1:20 ORGN **928.** How cinchona alkaloids steer the product distribution in the reactions of oxindoles with nitrosobenzene. **N. Celebi-Olcum**

1:40 ORGN **929.** N-heterocyclic carbene catalyzed ring opening polymerization of glycolide and lactide: A theoretical study. **X. Dong**, Y. Li, J.M. Grandner, K.N. Houk

2:00 ORGN **930.** Alkyne metathesis to delineate the effect of building block size on organic cage synthesis. **A. Yang**, J.S. Moore

2:20 ORGN **931.** Conjugated trimeric scaffolds accessible using indolyne cyclotrimerizations. **J. Lin**, T. Shah, A. Goetz, K.N. Houk, N.K. Garg

2:40 ORGN **932.** Non-bonding S–O interactions: A new element of stereocontrol and catalysis? **D. Walden**, E. Robinson, T. West, C. Fallan, J. Taylor, M. Greenhalgh, A.D. Smith, P. Ha-Yeon Cheong

3:00 ORGN **933.** Withdrawn.

3:20 ORGN **934.** Computational exploration of copper catalyzed azide-alkyne coupling reactions. **S. Bidwell**, H.P. Hratchian

3:40 ORGN **935.** Computational comparisons of Diels-Alder transition states for endiandric tetracycles using density functional theory. K.J. Kron, R.J. Cave, **D.A. Vosburg**

PHYS

Division of Physical Chemistry

J. Shea, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Elucidation of Mechanisms & Kinetics on Surfaces (see *CATL*, Sun, Mon, Tue, Wed, Thu)

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis (see *CATL*, Mon, Tue, Wed)

Nanoscience & Nanotechnology for Advanced Materials & Technologies (see *MPPG*, Mon)

Nanoscale Spectroscopic Characterization of Catalysts & Polymers (see *PMSE*, Sun, Mon)

SUNDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Cosponsored by INOR

S. Corcelli, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 PHYS **1.** Scanning tunneling microscopy of alkyl-substituted oligothiophenes on Au(111): Real-space visualization of molecular electronic structure. **B. Taber**, G. Nazin

8:50 PHYS **2.** Mixed-valence molecules: Direct imaging of intramolecular charge distribution by STM. **S. Kandel**

9:30 Intermission.

9:50 PHYS **3.** Spin effects on photo-induced electron and energy transfer processes in polynuclear donor-acceptor assemblies. **J.K. McCusker**

10:30 PHYS **4.** Energy transfer in quantum dot-molecule assemblies. **E.A. Weiss**, C. Wang, K. Lee, M. Kodaimati, S. Homan, G.C. Schatz

11:10 PHYS **5.** Nanocrystal taxonomy and ligand alphabet soup: Covalent bond classification system applied to surface chemistry. **N.C. Anderson**, N.R. Neale, J.S. Owen

Section B

Parc 55 San Francisco

Mason

Long Range Correlated Motions in Proteins

Protein Dynamics & Allostery

A. Markelz, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 PHYS **6.** Mind the gap: Building a bridge between physical and statistical models of allostery. M.A. Cuendet, G. Khelashvili, H. Weinstein, **M.V. LeVine**

9:35 PHYS **7.** Entropy in protein function. **A.J. Wand**

10:05 PHYS **8.** Predicting optimal allosteric stabilization sites with contact stabilization analysis. **A. Dickson**, C. Bailey, J. Karanicolas

10:25 Intermission.

10:40 PHYS **9.** Allosteric dynamics of AMPA receptors and coupling to membrane fluctuations. J. Lee, J. Krieger, I. Greger, **I. Bahar**

11:10 PHYS **10.** Understanding allosteric regulation of G protein-coupled receptors using molecular simulation. **A. Grossfield**

11:40 PHYS **11.** Opening of the intracellular gate affects the structure and ion occupancy of the selectivity filter of a potassium ion channel. **H.T. Kratochvil**, M.T. Zanni

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photosynthesis

K. Glusac, M. Olivucci, *Organizers*

D. S. Larsen, *Organizer, Presiding*

8:00 PHYS **12.** Probing ultrafast dynamics of photosynthetic reaction centers using two-dimensional electronic spectroscopy. **J.P. Ogilvie**, V. Policht, A. Niedringhaus, A. Loukianov

8:30 PHYS **13.** Structural and functional modularity of the orange carotenoid protein in governing cyanobacterial photoprotection. **C. Kerfeld**

9:00 PHYS **14.** Biomimetic designs and *In-Situ* x-ray structural characterization of catalysts for the artificial leaf. **D.M. Tiede**, G. Kwon, I. Kim, J. Emery, A.B. Martinson

9:30 PHYS **15.** Photophysics of coupled carotenoids. **M.J. Tauber**

10:00 Intermission.

10:20 PHYS **16.** Photochemical water oxidation by photosystem II. **G.W. Brudvig**

10:50 PHYS **17.** Pyridine Co-catalysis impacting CO_2 reduction over semiconductor photoelectrodes. **T. Senftle**, E.A. Carter

11:20 PHYS **18.** Energy transfer mechanisms in green sulphur bacteria. **D. Zigmantas**, J. Dostal, K. Zidek, K. Kim, M. Alcocer, D. Bina, H. Lokstein, J. Psencik

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulating Electrons on Large Scale

Cosponsored by COMP

O. V. Prezhdo, *Organizer*

A. V. Akimov, *Organizer, Presiding*

8:00 PHYS **19.** Spectroscopy of molecules at metal surfaces: Markovian and non-Markovian electron dynamics. **M. Pavanello**

8:40 PHYS **20.** Patches for realtime TDDFT: Correlation and a time-dependent Tamm-Dancoff approximation. **J. Parkhill**

9:20 Intermission.

9:35 PHYS **21.** Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states. M.G. Bayne, **A. Chakraborty**

10:15 PHYS **22.** Spectra from stochastic many-body methods. **V. Vlcek**, R. Baer, E. Rabani, D. Neuhauser

10:35 PHYS **23.** Description of quasiparticles in stochastic many-body methods. V. Vlcek, R. Baer, E. Rabani, **D. Neuhauser**

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Ahmed Zewail Award in Ultrafast Science & Technology: Symposium in honor of Stephen R. Leone

Cosponsored by PRES

J. E. Shea, *Organizer*

D. Zhong, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **24.** From ultrafast spectroscopy to structural dynamics. **M. Chergui**

8:45 PHYS **25.** In search of transition states of chemical reactions. A tribute to Ahmed Zewail. **L. Banares**

9:25 Intermission.

9:40 PHYS **26. Award Address** (Ahmed Zewail Award in Ultrafast Science & Technology sponsored by the Ahmed Zewail Endowment Fund by the Newport Corporation (Newport)). Ultrafast x-ray dynamics. **S.R. Leone**

10:40 PHYS **27.** Probed quantum systems from the inside: On the attosecond time scale. **P. Corkum**

11:20 PHYS **28.** Anion photoelectron/photodissociation spectroscopies: Ozonide solvation dynamics. **W.C. Lineberger**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Interfaces

A. T. Krummel, N. E. Levinger, *Organizers*

K. Gaffney, *Presiding*

8:00 Introductory Remarks.

8:20 PHYS **29.** Is the surface of clathrate hydrates hydrophilic or oleophilic? **V. Molinero**

9:00 PHYS **30.** Solvation and confinement effects on the thermodynamics of helix coil transitions of polyalanine in open nanotubes. D. Suvlu, S. Samaratunga, D. Thirumalai, **J.C. Rasaiah**

9:20 PHYS **31.** Ion-induced stabilization of palmitic acid monolayers. **H.C. Allen**, E. Adams, B. Wellen, A. Vidalis, T. Zhang

10:00 Intermission.

10:20 PHYS **32.** Quantitative prediction of position and orientation for a polyhedral nanoparticle at liquid/liquid interfaces. **S. Li**

11:00 PHYS **33.** Asymmetric electrowetting at the nanoscale: Molecular dynamics simulations of molecular fluids on graphene. **N. van der Vegt**

11:20 PHYS **34.** Rate theory on ion pairings at the liquid/vapor interface of water. **L.X. Dang**

Advanced X-Ray Techniques for Catalyst Characterization

Catalysts in Action

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Allosteric Regulation & Mechanisms

Sponsored by COMP, Cosponsored by PHYS

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Cosponsored by INOR

S. Corcelli, *Organizer*

S. Kandel, *Presiding*

1:30 PHYS **35.** Charge motion in disordered molecular solids. **M.A. Ratner**

2:10 PHYS **36.** Electronically excited states of organic molecules and transition-metal containing systems are a challenge for quantum chemistry. **L. Gagliardi**

2:50 Intermission.

3:10 PHYS **37.** Theoretical studies of homogeneous and heterogeneous multicenter electrocatalysts. **S. Hammes-Schiffer**

3:50 PHYS **38.** Spectroscopy and electron transfer processes in molecular systems of multi metal centers: Insight by *ab-initio* modeling. **B.D. Dunietz**

4:30 PHYS **39.** Efficient implementation and assessment of open-shell symmetry-adapted perturbation theory. **J.F. Gonthier**, L. Dos Anjos Cunha, C.D. Sherrill

Section B

Parc 55 San Francisco

Mason

Long Range Correlated Motions in Proteins

Protein-Solvent Modeling: Refinement through Comparison with Measurements

A. Markelz, *Organizer*

A. J. Wand, *Presiding*

1:30 PHYS **40.** Spectral analysis of correlated protein and protein-water vibrations in molecular dynamic simulations. **M. Heyden**

2:00 PHYS **41.** 2D-Raman-THz spectroscopy of water and aqueous salt solutions. A. Shalit, D. Sidler, **P. Hamm**

2:30 PHYS **42.** Correlated vibrational motion in the Fenna-Matthews-Olson complex. **B.S. Rolczynski**, H. Zheng, V.P. Singh, P. Navotnaya, J.R. Caram, K. Ashraf, A.T. Gardiner, R.J. Cogdell, G.S. Engel

2:50 PHYS **43.** Protein intramolecular vibrations couple to the dynamical transition. **M. Xu**, K. Niessen, Y. Deng, N. Michki, A. Markelz

3:10 PHYS **44.** Towards development of the *ab-initio*-based force field for biological systems. **P. Gurunathan**, L.V. Slipchenko

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photochemistry & Emerging Techniques

K. Glusac, M. Olivucci, *Organizers*

D. S. Larsen, *Organizer, Presiding*

1:30 PHYS **45.** Controlling the photostability of uracil with shaped light fields. D. Keefer, S. Thallmair, S. Matsika, **R. de Vivie-Riedle**

2:00 PHYS **46.** Using fundamental photochemistry to drive drug development and structural-biology applications. **C.E. Crespo-Hernandez**

2:30 PHYS **47.** Direct evidence of molecular charge accumulation during solar excitation of molecular dyes, and guidelines for obtaining large quantum yields. H. Chen, J.M. Cardon, **S. Ardo**

2:50 PHYS **48.** Operating photoswitches with sunlight. **S. Hecht PhD**

3:20 PHYS **49.** Fuel from water: The reductive side of water splitting and the light-driven generation of hydrogen. **R. Eisenberg**, H. Lv

3:50 Intermission.

4:10 PHYS **50.** Photochemical pathways for motion in E/Z photoswitchable thienyl-ethenes. **A.E. Bragg**

4:40 PHYS **51.** Combined experimental and theoretical study of the transient IR spectroscopy of 7-hydroxyquinoline in the first electronically excited singlet state. F. Hoffmann, M. Ekimova, G. Bekçioğlu-Neff, **E. Nibbering**, D. Sebastiani

5:00 PHYS **52.** Subensemble-Selective photochemistry by mixed IR/VIS two-dimensional spectroscopy. **J. Bredenbeck**

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulating Quantum Nuclei on Large Scale

Cosponsored by COMP

O. V. Prezhdo, *Organizer*

A. V. Akimov, *Organizer, Presiding*

1:30 PHYS **53.** Linearized path integral methods for capturing quantum effects in molecular dynamics simulations of condensed phase systems. **E. Geva**

2:10 PHYS **54.** Phase space vs. coordinate space approaches for overcoming exponential scaling in large quantum calculations. H. Larsson, B. Hartke, **D. Tannor**

2:50 PHYS **55.** Path integral methods for nonadiabatic dynamics: Quantum transitions from classical trajectories. **N. Ananth**

3:30 Intermission.

