquid interfaces. B. Derrick, S. Richert, S. Mosquera-Vasquez
    - **3:30 pm** [**355**] Investigating ultrafast radiolysis decent of a photocatalyst: Simulating 3-cyan-6-hydroxycoumarin with implicit and explicit ab initio solvent models. S. Hong, B. Nielsen, L. V. Slipchenko
    - **3:30 pm** [**356**] Photoinert kinetics in a GFP variant switched by ps changes in a low-barrier hydrocarbon bond. J. Pan, M. Vergna, D. Stoner-Ma, D. Madson, P. J. Tom, D. Larsen
    - **4:00 pm** [**357**] Designing ESPT molecules for full-color-molecular pixel system. S. Park, V. Khon
    - **4:30 pm** [**358**] Time-resolved fluorescence study of excited-state proton transfer. T. Huan
    - **5:20 pm** [**359**] Atypical modulations in the excited state intramolecular proton transfer by diffusive solvent relaxation in room temperature protic ionic liquids. N. Pal

**Section D**

- **Moscow Center, West Bldg.**
- **2006**
- **Renewable Energy Generation at the Interface Between Theory and Experiment**
- **Dye Sensitized Solar Cells**

**Chemists? What Have To Say To 21st Century Physical Chemists?**

- **Section F**

**Moscow Center, West Bldg.**
- **2010**

**Nano-Probes for Biological Systems**

**Chemical Bonds**

- **Section G**

**Moscow Center, West Bldg.**
- **2007**

**Control, Characterization, and Impact of Nanocrystal Surface Chemistry**

**Engineered Nanomaterials Interacting with Natural and Engineered Interfaces**

**Liquid State Theory: Symposium in Honor of Jay Rasaiha**

**Confining Gas, Proton Hydration and Complex Systems**

**Section A**
- **Moscow Center, West North Bldg.**
- **2006**
- **Photoinduced Proton Transfer in Chemistry and Biology**
  - Organized by COMP
  - Financially supported by Excess Material-Tech Corporation, Ltd
  - N. Levinger, P. Chou, K. Shobart, Organizers
  - **6:00 pm** [**380**] Interval of hydropilic and electrostatic interactions in the modulation of ground and excited state proton-depocronation equilibria of two positional isomers in their complexes with cucurbitas. V. Kart
  - **6:10 pm** [**381**] Novel state electron transfer in the isolated 7-azaindole-phenol Ni-bonded complex. C. Dedonder, M. Broquier, C. Jouvet, G. A. Pino
  - **6:20 pm** [**382**] Exploring water micro-solvation dynamics for imaging lipid domains in membranes. Y. Mity, V. Khon, G. Glushonkov, L. Richert, A. N. Klyosov
  - **6:30 pm** [**383**] Ultrafast dynamics of a bistable excited state intramolecular proton transfer involving quinolinium cations. C. Costa Corbelle, M. Mosquera, B. Fernandez, J. Perez Lustres, M. Rios Rodriguez, F. Rodriguez Prieto
  - **6:40 pm** [**384**] Photoinert control of conductivity in a hydrogen-bonded polycation gel. Effect of polyanions. E. Vagana, W. Wachtel, F. Dabkiew, A. Garkin, S. Ytzhak

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non-mass-dependent oxygen isotope effects in lar organisms: Spectroscopic and computational (P-glycoprotein).

Fer resonance energy transfer of liquid water and dissociations of pyrimidine and purine.

Theoretical prediction of polarizationizabilities of charge-transfer chromophores.

Studies of the spliceosomal U1A-SL2 interaction: An all-atomistic on-the-fly simulation of the complex and structural implications for the recognition of the splice site.

Superparamagnetic iron oxide nanoparticles for targeted drug delivery.

Low temperature dynamics and kinetics of short oligothiophenes: A combined physical approach: An all-atomistic on-the-fly simulation of the complex and structural implications for the recognition of the splice site.

On the water exchange rates in ion dissociations of pyrimidine and purine.

Determination of the conformation of the challenging case of the Cr dimer.

Quantum Monte Carlo calculations of the primary solvation shell of microhydrated iodide species.

Quantum studies on the metal oxide clusters.

Detailed quantum studies on the opening mechanism of the photodissociation of C=O bonds in highly activated 2,3-butanediol.

Investigation into the opening mechanism for the photoinduced charge transfer of the Cr dimer.