3:45 PHYS **56.** Molecular dynamics of large systems with quantum corrections for selected nuclei. **S. Garashchuk**

4:25 PHYS **57.** Nonadiabatic molecular dynamics with time-domain density functional theory. **O.V. Prezhdo**

5:05 PHYS **58.** Condensed phase non-adiabatic dynamics from temporally-interpolated memory kernels. **D. Hait**, M. Mavros, T.A. Van Voorhis

5:25 PHYS **59.** Preparation of a single highly vibrationally excited quantum state using Stark induced adiabatic Raman passage. **W. Perreault**, N. Mukherjee, R.N. Zare

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Ahmed Zewail Award in Ultrafast Science & Technology: Symposium in Honor of Stephen R. Leone

Cosponsored by PRES

J. E. Shea, *Organizer*

S. R. Leone, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS **60.** Ultrafast protein folding. **M. Gruebele**

2:10 PHYS **61.** How to turn a right hand into left: Chiral plasmons and more. **V.A. Apkarian**

2:45 PHYS **62.** Probing and controlling molecular electronic and vibrational states with shaped laser pulses. **M. Dantus**

3:20 Intermission.

3:35 PHYS **63.** Probing ultrafast photochemical processes in solution with femtosecond spectroscopies. **M.H. Khalil**

4:10 PHYS **64.** Better chemical filters for better life. **V. Stavros**, N.C. Cole-Filipiak, M. Staniforth, M. Horbury, N.D. Rodrigues, L.A. Baker, J. Woolley

4:45 PHYS **65.** Dynamics and mechanism of ultrafast water-protein interactions. **D. Zhong**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Liquids

A. T. Krummel, N. E. Levinger, *Organizers*

W. H. Thompson, *Presiding*

1:30 PHYS **66.** Measuring liquid density using optical Kerr effect spectroscopy. J.S. Bender, S. Cohen, X. He, B. Coasne, **J.T. Fourkas**

2:10 PHYS **67.** Combined FT-IR and soft-x-ray spectroscopic approach on aqueous ammonium and ammonia. M. Ekimova, W. Quevedo, L. Szyc, P. Wernet, M. Odelius, **E. Nibbering**

2:30 PHYS **68.** Structure and dynamics of glyme based electrolytes for sodium based rechargeable batteries. **R. Kumar**, R. Jorn, D.G. Kuroda

3:10 Intermission.

3:30 PHYS **69.** Ultrafast x-ray scattering studies of solvent and solvation dynamics. **K. Gaffney**, T.B. van Driel, K. Kjaer, R. Hartsock, A. Dohn, K. Moller, M. Nielsen, T. Harlang

4:10 PHYS **70.** Dramatic impact of confinement on sugars and carbohydrates in confined environments. **N.E. Levinger**, B.P. Wiebenga-Sanford

4:30 PHYS **71.** Solvation dynamics of hydrated electrons: Connecting hydrated electron structure to time-resolved photoelectron spectroscopy and temperature-dependent transient absorption experiments. **B.J. Schwartz**, C. Zho, E. Farr, W.J. Glover

Advanced X-Ray Techniques for Catalyst Characterization

Theory & Beyond

Sponsored by CATL, Cosponsored by PHYS

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Synthesis & Characterization of Materials for Energy Applications

In Operando & Surface Sensitive Analysis

Sponsored by ANYL, Cosponsored by PHYS

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

MONDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Cosponsored by INOR

S. Corcelli, *Organizer*

L. J. Webb, *Presiding*

8:00 PHYS **72.** Electrical transport in MOFs. **M. Dinca**, L. Sun, S. Park, G. Skorupskii, L. Xie, C. Hendon

8:40 PHYS **73.** Solar photochemistry of semiconductor nanocrystals coupled with redox catalysts. **G. Dukovic**

9:20 PHYS **74.** Charge transfer between hydrogen-bonded metal-metal quadruple bonds. L. Brown, A.J. Meijer, **N. Patmore**, K.B. Vincent, L. Wilkinson

10:00 Intermission.

10:20 PHYS **75.** Mixed-valency across hydrogen bonds: The effects of electron delocalization. **C.P. Kubiak**, T.M. Porter

‡ *Cooperative Cosponsorship*

11:00 PHYS **76.** Role of molecular assemblies in dye sensitized photoelectrosynthesis cells. **T.J. Meyer**, L. Alibabaei, M.K. Brennaman, B. Sherman, D. Wang, M. Eberhart, M. Sheridan, A. Nayak, Y. Wang

11:40 PHYS **77.** Synthesis and characterization of exactly doped semiconductor quantum dots. **A. Hassan**

Section B

Parc 55 San Francisco

Powell

Long Range Correlated Motions in Proteins

Measurement Techniques

A. Markelz, *Organizer*

M. Heyden, *Presiding*

9:00 PHYS **78. Award Address** (Nakanishi Prize sponsored by the Nakanishi Prize Endowment). Long range effects from *in vitro* to *in vivo*. **M. Gruebele**

9:40 PHYS **79.** Revealing large-amplitude motions using local probes. **C.H. Londergan**

10:00 Intermission.

10:15 PHYS **80.** Protein dynamics by femtosecond x-ray solution scattering and absorption. **M. Cammarata**, L. Balducci, M. Levantino

10:45 PHYS **81.** Biopolymer elasticities via terahertz spectroscopy. **T.M. Korter**

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photoreceptor Activity: Non-Rhodopsin Photosensors

K. Glusac, D. S. Larsen, *Organizers*

M. Olivucci, *Organizer, Presiding*

8:00 PHYS **82.** Ultrafast biological photomachine: Watching DNA repair in real time. **D. Zhong**

8:30 PHYS **83.** Using light as a trigger to understand biological mechanisms. **M. Sans**, D.C. Monteiro, J.J. Doyle, B.A. Yorke, A.R. Pearson

9:00 PHYS **84.** Unfolding of the C-terminal Ja helix in the LOV2 photoreceptor domain observed by time-resolved vibrational spectroscopy. P. Konold, T. Mathes, J. Weissenborn, M. Groot, P. Hegemann, **J. Kennis**

9:30 Intermission.

9:50 PHYS **85.** Ground state and photo-induced electron transfer in cryptochromes. R. Tazhigulov, **K.B. Bravaya**

10:20 PHYS **86.** Structure-guided design of infrared fluorophores based on the sunlight-driven photoreceptor phytochrome. **K.T. Forest**

10:50 PHYS **87.** Correlating secondary protein dynamics with cryokinetics measurements in cyanobacteriochromes. **D.S. Larsen**, N. Rockwell, J. Lagarias, P. Kim

11:10 PHYS **88.** Revealing the molecular identity of cryptochrome photoactivation reaction. **I. Solov'yov**

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Ab Initio & DFT

Cosponsored by COMP

O. V. Prezhdo, *Organizer*

A. V. Akimov, *Organizer, Presiding*

8:00 PHYS **89.** Highly accurate and efficient quantum chemical method based on non-orthogonal localized molecular orbitals. W. Yang, **F. Gu**

8:40 PHYS **90.** Ab Initio multiple spawning molecular dynamics with DFT for intersystem crossings. **D. Fedorov**, S.A. Varganov

9:00 PHYS **91.** Linear scaling calculations with the divide-and-conquer method and with non-orthogonal localized molecular orbitals. **W. Yang**

9:40 Intermission.

9:55 PHYS **92.** Parallel electron dynamics calculations with linear system-size scaling using the time-dependent Hartree-Fock method. **E. Rudberg**

10:35 PHYS **93.** Large-scale real-time TDDFT for studying non-equilibrium electron dynamics in condensed matters: Prospects and challenges in simulating extended systems. **Y. Kanai**, D. Yost, Y. Yao

11:15 PHYS **94.** Multi-petaflop/s quantum molecular dynamics simulations. **A. Nakano**

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Peter Debye Award in Physical Chemistry: Symposium in honor of Bruce J. Berne

Cosponsored by PRES

J. E. Shea, *Organizer*

G. Hummer, *Presiding*

8:00 PHYS **95. Award Address** (Peter Debye Award in Physical Chemistry sponsored by DuPont). Enhanced sampling for thermodynamics and kinetics of ligand-protein binding and unbinding. **B.J. Berne**

8:35 PHYS **96.** Use of molecular dynamics simulations in structure based drug discovery. **R. Friesner**

9:10 PHYS **97.** Free energy simulations of protein-ligand binding and solvation at the interface. **R.M. Levy**

9:45 PHYS **98.** How and when does a drug leave the binding pocket of a host protein. **P. Tiwary**

10:20 Intermission.

10:30 PHYS **99.** Molecular dynamics simulations of protein dynamics from femtoseconds to milliseconds. **G. Hummer**

11:05 PHYS **100.** Ultra-Coarse-Graining and its applications. **G.A. Voth**

11:40 PHYS **101.** Orderphobic effect: A general mechanism for membrane mediated forces between proteins. **D. Chandler**, K. Mandadapu

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Methods

A. T. Krummel, N. E. Levinger, *Organizers*

R. Kumar, *Presiding*

8:20 PHYS **102.** Chemical dynamics in Stochastic Hard Collision (SHC) solvents. **R. Hernandez**

9:00 PHYS **103.** Computing multi-dimensional optical spectra from classical trajectories. **R.F. Loring**

9:20 PHYS **104.** Collective behavior of nonequilibrium, nano-confined fluids. **D. Limmer**

10:00 Intermission.

10:20 PHYS **105.** Tests for, origins of, and corrections to non-Gaussian statistics. A.J. Schile, **W.H. Thompson**

11:00 PHYS **106.** Local structural dynamics revealed by solute-pump/solvent-probe spectroscopy. **X. Sun**, B.M. Ladanyi, R.M. Stratt

11:20 PHYS **107.** Coarse-graining of molecular liquids with integral equation theory. **M. Guenza**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Astrophysics of Ice & Dust

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

R. L. Hudson, *Presiding*

8:00 PHYS **108.** Production mechanisms for complex interstellar molecules. **E. Herbst**, C.N. Shingledecker

8:45 PHYS **109.** Thermally induced low temperature fragmentation reaction in solid phase: Possible answers to the non-detection of some interstellar chemical species. **L. Krim**

9:30 PHYS **110.** Ortho-to-para ratios of hydrogen molecules desorbed from ice at around 10 K: What happens on cosmic ice dust? **N. Watanabe**, H. Ueta, T. Hama, A. Kouchi

10:15 PHYS **111.** Gas-phase chemistry above interstellar and cometary ice analogs. **S.L. Widicus Weaver**, A.J. Mesko, H. Smith, S.N. Milam

10:45 PHYS **112.** Extreme Isotope Ratios in Meteoritic Material: A Gas-Phase Interstellar Origin? **L.M. Ziurys**, D.T. Halfen, T. Zega

Advanced X-Ray Techniques for Catalyst Characterization

Electro- & Photo-Catalysis

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Sponsored by COMP, Cosponsored by PHYS

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Catalytic Materials from Molecular Insight

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Strong Electron Correlation & Nonadiabatic Dynamics

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Coherent Multidimensional Spectroscopy in Materials Science

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MONDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Cosponsored by INOR

S. Corcelli, *Organizer*

E. Blair, *Presiding*

1:30 PHYS **113.** Probing vibrational coupling and relaxation in cyanide-bridged transition metal mixed-valence complexes. **M.H. Khalil**

2:10 PHYS **114.** Electrostatic and electrodynamic fields in lipid bilayer membranes. **L.J. Webb**

2:50 Intermission.

3:10 PHYS **115.** Voltage-gated switching of anion-molecule assemblies at interfaces and in solution. **A.H. Flood**

3:50 PHYS **116.** Radical chemistry and charge manipulation with an atomic force microscope. **L. Gross**, B. Schuler, N. Pavliček, S. Fatayer, Z. Majzik, N. Moll, G. Meyer

4:30 PHYS **117.** Revisiting the structure-properties relation in charge transport across large area molecular tunneling junctions. **J. Chen**, H. Yoon, M. Thuo

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Dynamics Relevant to Electron & Proton Transfer

A. V. Benderskii, J. Dawlaty, *Organizers*

S. T. Roberts, *Presiding*

1:30 PHYS **118.** Proton coupled electron transfer in photosynthetic oxygen evolution: Role for internal water and hydrogen bonded networks. **B.A. Barry**, U. Brahmachari, Z. Guo

2:10 PHYS **119.** Hydrated excess proton-ultrafast vibrational dynamics of the Zundel cation $H_5O_2^+$. F. Dahms, R. Costard, B. Fingerhut, E. Pines, **E. Nibbering**, T. Elsaesser

2:30 PHYS **120.** Dissecting the molecular structure and dynamics of aqueous systems through many-body molecular dynamics simulations. **F. Paesani**

3:10 Intermission.

3:30 PHYS **121.** Panoramic portrait of photochemical events in solution and proteins captured by femtosecond Raman spectroscopy. L. Tang, B.G. Oscar, Y. Wang, L. Zhu, W. Liu, **C. Fang**

4:10 PHYS **122.** Time-resolved infrared spectroscopy as a probe of nonequilibrium hydrogen-bond dynamics: A mixed quantum-classical study of alcohols in liquid solution. **E. Geva**

4:30 PHYS **123.** Alteration of photoacidic behavior of pyrenol dyes covalently bound in the nanoconfined, electrostatically-complicated tips of asymmetric nanopores. **C. Sanborn**, J.V. Chacko, S. Ardo

4:50 PHYS **124.** Photoinduced charge separation and recombination in DNA strands. **B. Kohler**

Section C

Parc 55 San Francisco

Hearst

Long Range Correlated Motions in Proteins

Dynamical Measurements & Calculations using Protein Crystals

A. Markelz, *Organizer*

M. Cammarata, *Presiding*

1:30 PHYS **125.** Fast and ultrafast structural investigations of trans to cis isomerizations in photoreactive proteins. **M. Schmidt**

2:00 PHYS **126.** Ultra-fast time-resolved serial femtosecond crystallography on myoglobin ligand dissociation. **I. Schlichting**

2:30 PHYS **127.** Photo-intermediate State Dependence of Picosecond Motions in Photoactive Proteins. **Y. Deng**, M. Xu, H. Liu, K. Niessen, M. Schmidt, R.E. Blankenship, A. Markelz

2:50 Intermission.

3:05 PHYS **128.** Non-thermal effect of terahertz radiation on crystals of lysozyme at room temperature and bovine trypsin at 100 K. **G. Katona**, I. Lundholm, W.Y. Wahlgren, M. Garcia Bonete, H. Rodilla, J. Stake, J. Vukusic, A. Duelli, H. Bassereh, G. Bourenkov, T. Schneider, R. Friedman

3:35 PHYS **129.** Effect of intermolecular interactions on mixing of intermolecular and intramolecular vibrations: Terahertz spectroscopy and solid-state density functional theory. F. Zhang, H. Wang, K. Tominaga, **M. Hayashi**

4:05 PHYS **130.** Mutation induced structure changes in histone proteins. **T. Yu**, G.C. Schatz, J. Licht

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Semiempirical & DFTB

Cosponsored by COMP

A. V. Akimov, *Organizer*

O. V. Prezhdo, *Organizer, Presiding*

1:30 PHYS **131.** Nonadiabatic molecular dynamics with tight-binding fragment molecular orbitals. **A.V. Akimov**

2:10 PHYS **132.** Fragment orbital-based surface hopping for simulation of charge carrier transport in materials and biomolecules. A. Carof, L. Scalfi, **J. Blumberger**

2:50 PHYS **133.** Nonadiabatic molecular mechanics/extended Hückel excited state quantum dynamics method. **L.G. Rego**, R. Oliboni, A. Torres, G. Bortolini

3:30 Intermission.

3:45 PHYS **134.** Chemical reaction simulations treated by linear-scaling Divide-and-Conquer Type Density-Functional Based Tight-Binding Molecular Dynamics (DC-DFTB-MD) method. **H. Nakai**

4:25 PHYS **135.** QM/MM simulations of electron/exciton transfer reactions. **M. Elstner**

5:05 PHYS **136.** Force field accelerated density functional theory molecular dynamics for simulation of reactive systems at extreme conditions. **R. Lindsey**, N. Goldman, L.E. Fried

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids: Symposium in honor of Salvatore Torquato

Cosponsored by PRES

J. E. Shea, *Organizer*

P. G. Debenedetti, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS **137.** Hard spheres under gravity. **F. Stillinger**

2:15 PHYS **138.** Inverse design of interactions for assembly. **T. Truskett**

2:55 PHYS **139.** Structure and dynamics in cold aqueous clusters: Quantum and classical perspectives. **P.J. Rossky**

3:35 Intermission.

3:50 PHYS **140.** Nano-scale drying and hydration phenomena. **P.G. Debenedetti**

4:30 PHYS **141. Award Address** (Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids sponsored by ExxonMobil Research & Engineering Company). Disordered hyperuniform materials: New states of amorphous matter. **S. Torquato**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Ionic Liquids

A. T. Krummel, N. E. Levinger, *Organizers*

M. Guenza, *Presiding*

1:30 PHYS **142.** Molecular geometries and electronic structures of ionic liquids: Bulk, vacuum interfaces, and ultrathin films. **E. Castner**

2:10 PHYS **143.** Heterogeneity in solvation by an ionic liquid: A qualitative distinction between inertial and diffusive dynamics. S. Verma, S. Corcelli, **M.A. Berg**

2:30 PHYS **144.** Solute dynamics in ionic liquids: Experiment and simulation. **M. Maroncelli**, C. Rumble, B. Conway, C. Uitvlugt

3:10 Intermission.

3:30 PHYS **145.** Dynamics and vibrational spectroscopy of solutes in ionic liquids. **S. Corcelli**

4:10 PHYS **146.** Photo-induced electron transfer by ions in ionic liquids. **B. Wu**, M. Maroncelli, E. Castner

4:30 PHYS **147.** Carbon dioxide dynamics in room temperature ionic liquids and supported ionic liquid membranes: 2D IR and polarization selective pump-prove experiments. **M.D. Fayer**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Kuiper Belt Objects & Comets

M. S. Gudipati, *Organizer*

R. Kaiser, *Organizer, Presiding*

N. Watanabe, *Presiding*

1:30 PHYS **148.** Chemistry in protoplanetary disks. **T.K. Henning**

2:15 PHYS **149.** Chemical evolution of organic materials from protoplanetary disk to small bodies recorded in Antarctic micrometeorites. **H. Yabuta**

3:00 PHYS **150.** Energetic gas-surface encounters at ice interfaces. G. Langlois, R.S. Thompson, W. Li, K. Gibson, D.R. Killelea, H. Yuan, **S.J. Sibener**

3:45 PHYS **151.** Adsorption, diffusion, aggregation, and desorption of simple molecules (CO_2, CO, O_2, etc.) on interstellar ice analogs. **G. Vidali**, J. He, S. Emtiaz

4:30 PHYS **152.** Synthesizing the basic PAH unit. **B. Sivaraman**

Advanced X-Ray Techniques for Catalyst Characterization

New Methodologies

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

Sponsored by COMP, Cosponsored by PHYS

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

J. E. Shea, *Organizer*

8:00 - 10:00

39, 59. See previous listings.

169, 220, 241, 247, 338, 367-368, 380-381, 396, 453, 465, 470, 478, 493, 499, 505, 511, 515, 523, 532, 541. See subsequent listings.

TUESDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Applications & Devices

Cosponsored by INOR

S. Corcelli, *Organizer*

S. Roy, *Presiding*

8:00 PHYS **153.** Investigation of quantum-dot cellular automata networks using a quantum annealing processor. J. Retallick, **K. Walus**

8:40 PHYS **154.** Multistable mixed-valence molecular entities for quantum cellular automata: Vibronic localization in isolated and coupled cells. **B. Tsukerblat**, A. Palii

9:20 Intermission.

9:40 PHYS **155.** Fully-quantum, non-equilibrium model of vibration-coupled, electric-field-driven electron transfer in mixed-valence molecules. **E. Blair**

‡ *Cooperative Cosponsorship*

10:20 PHYS **156.** Properties of multiple silicon atom artificial molecules on a silicon surface. **R.A. Wolkow**

11:00 PHYS **157.** Mixed-valence molecules could be the replacement for the transistor. **C. Lent**

Section B

Parc 55 San Francisco
Mission I

Spectroscopy of Complex Systems

Exciton Dynamics & Dissociation in Heterogeneous Systems

A. V. Benderskii, J. Dawlaty, *Organizers*

P. B. Petersen, *Presiding*

8:00 PHYS **158.** Extracting triplet excitons produced by singlet exciton fission from perylenediimide thin films. A.K. Le, J.A. Bender, A.P. Moon, R. Pandey, **S.T. Roberts**

8:40 PHYS **159.** Resonance Raman study of exciton-phonon coupling in CdSe and ZnSe quantum dots and their alloys. K. Gong, D.F. Kelley, **A.M. Kelley**

9:00 PHYS **160.** Probes of structure, disorder, and dynamics of excited states in conjugated materials. **A.E. Bragg**

9:40 Intermission.

10:00 PHYS **161.** Probing the mechanism of singlet fission with femtosecond stimulated Raman spectroscopy. **R.R. Frontiera**, S.M. Hart, W.R. Silva, K. Bera, S. Kwang, A. Cassabaum

10:40 PHYS **162.** Interfacial disorder drives charge separation in molecular semiconductors. **A. Willard**, C. Lee, L. Shi

11:20 PHYS **163.** Intermolecular vibronic coherence transfer in an organic electrode material. **A. Rury**, J. Dawlaty

11:40 PHYS **164.** When a single structure is not sufficient: Effect of thermal deformation on excitonic properties of semiconductor nanoparticles. J. Scher, A. Srihari, M.G. Bayne, S. Nangia, **A. Chakraborty**

Section C

Parc 55 San Francisco
Hearst

Long Range Correlated Motions in Proteins

Catalysis

A. Markelz, *Organizer*

A. Grossfield, *Presiding*

9:00 PHYS **165.** Motions in proteins and drug design. **J. Smith**

9:30 PHYS **166.** Evolution and designing enzymes for rapid protein dynamics and catalysis. **S.D. Schwartz**

10:00 PHYS **167.** Sensitivity to protein vibration directionality and the relation to function. **K.A. Niessen**, M. Xu, Y. Deng, E. Snell, A. Markelz

10:20 PHYS **168.** Role of statistical fluctuations and electrostatics in the improvements of de novo enzyme catalysis. **T.L. Head-Gordon**

10:50 PHYS **169.** Withdrawn.

Section D

Parc 55 San Francisco
Divisadero

Quantum Dynamics in Large Scale Systems

Simulations in Materials Systems

Cosponsored by COMP

A. V. Akimov, *Organizer*

O. V. Prezhdo, *Organizer, Presiding*

8:00 PHYS **170.** Relating chromophoric and structural disorder in conjugated polymers. **L. Simine**, P.J. Rossky

8:20 PHYS **171.** Dynamics of organic materials with optical activity: Advances, appraisal, applications. **M. Barbatti**

9:00 PHYS **172.** Charge transfer and singlet fission quantum dynamics in organic photovoltaic. **P. Huo**

9:40 PHYS **173.** Theoretical investigation of electron-nuclear dynamics in the neutral and cationic $[Au_{25}(SH)_{18}]^{q}$ [q = 0, +1] thiolate-protected gold nanoclusters. **R.D. Senanayake**, A.V. Akimov, C.M. Aikens

10:00 Intermission.