Electron stimulated desorption study of the relative energy of C=O bonds in highly activated 2,3-butanediol.
Section A
Moscone Center, West Bldg.
2000
The Future of Computational Chemistry
Cosponsored by COMP
T. Crawford, W. Frank, Organizers
E. Valeur, Presiding
8:30 PHYS 615. First principles simulation of mineral/fluid interactions: Methods development, application to metal oxide surfaces, and analysis of observations. J. Waare, Y. Chen, E. Bylaska, J. Waare, J. Fulton
8:50 PHYS 616. Evolution and revolution in massively parallel coupled cluster codes. J. Hammond
9:30 PHYS 617. Ab initio excited state green's function methods and their scaling on massively parallel architectures. S. Ismail-Beigi
10:00 PHYS 618. Coarse-grained electron simulations: Many-body potentials with chemical accuracy for condensed phase processes. E. Pantazis
10:20 Intermission.
11:10 PHYS 620. Improving the time scales of ab initio molecular dynamics simulations for actinide and geochemical systems: Free energy, and parallel in time algorithms. E. J. Bylaska, J. Chen, H. Weiss, J. Gordon
11:40 PHYS 621. Quantum reaction dynamics of nanoscale materials. J. Jakowski, S. Garachuk, W. Bang, B. G. Sumpter
Section B
Moscone Center, West Bldg.
2002
Physical Chemistry of Ionic Liquids
Transport Phenomena and Dielectric Behavior
Cosponsored by ENVR and PHYS
J. Wishart, E. Castron, E. Maginn, C. Margulis, Organizers
R. Batts, Presiding
8:00 PHYS 622. Computational study of diffusive behavior of choline-based ILs. F. Yan
8:20 PHYS 623. Ion pairing in protic ionic liquids: The effects of solvent polarity, solvent concentration, and temperature. R. Ludwig, P. Stange, K. Furnino, K. Wittke, W. Point, V. Fossog, R. Hampfmann
8:55 PHYS 624. Charge transport in ionic liquids. M. Watanabe
9:30 PHYS 625. Dielectric loss and IR spectroscopy of ionic liquids: A computational study. H. Kim, Y. Shim, H. Kim, N. Dhumal
10:05 Intermission.
10:25 PHYS 626. Developing low viscous ionic liquids: Viscosity dependence upon the mass of the ions. N. Ignatiev, M. Schultz, P. Barthen, W. Frank, E. Barnhardt, H. Wittler
10:45 PHYS 627. Insights into the electrochemical stability of ionic liquids from first principles calculations and molecular dynamics simulations. S. Ong, Y. Wu, O. Andreussi, N. Marzari, G. Ceder
11:20 PHYS 628. Molecular dynamics studies of dynamic properties in ionic liquids. Y. Zhang, E. Maginn
Section C
Moscone Center, West Bldg.
2004
Renevalable Energy Generation at the Interface Between Theory and Experiment
Bulk Heterojunction Solar Cells and New Discoveries in Solar Energy
Cosponsored by ENVR and WWI
A. Morris, Organizer
J. Muennick, Organizer, Presiding
8:45 Introductory Remarks.
9:00 PHYS 630. General strategy for self-assembled highly oriented nanocrystalline semiconductor polymers with high mobility. A. Heeger
9:30 PHYS 631. Charge transport in Ti-conjugated materials: A theoretical model. J. Breda
10:40 Intermission.
11:00 PHYS 634. Electron and hole mobilities at a semiconductor surface with adsorbed metal clusters. Adapting methods relevant to experimental measurements. D. A. Micha, R. H. Holmes, T. Vatcheva
11:20 PHYS 635. Hole transfer limitations in thin film solid state solar cells. P. V. Kamar, J. Christians, J. Manser
Section D
Moscone Center, West Bldg.
2006
Computational Spectroscopy
Condensed Phase
Cosponsored by COMP
C. Jarrod, J. Stanton, Organizers
S. S. Xantheas, Presiding
8:00 PHYS 637. Surface-enhanced Raman scattering: The importance of the molecule. K. Willett
8:40 PHYS 638. Using electronic structure, quantum mechanics, classical mechanics, and statistical mechanics to calculate vibrational spectroscopy of water. J. L. Skinner
9:00 PHYS 639. Computing electronic excitations in the condensed phase. C. Iabon
9:30 Intermission.
10:00 PHYS 640. Spectroscopy of adsorbates on semiconductor surfaces: From small clusters to electronic spread-over. K. Rauthschmitt
10:40 PHYS 641. Photoexcitations in semicon- ductors and insulators from first principles. M. Govoni, G. Galli
11:20 PHYS 642. Understanding the struc- tural-activity relationships of silica supported metal catalysts from theory and spectroscopy. U. Das
Section E
Moscone Center, West Bldg.
2004
Photoinduced Proton Transfer in Chemistry and Biology
Cosponsored by COMP Financially supported by Exceed Material-Tech Corporation, Ltd
J. Wishart, E. Castron, E. Maginn, C. Margulis, Organizers
8:00 PHYS 643. Tautomerism in porphycenes. J. Walk
10:55 PHYS 648. Photo-induced redox pro- cess from fluorescent proteins from the GFP family. A. Krylov
Chemistry of Atmospheric Nitrogen-Containing Compounds
Cosponsored by ENVR, Cosponsored by PHYS
11:40 PHYS 650. Insights into the exciting with Natural and Engineered Interfaces
Cosponsored by COMP and PhysChem
Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage: Interfacial Transport Dynamics
Section F
Moscone Center, West Bldg.
2004
Photoinduced Proton Transfer in Chemistry and Biology
Cosponsored by COMP Financially supported by Exceed Material-Tech Corporation, Ltd
J. Wishart, E. Castron, E. Maginn, C. Margulis, Organizers
K. Glusac, Presiding
1:30 PHYS 666. Photoinduced fragmentation of protonated peptides: The bouncing ball. N. L. Burke, J. C. Dean, S. A. McClellan, T. Zwer
2:05 PHYS 667. Interfacial charge transfer: A molecular view of state proton transfer (ESPT). L. M. Tolbert
2:30 PHYS 668. Excited state proton transfer and two color fluorescence of therapeutically potent plant flavonoids: Applications toward understanding their interactions with representative bio-relevant targets and nano-vehicles for drug delivery. P. K. Sengupta
4:00 PHYS 670. Mid-IR absorption spectroscopy of hydrocarbon bounded in complex and excited states of hydrocarbons. D. Pintet, F. M. Kiefer, J. T. Hynes, E. Pire
4:35 PHYS 671. Proton transfer studies of cyano-substituted hydrides. M. Zahid, S. Asima, A. Mandha, G. Gramp
5:20 PHYS 672. Elucidation of the dynamic role of alcohol molecular clusters in non-aqueous acid-base reactions. D. Ok
9:00 PHYS 673. Control, Characterization, and Impact of Nanocrystal Surface Chemistry
Cosponsored by COLI, Cosponsored by PHYS
Engineered Nanomaterials Interacting with Natural and Engineered Interfaces
Cosponsored by COMP and PHYS
edQuantum Program
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