10:15 PHYS **174.** Mapping nuclear dynamics in nonadiabatic molecular dynamics simulations. **G. Tao**

10:55 PHYS **175.** Theoretical investigation of novel CdSe/$Cd_{1-x}Zn_xS$ seeded nanorods exhibiting high quantum-yield, high polarization, and minimal blinking. I. Hadar, **J.P. Philbin**, Y. Panfil, H. Eshet, E. Rabani, U. Banin

11:15 PHYS **176.** Strong binding of CdSe quantum dots to single-walled carbon nanotubes. **B. Rudshteyn**, S. Azoz, W. Ding, F. Ren, M. Askerka, A. Matula, N. Marinkovic, G.L. Haller, L. Pfefferle, V.S. Batista

11:35 PHYS **177.** Exciton transport in disordered molecular systems in couple with the quantum fluctuating electromagnetic field of metal surface. **X. Chen**, A. Poudel, M.A. Ratner

Section E

Parc 55 San Francisco
Embarcadero

PHYS Division Awards Symposium

ACS Award in Theoretical Chemistry: Symposium in honor of Peter Pulay

Cosponsored by PRES

J. E. Shea, *Organizer*

S. Hirata, *Presiding*

8:00 PHYS **178.** Paradigm changes in the methodology of computational quantum chemistry: A tribute to the contributions by Peter Pulay. **W.E. Meyer**

8:30 PHYS **179.** Density cumulant functional theory. **H.F. Schaefer**

9:00 PHYS **180.** 34 years of local electron correlation: From Peter Pulay's pioneering work to the state-of-the-art. **H. Werner**

9:30 Intermission.

10:00 PHYS **181.** Merging symmetry projection methods with coupled cluster theory. **G.E. Scuseria**

10:30 PHYS **182.** Scalable electron-correlation methods and instabilities versus strong correlation: A legacy of Peter Pulay. **S. Hirata**

11:00 PHYS **183. Award Address** (ACS Award in Theoretical Chemistry sponsored by the ACS Division of Physical Chemistry). Molecular properties from quantum mechanical calculations 1967 - 2017: Synergy, successes, and challenges. **P. Pulay**

Section F

Parc 55 San Francisco
Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Extreme Environments

A. T. Krummel, N. E. Levinger, *Organizers*

M. McCullagh, *Presiding*

8:00 PHYS **184.** Why do isotropic liquid crystals resemble supercooled liquids? **R.M. Stratt**

8:40 PHYS **185.** Relaxation and self-diffusion of liquids and supercooled liquids derived from picosecond timescale dynamics. **M.T. Cicerone**, M. Tyagi, M. Zhi, J.S. Bender

9:00 PHYS **186.** Fundamental differences between glassy dynamics in two and three dimensions. **G. Szamel**

9:20 PHYS **187.** Wetting behavior of alkane–water nanodroplets and planar interfaces. P. Neupane, F. Hrahsheh, **G. Wilemski**

10:00 Intermission.

10:20 PHYS **188.** Supercooled water: Three-body interactions, IR spectra in no man's land, and the liquid-liquid critical point. **J.L. Skinner**

11:00 PHYS **189.** Electronically coarse grained model, including all quantum mechanical fluctuations necessary for long-range forces, describes water's properties from ice to the supercritical regime. **G.J. Martyna**

11:20 PHYS **190.** Thermodynamic forces between plant cell wall constituents. **M.S. Skaf**

Section G

Parc 55 San Francisco
Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Condensed Materials in the Outer Solar System

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

B. L. Henderson, *Presiding*

8:00 PHYS **191.** Chemistry and processes in the Pluto system. **W. Grundy**, D. Cruikshank, C. Olkin, S. Stern, K. Ennico-Smith, L. Young, H.A. Weaver

8:45 PHYS **192.** Links between the ices of comet 67P/Churyumov-Gerasimenko and the interstellar medium from Rosetta/ROSINA observations. **M. Rubin**, K. Altwegg, H. Balsiger, J. Berthelier, M. Combi, J. De Keyser, B. Fiethe, S. Fuselier, S. Gasc, T. Gombosi, K. Hansen, U. Mall, H. Rème, M. Schuhmann, I. Schroeder, T. Sémon, C. Tzou, J.H. Waite, S. Wampfler, P. Wurz

9:30 PHYS **193.** Aerosol impact spectrometer – A variable velocity nanoparticle accelerator. **R.E. Continetti**

10:15 PHYS **194.** Self-Assembly of prebiotic organic materials from impact events of amino acid solutions. **N. Goldman**

10:45 PHYS **195.** Comparison of gas phase and condensed phase species: Sgr B2(N) vs. Comet 67P. **D.T. Halfen**, J. Bernal, L.M. Ziurys

11:15 PHYS **196.** Results from recent experiments on electron-stimulated desorption from icy & rocky surfaces. **C. Bennett**, M.J. Poston, T.M. Orlando

Advanced X-Ray Techniques for Catalyst Characterization

New Methodologies

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

Sponsored by COMP, Cosponsored by PHYS

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG² and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

TUESDAY AFTERNOON

Section A

Parc 55 San Francisco
Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Cosponsored by INOR

S. Corcelli, *Organizer*

C. Lent, *Presiding*

1:30 PHYS **197.** Information propagation in molecular field coupled nanocomputing logic. **M. Graziano**, R. Wang, G. Piccinini

2:10 PHYS **198.** Organic semiconductors: Singlets and triplets and charges, oh my! **T.A. Van Voorhis**, P. de Silva, T. Zhu

2:50 Intermission.

3:10 PHYS **199.** Theoretical study of dyamics in molecular junctions: Effects of molecule and electrode microstructure on electron transport. A. Becker, J. Kern, **S. Roy**

3:50 PHYS **200.** Practical approaches for studying photochemistry of large molecules in solution and some nice applications. **J.E. Subotnik**, A. Jain, G.R. Medders

4:30 PHYS **201.** Nonadiabatic electron-transfer in mixed-valence molecules. **S. Corcelli**

Section B

Parc 55 San Francisco

Mission I

Spectroscopy of Complex Systems

Exciton Dynamics & Dissociation in Heterogeneous Systems

A. V. Benderskii, J. Dawlaty, *Organizers*

A. Rury, *Presiding*

1:30 PHYS **202.** Multiresonant coherent multidimensional spectroscopy of cobalamin. **J.C. Wright**, J. Handali, N. Neff-Mallon

2:10 PHYS **203.** Two dimensional spectroscopy of photosynthetic light harvesting antennae. **G.S. Engel**

2:30 PHYS **204.** Mixed quantum/semiclassical simulations of ultrafast dynamics and spectroscopic signals. **J.A. Cina**, P.A. Kovac

3:10 Intermission.

3:30 PHYS **205.** Harnessing shared vibrations to control energy transfer. **D.M. Jonas**

4:10 PHYS **206.** Accessing excitonic structure of a photosynthetic Fenna-Matthews-Olson pigment-protein complex by time-resolved circular dichroism spectroscopy. **S. Savikhin**, V. Stadnytskyi, G. Orf, R.E. Blankenship

4:30 PHYS **207.** Withdrawn.

4:50 PHYS **208.** Ultrafast 2D white light spatial imaging of single nano-structures. **A.C. Jones**, N.M. Kearns, M.T. Zanni

5:10 PHYS **209.** Probing ultrafast electron dynamics at surfaces using soft x-ray transient reflectivity spectroscopy. **L. Baker**, J. Husek, S. Biswas, A. Cirri

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photoreceptor Activity: Rhodopsins Photosensors

K. Glusac, D. S. Larsen, *Organizers*

M. Olivucci, *Organizer, Presiding*

1:30 PHYS **210.** Photoactivation mechanisms of rhodopsins from time-resolved optical absorption spectroscopy. **D.S. Kliger**

2:10 PHYS **211.** Unexpected rhodopsin functions initiated by common retinal photoisomerization. **H. Kandori**

2:50 PHYS **212.** Evidence for a vibrational phase isotope effect on the photochemistry of vision. **R.A. Mathies**, C. Schnedermann, M. Liebel, K.M. Spillane, P. Kukura, I. Fernandez, J. Lugtenburg

3:30 Intermission.

3:50 PHYS **213.** Effect of point mutations on the ultrafast photo-isomerization of anabaena sensory rhodopsin. **S. Haacke**, D. Agathengelou, J. Leonard, H. Kandori, K. Jung

4:30 PHYS **214.** Understanding and designing color variants of retinal binding proteins by molecular simulations. **S. Hayashi**

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulations in Biological Systems

Cosponsored by COMP

A. V. Akimov, *Organizer*

O. V. Prezhdo, *Organizer, Presiding*

1:30 PHYS **215.** Importance of polarizable embedding in biological systems: Excitonic interactions in photosynthetic proteins. **L.V. Slipchenko**

2:10 PHYS **216.** Improving density functional tight binding predictions of free energy surfaces for peptide condensation reactions in solution. **M. Kroonblawd**, N. Goldman

2:30 PHYS **217.** Energy profiles for modeling transient kinetic studies of chemical reactions in proteins. **A. Nemukhin**

3:10 Intermission.

3:25 PHYS **218.** QM/MM dynamics for metalloproteins, so far without quantum dynamics. C.E. Valdez, M.R. Nechay, A. Morgenstern, M. Eberhart, **A. Alexandrova**

4:05 PHYS **219.** Quantum mechanical force fields for condensed phase molecular simulations. **D.M. York**

4:45 PHYS **220.** Single ion solvation free energies with ab initio molecular dynamics. **T.T. Duignan**, M.D. Baer, G.K. Schenter, C.J. Mundy

5:05 PHYS **221.** Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules. **Y. Li**, L. Xiang, J.L. Palma, Y. Asai, N. Tao

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

E. Bright Wilson Award: Symposium in honor of David J. Nesbitt

Cosponsored by PRES

J. E. Shea, *Organizer*

M. I. Lester, *Presiding*

1:30 PHYS **222.** Always acetylene! **R. Field**, J. Baraban, B. Changala, Z. Du, J. Jiang, A. Merer, A. Muthike, C. Saladrigas

2:05 PHYS **223.** Unimolecular decay of Criegee intermediates to hydroxyl radical products. **M.I. Lester**

2:40 PHYS **224. Award Address** (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). Good, good, good rovibrations! **D.J. Nesbitt**

3:25 Intermission.

3:45 PHYS **225.** Properties of molecular clusters from broadband molecular rotational spectroscopy. **B.H. Pate**

4:20 PHYS **226.** Formation of exotic networks of water clusters in helium droplets facilitated by the presence of neon atoms. **G.E. Douberly**, S. Xantheas

4:55 PHYS **227.** Spectroscopic resolution attosecond measurements. **S.R. Leone**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Interfaces

A. T. Krummel, N. E. Levinger, *Organizers*

M. Berg, *Presiding*

1:30 PHYS **228.** Chemical processes at environmental water-air interfaces. **V. Vaida**, E. Griffith, R. Rapf, R. Perkins

2:10 PHYS **229.** Quantifying the catalyst's role in inverse phase transfer catalysis with computer simulations. **J.J. Karnes**, I. Benjamin

2:30 PHYS **230.** Visualization of charge motion in nanostructures with pump-probe microscopy. **J.M. Papanikolas**

3:10 Intermission.

3:30 PHYS **231.** Ice: The common solid we hardly know. **M.J. Shultz**, P.J. Bisson, J. Marmolejos, A. Brumberg

4:10 PHYS **232.** Solvation dynamics of aqueous solutions in extreme hydrophilic confinement. **R.C. Remsing**

4:30 PHYS **233.** Dynamics and structure of water in confined environments. **A. Luzar**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Chemistry of Condensates on the Terrestrial Planets

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

N. Goldman, *Presiding*

1:30 PHYS **234.** Quantum chemistry and ab initio molecular dynamics simulations of reactive chemistry in ionized clusters: From acetylene clusters to aromatics. T. Stein, M. Ahmed, **M.P. Head-Gordon**

2:15 PHYS **235.** Nucleobase synthesis via UV-induced oxidation of their precursors in astrophysical ices: A quantum chemical perspective. **P. Bera**, T. Stein, M.P. Head-Gordon, T.J. Lee

3:00 PHYS **236.** Theoretical cluster studies of charge shift reactions in astrophysical ices. **D.E. Woon**

3:45 PHYS **237.** Formation of formamide NH_2CHO catalyzed by icy grain particles: Atomistic insights from quantum chemical simulations. **A. Rimola**, V. Taquet, C. Ceccarelli, N. Balucani, P. Ugliengo

4:15 PHYS **238.** Adsorption and catalysis of noble gas atoms and electrons on PAH surfaces. **R.C. Fortenberry**, G.T. Filipek, II, C.M. Novak, M.M. Moore, M.L. Theis, T.J. Lee

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Cosponsored by INOR

S. Corcelli, *Organizer*

M. Lieberman, *Presiding*

8:00 PHYS **239.** Structural insight into electronic communication and energy transfer in metal organic framework arrays. **A.J. Morris**, J.M. Rowe

8:40 PHYS **240.** Nano-Confinement inside molecular metal oxide clusters: Dynamics and modified encapsulation behavior. **P. Yin**

9:00 PHYS **241.** Investigating the transformations of polyoxoanions using mass spectrometry and molecular dynamics. **L. Vilà Nadal**, L. Cronin

9:20 PHYS **242.** Charge localization vs delocalization in tetranuclear mixed-valence complexes: A spectroscopic study. **C. Lapinte**, J. Hamon, R. Makhoul, P. Hamon

10:00 Intermission.

10:20 PHYS **243.** Closo-$Si_{12}C_{12}$ Molecule from cluster to crystal: Structure and properties of closo-$Si_{12}C_{12}$ siloxane polymers. **X.F. Duan**, L.W. Burggraf

10:40 PHYS **244.** Layer-by-layer assembled MOFs. Building ordered chromophoric arrays and propagating molecular excitons. S. Goswami, O.K. Farha, **J.T. Hupp**

11:20 PHYS **245.** Lanthanide-based single-molecule magnets with high blocking temperatures. S. Demir, C. Gould, L.E. Darago, M.I. Gonzalez, K.R. Meihaus, J. Zadrozny, M. Nippe, J.D. Rinehart, **J.R. Long**

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Effects of Nanoconfinement & Local Asymmetry on Dynamics & Chemistry: Local E-Fields

A. V. Benderskii, J. Dawlaty, *Organizers*

A. Rury, *Presiding*

8:00 PHYS **246.** Electric fields and enzyme catalysis. **S.G. Boxer**

8:40 PHYS **247.** Vibrational sum frequency generation Stark shift spectroscopy: Measuring the electric field at a metal-dielectric interface. **S.A. Sorenson**, J. Patrow, J. Dawlaty

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

9:00 PHYS **248.** Probing electrostatics along the catalytic cycle of an enzyme with site-specific nitrile probes. **S. Hammes-Schiffer**

9:40 Intermission.

10:00 PHYS **249.** Calibrating the vibrational Stark effect of nitrile probes in the presence of hydrogen bonding with independently measured electric fields in green fluorescent protein. **L.J. Webb**

10:40 PHYS **250.** Non-linear SFG spectroscopy of mineral/water interfaces containing electrolytes & tera-hertz spectroscopy in liquid water: A DFT-MD theoretical perspective. **M.P. Gaigeot**

11:00 PHYS **251.** Atomistic electrodynamic-quantum mechanical approaches for simulating surface-enhanced hyper-Raman scattering: Theory and application. **Z. Hu**, D. Chulhai, L. Jensen

11:20 PHYS **252.** Attosecond quantum kinetics of photoexcited Germanium. **P. Kraus**, C. Kaplan, M.W. Zuerch, H. Chang, L.J. Borja, M.F. Jager, S. Cushing, D.M. Neumark, S.R. Leone

11:40 PHYS **253.** Driving delocalized dynamics using the orbital angular momentum of light. **B.S. Rolczynski**, P. Navotnaya, G.S. Engel

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Excited-State Dynamics & Microscopy

K. Glusac, D. S. Larsen, M. Olivucci, *Organizers*

S. Haacke, *Presiding*

8:00 PHYS **254.** Electronic energy redistribution in conjugated molecules and the effect of an energy gradient. **V.D. Kleiman**

8:30 PHYS **255.** Space- and time-resolved spectroscopy of energy transfer. **T. Brixner**

9:00 PHYS **256.** Ultrafast vibronic microspectroscopy of nanostructured electronic materials. C. Schnedermann, J. Lim, A. Rao, **P. Kukura**

9:30 PHYS **257.** Ultrafast spectroscopic observation of cysteine-based redox regulation of coherent energy transfer in a photosynthetic antenna complex. **J.P. Otto**, M.A. Allodi, R.G. Saer, S.H. Sohail, R.E. Blankenship, G.S. Engel

9:50 PHYS **258.** Resolving the detailed 2D spectral structure of the Fenna-Matthews-Olson complex. **B.S. Rolczynski**, S. Yeh, P. Navotnaya, K. Ashraf, A.T. Gardiner, R.J. Cogdell, G.S. Engel

10:10 Intermission.

10:30 PHYS **259.** Electronic and geometric dynamics of transition metal complexes for solar energy conversion. **L.X. Chen**, M. Shelby, D. Hayes, R. Hadt, P. Kim, S. Brown-Xu, J. Hong, M. Kelley

11:00 PHYS **260.** Torsional dynamics, intramolecular charge transfer, and solvent friction in the S_2 ($1^1B_u^+$) excited state of peridinin: A mechanism for enhanced mid-visible light harvesting in the peridinin–chlorophyll a protein. **W.F. Beck**, J.D. Roscioli, S. Ghosh, M.M. Bishop, A.M. LaFountain, H.A. Frank

11:20 PHYS **261.** Probing the dynamics of higher-lying excited states. **C.G. Elles**, T.J. Quincy, M.S. Barclay

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Metamaterials & Information Technology

P. K. Jain, *Organizer*

C. J. Murphy, *Organizer, Presiding*

8:00 PHYS **262.** Film-Coupled nanocubes: From ultrafast spontaneous emission to perfect absorbers. **M.H. Mikkelsen**

8:35 PHYS **263.** Dynamic plasmonic metamaterials with broken symmetry created via directed self-assembly. **D.B. Litt**, M.R. Jones, M. Hentschel, P. Alivisatos

8:55 PHYS **264.** Towards all-optical chiral resolution with achiral plasmonic and dielectric nanostructures. **J. Dionne**

9:30 PHYS **265.** Magneto-Optical response of cobalt interacting with plasmonic nanoparticle superlattices. **M.B. Ross**, C.A. Mirkin, G.C. Schatz

9:50 Intermission.

10:05 PHYS **266.** Heat-assisted magnetic recording: Next-generation mass storage technology. **M. Re**, J. Thiele, G. Ju, C. Rea, T. Rausch, M. Siegler, E. Gage

10:40 PHYS **267.** Near field thermal imaging: Sub-diffraction and steady state thermal measurements on optically excited gold nanostructures. S. Baral, A. Rafiei Miandashti, **H.H. Richardson**

11:00 PHYS **268.** Plasmonic transition metal nitrides for harsh-environment photonic applications. U. Guler, H. Reddy, K. Chaudhury, A. Naldoni, A. Kildishev, V. Shalaev, **A. Boltasseva**

11:35 PHYS **269.** Far-field supperresolution detection of plasmonic near-fields. **R.C. Boutelle**, D. Neuhauser, S. Weiss

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Francis P. Garvan–John M. Olin Medal: Symposium in honor of Barbara J. Finlayson-Pitt

Cosponsored by PRES

J. E. Shea, *Organizer*

S. A. Nizkorodov, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **270. Award Address** (Francis P. Garvan–John M. Olin Medal sponsored by Francis P. Garvan–John M. Olin Medal Endowment). From active molecules to atmospheric models: The central role of molecular level understanding in improving human health and welfare. **B.J. Finlayson Pitts**

8:40 PHYS **271.** Towards molecular-level understanding of growth, formation and properties of atmospheric acid-base particles. **R.B. Gerber**, J. Xu, K. Arquero, B.J. Finlayson Pitts

9:05 PHYS **272.** Atmospheric photochemistry of pyruvic acid and related oxoacids. **V. Vaida**, A. Reed Harris, R. Rapf, R. Perkins

9:30 PHYS **273.** Enhanced reactivity in aqueous aerosols: Why bulk-phase aqueous measurements can mislead us. **D.O. Dehaan**

9:55 Intermission.

10:15 PHYS **274.** Studies of halogen chemistry in the Arctic. **P.B. Shepson**

10:45 PHYS **275.** Molecular dynamics simulation studies of ions and acids at atmospherically relevant aqueous solution-air interfaces. **D. Tobias**

11:10 PHYS **276.** Composition and chemistry of the liquid/vapor interface of aqueous solutions. **J.C. Hemminger**

11:35 PHYS **277.** Organic photochemistry in atmospheric particulate matter. **S.A. Nizkorodov**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Complex Systems

A. T. Krummel, N. E. Levinger, *Organizers*

R. Remsing, *Presiding*

8:20 PHYS **278.** Biomolecular hydration shells: Dynamics and effect on biochemical function. **D. Laage**

9:00 PHYS **279.** Probing PDI nanoaggregate structures by combining MD simulations & 2D IR spectroscopy. **A.T. Krummel**

9:20 PHYS **280.** Biological water or rather water in biology? **P. Jungwirth**

10:00 Intermission.

10:20 PHYS **281.** Bottom-up treatment of nonpolar solvation for molecular dynamics simulations. P.T. Lake, **M. McCullagh**

11:00 PHYS **282.** Magnesium fluctuations modulate RNA dynamics in riboswitch. **U. Mohanty**

11:20 PHYS **283.** Depolarized light scattering and terahertz absorption of protein solutions. **D.V. Matyushov**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Physical Properties of Condensed Super Volatiles on Pluto: From the New Horizon Mission

M. S. Gudipati, *Organizer*

R. Kaiser, *Organizer, Presiding*

G. Vidali, *Presiding*

8:00 PHYS **284.** Probing molecular growth and charge transfer processes with vacuum ultraviolet mass spectrometry. **M. Ahmed**

8:45 PHYS **285.** Chemical processing in interstellar grains via electron and UV radiation. **B.L. Henderson**, M.S. Gudipati

9:30 PHYS **286.** Photon-stimulated processes on planetary surfaces and in astrophysical environments. **T.M. Orlando**, C. Bennett, J. McLain, M. Sarantos

10:15 PHYS **287.** Chemical functionalization and catalytic activity of polycyclic aromatic hydrocarbons on dust grain surfaces. **L. Hornekaer**, J.H. Jørgensen, A.W. Skov

11:00 PHYS **288.** PAHs, Dust and ice in the solar system. **A. Mattioda**, G. Cruz-Diaz, A. Ricca Bauschlicher, A. de Barros, S. Erickson, P. van Vliet, E. da Silveira, A. Cook

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Cosponsored by INOR

S. Corcelli, *Organizer, Presiding*

1:30 PHYS **289.** Pyrolysis of DNA origami drives carbon atoms into the substrate forming silicon carbide replicas. M.A. Pillers, **M. Lieberman**

2:10 PHYS **290.** Self-assembled crystals that perform molecular rotor-based computations. **E.H. Sykes**, N. Wasio

2:50 Intermission.

3:10 PHYS **291.** Simulation of static and dynamic behavior of molecular quantum-dot cellular automata made of Fe and Ru mixed-valence complexes. **K. Tokunaga**

3:50 PHYS **292.** New reactions in surface chemistry. **F. Rosei**

4:30 PHYS **293.** Electron transfer in the molecular quantum-dot cellular automata: The competition between Coulomb effect and nuclear relaxation. **Y. Lu**, C. Lent

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Effects of Nanoconfinement & Local Asymmetry on Dynamics & Chemistry

A. V. Benderskii, *Organizer*

J. Dawlaty, *Organizer, Presiding*

1:30 PHYS **294.** Dynamics of room temperature ionic liquids measured with two dimensional infrared spectroscopy: The influence of electric fields on observables. **M.D. Fayer**

2:10 PHYS **295.** Environmental effects on the structure of nanoemulsion interfaces. **A. Carpenter**, J. Hensel, R. Ciszewski, B. Schabes, G.L. Richmond

2:30 PHYS **296.** Simulations of the vibrational spectroscopy of water at silica interfaces. J.A. Harvey, P.C. Burris, P. Wimalasiri, **W.H. Thompson**

3:10 Intermission.

3:30 PHYS **297.** Spectroscopic insight into efficiency limiting factors in light-driven H_2 generation using 1D and 2D multicomponent semiconductor/catalyst nanoheterostructures. **T. Lian**

4:10 PHYS **298.** Transition from molecular vibrations to phonons in atomically-precise cadmium selenide quantum dots. A. Beecher, R.A. Dziatko, M.L. Steigerwald, J.S. Owen, **A. Crowther**

4:30 PHYS **299.** Single-molecule exploration of the regulation of photosynthetic light harvesting. **G. Schlau-Cohen**

4:50 PHYS **300.** Linear and nonlinear spectroscopy of multicolor photoresists. Z. Tomova, N. Liaros, S. Gutierrez Razo, H. Ogden, S. Wolf, M. Thum, **J.T. Fourkas**, A.S. Mullin, D. Falvey, J. Petersen

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Exciton Photodynamics: Soft Materials

D. S. Larsen, M. Olivucci, *Organizers*

K. Glusac, *Organizer, Presiding*

1:30 PHYS **301.** What happens to triplet excitons after singlet fission? **C.J. Bardeen**

2:00 PHYS **302.** Introducing a general spin-correct spin-flip configuration interaction method that includes dynamic correlation. **J. Mato**, M.S. Gordon

2:20 PHYS **303.** Excitonic triplet-triplet couplings in dimeric and aggregated dyes: Experiment and theory. **L.V. Slipchenko**, D.A. Hartzler, S. Savikhin

2:40 PHYS **304.** Singlet fission: Optimal choice of mutual disposition of chromophores. Z. Havlas, P. Felkel, E. Buchanan, **J. Michl**

3:10 PHYS **305.** Dynamics of electronic excitations at organic-inorganic interfaces. **D. Kilin**, Y. Han, D. Vogel, A. Forde, B. Disrud, S.J. Jensen, W. Sapp, A.R. Erck

3:30 Intermission.

3:50 PHYS **306.** Conical intersections and non-radiative recombination in semiconductor nanocrystals. **B.G. Levine**, Y. Shu, B. Fales, W. Peng

4:20 PHYS **307.** Insights into the mechanism of photovoltaic action from photoacid-functionalized ion-exchange materials. **W.N. White**, C. Sanborn, D. Fabian, S. Ardo

4:40 PHYS **308.** Role of the protein in light-driven biological functions: A quantum chemical view. **B. Mennucci**

5:10 PHYS **309.** Understanding the quantum dynamics of photosynthetic energy transfer with realistic environment interactions. **P. Huo**, D. Coker, M. Lee

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Surface Chemistry, Sensors & Diagnostics

C. J. Murphy, *Organizer*

P. K. Jain, *Organizer, Presiding*

1:30 PHYS **310.** Plasmonic nanomaterials for ultrasensitive biosensing. **M. Stevens**

2:05 PHYS **311.** Dependence of the plasmonic properties of two silver nanocubes on their separation, relative orientation, refractive index of the substrate and propagation direction of the exciting light. **N. Hooshmand**

2:25 PHYS **312.** Controlling chirality of aluminum plasmonic architectures based on copper mask nanosphere template lithography. **J.S. Shumaker-Parry**

3:00 PHYS **313.** Understanding molecule-plasmon coupling in surface-enhanced femtosecond stimulated Raman scattering: Combined experimental-theoretical studies. **M.O. McAnally**, G.C. Schatz, R.P. Van Duyne

3:20 Intermission.

3:35 PHYS **314.** Commercialization of optically tailored plasmonic nanoparticles for diagnostic assays and therapeutics. **S. Oldenburg**, R.K. Baldwin, A.E. Saunders, J.M. Werle, R.T. Decker

4:10 PHYS **315.** Novel numerical method for electron energy-loss spectroscopy calculation: EELS-FDTD. **N. Large**, A. Manjavacas, E. Ringe, G.C. Schatz, S.X. Wang, P.J. Nordlander

4:30 PHYS **316.** SERS sensors for direct detection of environmental contaminants. **A.J. Haes**, T. Forbes, G. Lu

5:05 PHYS **317.** Plasmon-induced excited-state heterogeneous catalysis on surface-doped metallic nanoparticles. **J. Martirez**, E.A. Carter

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Water

N. E. Levinger, *Organizer*

A. T. Krummel, *Organizer, Presiding*

1:30 PHYS **318.** Mechanisms of electronic excited state relaxation in water clusters. **P.J. Rossky**

2:10 PHYS **319.** Withdrawn.

2:30 PHYS **320.** Solvation structure and photochemical dynamics of seeded molecular clusters. **G. Peslherbe**

3:10 Intermission.

3:30 PHYS **321.** Solvation dynamics revisited: An energy flux approach. **J.T. Hynes**, R. Rey

4:10 PHYS **322.** Connecting features of a water molecule with the anomalous properties of liquid water by comparing different water models in computer simulations. **T. Ichiye**

4:30 PHYS **323.** Hydration-shell vibrational spectroscopy of water-mediated interactions. **D. Ben-Amotz**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Chemical Composition & Evolution of Comets 67P/CG: As Observed by the Rosetta Mission

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

L. Hornekaer, *Presiding*

1:30 PHYS **324.** Sugar derivatives in residues produced from the UV irradiation of astrophysical ice analogs. **M. Nuevo**, S.A. Sandford, J. Saunders, G. Cooper

2:15 PHYS **325.** Protonation and ionization of organic reactive molecules in low-density amorphous water ice. **W.W. Sander**, P. Costa, M.S. Gudipati

3:00 PHYS **326.** Radiation chemistry and redox reactions in icy molecular solids. **R.L. Hudson**, M. Loeffler

3:45 PHYS **327.** Electron induced chemistry in interstellar and cometary ices. **N.J. Mason**

4:30 PHYS **328.** Non-Ionizing UV (< 7 eV) photochemistry of cosmic ice analogs of ammonia. **H. Cumberbatch**, **A. Bao**, C. Arumainayagam

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY EVENING

Section A

Moscone Center

Hall D

PHYS Poster Session

J. E. Shea, *Organizer*

7:00 - 9:00

PHYS **329.** Study of the O(^{3}P) initiated oxidation of 2-methylfuran via synchrotron multiplexed photoionization mass spectrometry. Y. Fathi, **K. Nwachuku**, G. Meloni

PHYS **330.** Photo-induced phase transitions of spin-crossover nanoparticles within the thermal hysteresis loop. **A.D. Mena**, D.A. Munteanu, R.M. van der Veen, T. Dixon, C.M. Gentle

PHYS **331.** Insight into the role of water in the photogeneration and properties of bifunctional quinone methides: A time-resolved spectroscopic study of a binol quinone methide. **L. Du**, X. Zhang, J. Xue, D.L. Phillips

PHYS **332.** Electronic dynamics in bulk GaAs induced by light with orbital angular momentum. **P. Navotnaya**, B.S. Rolczynski, G.S. Engel

PHYS **333.** Equivalency of the kinetic schemes: Mathematical formulation. **V.D. Dergachev**, A. Petrov, I. Dergachev, S.A. Varganov

PHYS **334.** Water, hydrogen-bonding networks, redox-active tyrosines, and proton coupled electron transfer reactions in the photosynthetic water oxidizing complex. **Z. Guo**, B.A. Barry

PHYS **335.** Withdrawn.

PHYS **336.** Accessing chiral information in macromolecules via time-resolved circular dichroism spectroscopy. **V. Stadnytskyi**, G. Orf, R.E. Blankenship, S. Savikhin

PHYS **337.** Methylglyoxal hydration state equilibrium at the air-water interface. **B. Gordon**, G. Lindquist, N.A. Valley, S. Wren, G.L. Richmond

PHYS **338.** Simulating transient x-ray absorption spectroscopy of photo-excited chemical dynamics in molecular systems. **S. Pemmaraju**, D. Prendergast

PHYS **339.** Characterization of the structure and dynamics of AOT reverse micelles in heavy alkanes. **I. Sitarik**, K. Obray, J. Diverdi

PHYS **340.** Exploring the role of asymetrically coordinated photoactive metal centers in photoinduced electron transfer reactions: A spectroscopic perspective. **B. Dietzek**

PHYS **341.** Chemistry of aerosolized room-temperature ionic liquids. **S. Chambreau**, G.L. Vaghjiani, D. Popolan-Vaida, S.R. Leone

PHYS **342.** Electron irradiation effects in icy regoliths: The PacMan anomalies on the icy Saturnian moons. **M.J. Schaible**, R.E. Johnson, L. Zhigilei

PHYS **343.** Effects of thermal broadening and photoluminescence in functionalized silicon nanocrystals. **D. Vogel**, D. Kilin

PHYS **344.** Undistorted fluorescence yield detected soft x-ray absorption spectroscopy: Direct detection of outer (3d->2p), inner (3s->2p) and inverse partial fluorescence yield using TES based spectrometers. **C. Titus**

PHYS **345.** Charge transfer dynamics at perovskite quantum dot and Spiro-MeOTAD interface. **D. Vogel**, D. Kilin

PHYS **346.** Withdrawn.

PHYS **347.** Binary mixtures consisting of glass-forming constituent and crystal-forming constituent: Density, rheology and phase transitions in poly(propylene glycol) – water system. **B.H. Milosavljevic**, S. Lovrinic

PHYS **348.** Simplifying calculations of IR and Raman spectra from DFT-based molecular dynamics simulations. **D.R. Galimberti**

PHYS **349.** Transient absorption spectroscopy with realtime TDDFT: Perovskites and Pauli bleaches. **J. Parkhill**

PHYS **350.** New mechanism for glass formation. **I.C. Sanchez**

PHYS **351.** Withdrawn.

PHYS **352.** Role of chloride ion in photosynthetic oxygen-evolution. **U. Brahmachari**, J.F. Gonthier, C. Sherrill, B.A. Barry

PHYS **353.** Theoretical ^{15}N isotropic chemical shift: Challenging the calculation of liquid state references. **F. Jolibois**, I. Gerber

PHYS **354.** Computational studies on chemistry of graphene surface. **B.Q. Pham**, M.S. Gordon

‡ *Cooperative Cosponsorship*

PHYS **355.** Proposed two-dimensional topological insulator in SiTe. **Y. Ma**, T. Heine

PHYS **356.** Sunlight-Driven synthesis of oligomers from oxoacids in aqueous environments. **R. Rapf**, R. Perkins, V. Vaida

PHYS **357.** Ultrafast electron transfer in a model organic semiconductor: An experimental and theoretical examination. **V. Duong**, D. Nordlund, D. Prendergast, A. Ayzner

PHYS **358.** Optoelectronic structures of hybrid lead iodide perovskites probed by electron-rotor interaction. **J. Gong**, M. Yang, X. Ma, R.D. Schaller, G. Liu, L. Kong, Y. Yang, M.C. Beard, M. Lesslie, Y. Dai, B. Huang, K. Zhu, T. Xu

PHYS **359.** Spectroscopic and theoretical investigations of the intramolecular π-type hydrogen bonding in cyclic and bicyclic molecules. **J. Laane**, E.J. Ocola, A. Al-Saadi

PHYS **360.** Withdrawn.

PHYS **361.** Polarization anisotropy measurements for determining the orientation of guest molecules in a self-assembled bis-urea macrocycle host. **P. Kittikhunnatham**, B. Som, L.S. Shimizu, A. Greytak

PHYS **362.** Withdrawn.

PHYS **363.** Effects of exciton-delocalizing ligands on intraband relaxation in semiconductor nanocrystals. **M.S. Azzaro**, M.C. Babin, S.T. Roberts

PHYS **364.** Nonlinear interferometer for complex signal measurement. **M.J. Shultz**, J. Wang, P.J. Bisson, J. Marmolejos

PHYS **365.** Withdrawn.

PHYS **366.** Efficient geometry minimization and transition structure optimization using interpolated potential energy surfaces. **J. Zheng**, M.J. Frisch

PHYS **367.** Photon induced aerosol formation: Photochemically driven reactions of sulfur dioxide with water and organics. **J.A. Kroll**, V. Vaida

PHYS **368.** Angular dependence of ionization by short, intense pulses of linear and circularly polarized light simulated by time-dependent configuration interaction with an absorbing potential. **H.B. Schlegel**, P. Krause, P. Hoerner, Q. Liao, W. Li

PHYS **369.** Ultrafast transient absorption spectroscopy investigation of excited state dynamics of methyl ammonium lead bromide perovskite nanostructures. **H. Telfah**, J. Liu, A. Jamhawi, J. Strain, M. Teunis, R. Sardar

PHYS **370.** Modelling photodetachment processes in transition metal oxide clusters. **L.M. Thompson**, H.P. Hratchian

PHYS **371.** Lock and key bidentate binding of ligands on nanocrystals. **X. Li**, A. Fast, D. Fishman, Z. Huang, M. Tang

PHYS **372.** Multiple *cis* and *trans* conformations of caprylolactam and their role in deuterium isotope effect predictions in ^{13}C NMR. **E. Kleist**, B.S. Hudson

PHYS **373.** ϕ Photoreduction of $CHCl_3$ initiated by illumination of SPEEK/PVA and SPEEK/HCO_2^- system via a free radical mechanism. **M. Islam**

PHYS **374.** Withdrawn.

PHYS **375.** Tunable molecular separation by photoswitchable MOF membranes. **L. Heinke**

PHYS **376.** Nanoscale MoS_2towards emerging organic optoelectronics. A. Salam, **S. Pal**

PHYS **377.** Chiroptical investigation of sulfone-bridged heterohelicene. **A. Kim**, E. Mohammad, M. Vargas, A.G. Petrovic, B. Gliemann, M. Kivala

PHYS **378.** Withdrawn.

PHYS **379.** Tryptophan-to-tryptophan energy Transfer in UV-B photoreceptor UVR8. **X. Li**, D. Zhong

PHYS **380.** Withdrawn.

PHYS **381.** Withdrawn.

PHYS **382.** Accessing spatial heterogeneity in halide lead perovskite thin films with multimodal optical imaging. **Y. Ma**, M. Simpson, B. Doughty, S. Das, B. Yang, K. Xiao

PHYS **383.** Non-intrusive detection of polyatomic combustion intermediates via photoionization out of Rydberg states. **F. Rudakov**

PHYS **384.** Description of hydration water in protein (GFP) solution. **J. Nickels**, S. Perticaroli, G. Ehlers, C.B. Stanley, E. Mamontov, H.M. O'Neill, Q. Zhang, D. Myles, J. Katsaras

PHYS **385.** Raman studies of the photopolymerization of 1,4-diiodobuta-1,3-diene in crystalline urea inclusion compounds. **S. Dinca**, D.G. Allis, M.B. Sponsler, B.S. Hudson

PHYS **386.** Unequal hole and electron diffusion in lead bromide perovskites. **G. Elbaz**, D. Straus, O.E. Semonin, T. Hull, D. Paley, P. Kim, J.S. Owen, C.R. Kagan, X. Roy

PHYS **387.** First-principles calculations of the K-edge XANES spectra for aqueous Na^+ and for ion pairs of Ca^{2+} with either carbonate or bicarbonate. **M. Galib**, N. Govind, J. Fulton

PHYS **388.** Photoinduced charge transfer rates in light-harvesting carotenoid-porphyrin-C_{60} molecular triad. **X. Sun**, E. Geva

PHYS **389.** Inelastic neutron scattering analysis of tautomeric polymorphic crystals: The strange case of barbituric acid. **B.S. Hudson**, Y. Cheng

PHYS **390.** Exciton imaging in polycrystalline semiconducting organic thin films using optical resonance Imaging. **M.A. Allodi**, R.J. Mazukski, P.D. Dahlberg, H. Davis, J. Otto, G.S. Engel

PHYS **391.** Withdrawn.

PHYS **392.** High-Resolution infrared spectroscopy of carbon sulfur clusters. **J.B. Dudek**, J. Kozubal, T. Salomon, S. Fanghänel, S. Thorwirth

PHYS **393.** Electronic structure of iron-sulfur clusters revealed by 2p3d resonant inelastic x-ray scattering: Implications for biological nitrogen fixation. **B. Van Kuiken**, A. Hahn, S. DeBeer

PHYS **394.** Vacuum ultraviolet spectroscopy of the lowest-lying electronic state in sub-critical and supercritical water. **T.W. Marin**, I. Janik, D.M. Bartels, D. Chipman

PHYS **395.** Molecular simulations of Aβ-hIAPP cross-seeding assemblies on lipid membranes. **M. Zhang**, R. Hu, B. Ren, F. Yang, K. Chu, J. Zheng

PHYS **396.** Femtosecond stimulated Raman Spectroscopy of light harvesting complexes: Good vibrations in photosynthesis. **J. Artes Vivancos**, Y. Hontani, R. van Grondelle, J. Kennis

PHYS **397.** Synthesis and charge carrier dynamics of organolead bromide perovskite/graphitic carbon nitride nanoheterostructures for photocatalytic CO_2 reduction. **Y. Pu**

PHYS **398.** Partitioning, clustering, and hydrophobicity in mixtures of phospholipids and aromatics at water interfaces. **R. Perkins**, V. Vaida

PHYS **399.** Density fluctuations of carbon dioxide in cylindrical nanopore. **Y. Dai**, X. Xu, Y. Liu

PHYS **400.** From primordial soup to replicating DNA: Analyzing a proposed precursor of modern nucleotides. **K. Gochenour**, M.P. Callahan, K.E. Smith, D.K. Elliott, G.E. Lindberg

PHYS **401.** Investigation of electric potential induced by flowing water droplet on electrolyte-insulator-semiconductor structure. **J. Park**, Y. Yang, Y. Kim

PHYS **402.** Effect of salt and pH on the self-assembly of myristic acid. **B. Williamson**, R. Rapf, R. Perkins, V. Vaida

PHYS **403.** Confined phase separation of aqueous-organic nanodroplets. **F. Hrahsheh**, Y. Sani Wudil, G. Wilemski

PHYS **404.** Molecular properties of a light-gated cation channel from cryptophyta *Guillardia theta*. **Y. Yamauchi**, M. Konno, S. Ito, Y. Kato, S. Tsunoda, K. Inoue, H. Kandori

PHYS **405.** Triboelectric hydrogen gas detection using palladium functionalized surface. S. Shin, Y. Kwon, J. Jung, **J. Nah**

PHYS **406.** Asymmetric solvent-mediated electron-transfer chemical doping of graphene. **R.A. Dziatko**, **K. Harris**, M. Gibson, J. Karten, B. Janicek, A. Crowther

PHYS **407.** Nondestructive testing with second harmonic generation. **S.D. Smith**, S. Averett, J.E. Patterson

PHYS **408.** Nature of two diffuse interstellar bands revealed by electronic transitions in C_{60}^+. **S. Ahmadvand**, **A.O. Lykhin**, **S.A. Varganov**

PHYS **409.** Specific peptide-bond dissociation and effects of a phenyl group of some peptide model molecules. **C. Liu**, Y. Chiang, H. Lin

PHYS **410.** Vapor-liquid and liquid-liquid equilibria for a langmuir monolayer of pentadecanoic acid: A Monte Carlo study. **M.S. Minkara**, J. Siepmann

PHYS **411.** Withdrawn.

PHYS **412.** Excited-state dynamics of carotenoid dimers. **S.J. Doyle**, M.J. Tauber

PHYS **413.** Experimental and computational investigation of the competitive unimolecular reactions of CHF_2CHF_2 and CHF_2CF_3. C.A. Smith, G.L. Heard, **B.E. Holmes**

PHYS **414.** Transient grating spectroscopy of spheroidene and spheroidenone: The role of the carbonyl group in the excited state electronic and vibrational dynamics of carotenoids. S.D. Khosravi, M.M. Bishop, A.M. LaFountain, D. Busa, S. Suresh, D. Turner, G.N. Gibson, **H.A. Frank**, N. Berrah

PHYS **415.** ITC investigations on the dependence of temperature and osmometry on the structure and stability of the DNA I-motif. **T. Sutorius**

PHYS **416.** Theoretical investigation of RecA filaments search for DNA breaks. **M. Kochugaeva**, A. Shvets, A. Kolomeisky

PHYS **417.** Withdrawn.

PHYS **418.** Theoretical study on the reaction of silylidyne radical (SiH) with dimethylacetylene (CH_3CCCH_3). **Y. Lin**, M. Wu, B. Sun, A.H. Chang, R. Kaiser

PHYS **419.** Cl-initiated oxidation of propargylamine via synchrotron multiplexed photoionization mass spectrometry. **C. Price**

PHYS **420.** Withdrawn.

PHYS **421.** Investigation of glass structures using Raman spectroscopy. **V. Torres**, M.D. Sonntag

PHYS **422.** Ultrafast photoreleasing of the quinoline-derived phototrigger with sensitivity toward 2-photon excitation. **X. Lan**

PHYS **423.** Singlet/Triplet excited state mediated dehalogenation reactions of itraconazole in acetonitrile and aqueous solutions studied by time-resolved spectroscopy. **Z. Ruixue**, M. Li, L. Du, D.L. Phillips

PHYS **424.** Nanomorphology stabilization through the solvent additives and fixing agent interlayer for efficient organic and perovskite photovoltaic devices. **D. Wang**, W. Jang, S. Ahn, S. Park, J. Park

PHYS **425.** Quantum mechanical calculations of the effects of humidity on HNO_3 chemisorbed onto TiO_2. **C.J. Ostaszewski**, N.M. Stuart, J.G. Navea

PHYS **426.** Computational investigation of hydroperoxyl radical reacting with acetyl peroxy radical. **M.P. DeVault**, K.T. Kuwata

PHYS **427.** Computational study of hydride binding to the active site of lactate racemase. **R.C. Mauban**, S.A. Varganov

PHYS **428.** Temperature dependence of the hydrated electron's excited-state relaxation: Distinguishing cavity and non-cavity models. **C. Zho**, E.P. Farr, W.J. Glover, B.J. Schwartz

PHYS **429.** Excited state proton transfer kinetics of amino-naphthols in aqueous reverse micelles. **A.P. Poblete**, K. Takematsu

PHYS **430.** Photochemical reactivity of oxoacids in aqueous solution as a function of pH. **M.R. Dooley**, **R. Rapf**, R. Perkins, V. Vaida

PHYS **431.** Prevention of fibrillation of the amyloid-β (25-35) peptide by graphene oxide. **S. Bag**, S. DasGupta, S. Dasgupta

PHYS **432.** FTIR analysis of internal water molecules of a light-driven sodium pump KR2. **S. Tomida**, S. Ito, K. Inoue, H. Kandori

PHYS **433.** Kinetic modeling of the atmospheric oxidation pathways of dimethyl disulfide and dimethyl sulfide. **J.A. Berlanga**

TECHNICAL PROGRAM

PHYS **434.** Withdrawn.

PHYS **435.** Photoaddition of methanol to the stilbenes: Involvement of a common twisted intermediate. **S. Gupta**, D. Boose, J. Saltiel

PHYS **436.** Utilizing electron spin echo envelope modulation to distinguish between the local secondary structures of an α-helix and an amphipathic 310-helical peptide. **S. Rafferty**

PHYS **437.** Hybrid nano-biosystems: An investigation of the impact of quantum dots on the bacteriorhodopsin photocycle. **T.J. Wax**, J.A. Greco, S. Chen, J. Zhao, R.R. Birge

PHYS **438.** Thermal study of the decomposition of (HTPB) hybrid rocket fuel in the presence of azo-tetrazolate based high nitrogen content high energy materials. **M. Yousef**, K. Hudson

PHYS **439.** Metal free, redox-active, viologen-based, Deep Eutectic Solvents (DES). **L.N. Matsushima**, J.C. Goeltz

PHYS **440.** Optical transitions in bulk semiconductors induced by light carrying orbital angular momentum. **P. Navotnaya**, B.S. Rolczynski, G.S. Engel

PHYS **441.** Core-shell MoS_2/CdS nanorods with extraordinary high photocatalytic activity for hydrogen production under visible-light. **Z. Yan**

PHYS **442.** Developing and implementing methods for Markov state model construction and conformational sampling to extract the kinetics of protein-protein interactions. **Z. He**

PHYS **443.** Decomposition of contributions from core-levels exhibiting spin-orbit splitting in XUV core-level spectroscopy. **H. Chang**, M.W. Zuerch, P. Kraus, C. Kaplan, L.J. Borja, S. Cushing, D.M. Neumark, S.R. Leone

PHYS **444.** Withdrawn.

PHYS **445.** Unusual pattern formation in the cadmium hydroxide system. **B. Bohner**, Á. Tóth, D. Horvath

PHYS **446.** Photofragmentation dynamics of tetranitromethane. **Y. Han**, B. Rasulev, D. Kilin

PHYS **447.** Can zwitterionic cyclic polymers show aggregation in solution? **P. Du**, A. Li, X. Li, R. Kumar, D. Zhang

PHYS **448.** Molecular dynamics of reaction between hydrogen peroxide and zigzag carbon nanotube. **B. Disrud**, D. Kilin

PHYS **449.** Photophysical studies of nitro substituted porphyrinoids. **A. Aggarwal**, **C. Farley**, C.M. Drain

PHYS **450.** First-principles calculations of electron transfer rates. **S. Chaudhuri**, S. Hedström, D.D. Mendez, H.P. Hendrickson, K. Jung, V.S. Batista

PHYS **451.** Proton diffusion from pH gradients on litmus paper. **S. Ostresh**

PHYS **452.** Estimating the redox potentials of organic dyes in dichloromethane. **F.A. Rodriguez Ortiz**, D. Méndez-Hernández

PHYS **453.** Photo-conductivity measurements of water-rich ices at cryogenic temperatures. **D. Marchione**, R. Yang, M.S. Gudipati

PHYS **454.** Solution behavior and self-assembly of nanoscale macroions into "Blackberry" structure through charge mediated attractions. **S. Eghtesadi**, P. Yin, D. Li, F. Haso, Y. Gao, T. Liu

PHYS **455.** Analyzing phosphorylation of prebiotic molecules by schreibersite with polarization-modulation: Infrared reflection-absorption spectroscopy. **K. Slavicinska**, T.J. Beckman, H.L. Abbott-Lyon

PHYS **456.** Spectroscopic characterization of the physical and photo-physical properties of pewly peveloped platinum pincer complexes. **S.A. Autry**, M. Zhang, V. Dixit, T.K. Hollis, C.E. Webster, N. Hammer

PHYS **457.** Studies of nanoparticle impact dynamics with the aerosol impact spectrometer. **M.E. Miller**, B.D. Adamson, R.E. Continetti

PHYS **458.** Synchrotron multiplexed photoionization mass spectrometry of Cl-initiated oxidation of tetrahydropyrane (THP) at 298, 550, and 650 K. **A. Otten**

PHYS **459.** Charge carrier dynamics in highly luminescent cesium lead halide nanocrystals. **N. Gibson**

PHYS **460.** Photoionization and photodissocation of xylyl (methylbenzyl) bromide radicals using VUV synchrotron radiation. **Y. Fathi**, G. Meloni, P. Hemberger

PHYS **461.** Solvent thermodynamic driving force controls stacking interactions between polyaromatics. A. Rury, C.E. Ferry, **J.R. Hunt**, M. Lee, D. Mondal, S. O'Connell, E.N. Phan, Z. Peng, P. Pokhilko, D. Sylvinson, Y. Zhou, C.H. Mak

PHYS **462.** Withdrawn.

PHYS **463.** Si-SiO_x-Al_2O_3 Composite with carbon coating as an anode material for Li-ion batteries. **K. Kim**, J. Kim

PHYS **464.** Non-Thermal plasma for the heterogeneous chemistry of chemisorbed volatile compounds with free-radicals. **C. Bennett-Caso**, J.R. Borgatta, J.G. Navea

PHYS **465.** Excited-state investigation of the ultrafast electrocyclization reaction for a molecular photochromic switch. **C. Jones**, V.A. Spata, S. Matsika

PHYS **466.** PhotochemCAD 3. digital database of >1000 absorption and fluorescence spectra of diverse natural and synthetic tetrapyrrole macrocycles. **M. Taniguchi**, H. Du, J.S. Lindsey

PHYS **467.** Nonadiabatic dynamics in the formation of the elusive disilavinylidene molecule (H_2SiSi). C. Kang-Heng, **L. Lin**, A.H. Chang, R. Kaiser

PHYS **468.** Nonadiabatic dynamics of $Si(^3P) + Si_2H_6$ reaction. B. Sun, **C. Jimmy**

PHYS **469.** In-situ x-ray spectroscopy study of electrodeposited Ni-Fe hydroxide catalysts for electrochemical oxygen evolution reaction. **K. Nie**

PHYS **470.** Two-Dimensional electronic spectroscopy of BODIPY dye derivatives: Characterizing photophysics and solvent dependence. **Y. Lee**, S. Das, R.M. Malamakal, S. Meloni, D.M. Chenoweth, J.M. Anna

PHYS **471.** MRCI study of the ground state and low-lying states of Si_2H. **D. Corey**, J. Song

PHYS **472.** Apparent molar volumes and isentropic compressions of cyclic ethers in aqueous solutions from 288.15 K to 313.15 K at atmospheric pressure. **L. Brown**, P. Bernal

PHYS **473.** Electrochemical impedance spectroscopy of bipolar membranes for water and CO_2 electrolysis. **Z. Yan**, L. Zhu, C.C. Li, M. Hickner, T. Mallouk

PHYS **474.** Excited-State proton transfer in aminonaphthols. **M. Groves**, H.E. Rudel, K. Takematsu

PHYS **475.** Experimental determination of the aqueous redox potentials of environmentally relevant organic pollutants via high-speed cyclic voltammetry. **M. Paul**, D. Ruuska, S.N. Eustis

PHYS **476.** Brillouin spectroscopy of bamboo fibers. **D. Williams**, N. Rahbar, K.J. Koski

PHYS **477.** Anisotropic optical response from asymmetrical assembly of gold-silica-quantum dot nanostructure. **Y. Luo**

PHYS **478.** Enhanced sampling method with hybrid non-equilibrium molecular dynamics/Monte Carlo. **D. Suh**, C. Chipot, B. Roux

PHYS **479.** Novel approach to investigate the single molecule photophysics of bare CdSe quantum dots. **B. Mehlenbacher**, J.J. Peterson

PHYS **480.** Synthesis of iron series phosphate micro-nano-materials and their potential applications for electrochemical energy storage. **H. Xue**, Y. Yan, H. Pang

PHYS **481.** New inorganic pH indicator based on ferricyanide intercalated zinc-aluminum layered double hydroxide. **N.A. Ibrahim**, A. Chaparadza

PHYS **482.** Many-Body expansion combined with neural networks. **K. Yao**, J. Herr, J. Parkhill

PHYS **483.** Albumin based nanoparticles as a delivery vehicle for flavonoids and their anticancer activity. **P. Ghosh**, S. Dasgupta

PHYS **484.** Stability of bovine serum albumin solutions in presence of salts: A calorimetric and solubility study. T. Janc, V. Vlachy, **M. Luksic**

PHYS **485.** Noninvasive detection of aluminum sensitization using SHG. **A. Farnsworth**, S. Averett, K. Rellaford, S.D. Smith, J.E. Patterson

PHYS **486.** Feasibility of *in situ* magnetic resonance imaging of semi-industrial chemical reactors at milli-Tesla magnetic fields. **D. Barskiy**

PHYS **487.** Influence of pH on the photochromic reaction dynamics of phenylamine-substituted diarylethene derivatives. **S. Mahvidi**, C.J. Otolski, Y. Yokoyama, F. Nourmohammadian, C.G. Elles

PHYS **488.** Ultrafast energy relaxation dynamics and wave-packet motion in Pt(II) bimetallic complexes. P. Kim, S. Brown-Xu, A. Chakraborty, **F.N. Castellano**, **L.X. Chen**

PHYS **489.** Investigation on pyrolsis of jet propellant 8. **D. Belisario-Lara**, A.M. Mebel

PHYS **490.** Post-Marcus charge transfer dynamics via the generalized quantum master equation. **E. Mulvihill**, E. Geva, A. Schubert, X. Sun, A. Kananenka

PHYS **491.** Withdrawn.

PHYS **492.** Molecule-nanocrystal photon upconversion sensitized by CdSe/CdS core-shell nanocrystals. **Z. Huang**, M.L. Tang

PHYS **493.** Bath gas and pressure dependence of the anomalous isotopic composition of ozone. **A.H. Kazez**, K.A. Boering

PHYS **494.** Jet-cooled high resolution infrared spectroscopy of small van der Waals SF_6 clusters. **A. Turner**, Y. Berger, V. Boudon, L. Bruel, M. Gaveau, M. Mons, A. Potapov, P. Asselin

PHYS **495.** Withdrawn.

PHYS **496.** Ultrafast photophysics of plasmonic aluminum nanoparticles. **K. Smith**, Y. Cheng, E. Arinze, S. Thon, A.E. Bragg

PHYS **497.** Modeling of hydrodynamic interactions in biological systems. **M. Dlugosz**

PHYS **498.** Optimization of energy transfer in DNA-dye excitonic circuits. **W. Bricker**, J. Banal, R. Veneziano, K. Pan, M. Bathe

PHYS **499.** Theoretical investigation of vibrational frequency shifts as probes of charge transfer in organic systems. **K. Williams**, E. Geva

PHYS **500.** Theoretical study on photoluminescence properties of double salts of silver and gold complexes. **S. Chen**, B. Sun, A.H. Chang, I.J. Lin

PHYS **501.** Computations of the hyperpolarizability of nonlinear optical chromophores aggregates. **X.A. Sosa Vazquez**, J. Maat, C. Isborn

PHYS **502.** Surface-Enhanced Raman scattering analysis of DNA modifications in the presence of carboplatin. **N. Mirsaleh-Kohan**, S. Khan, M. Torres, M. Duplanty, P. Hall, M. Garrett

PHYS **503.** Water solubilization of $CuInS_2$/ZnS QDs and bioconjugation to fibroblast growth factor studied by FRET. **C. Robinson**, M. Mohale, A. Nguyen, C.D. Heyes

PHYS **504.** Nonradiative relaxation in real-time electronic dynamics OSCF2: Organolead triiodide perovskite. **T.S. Nguyen**, J. Parkhill

PHYS **505.** Characterization of α-hemolysin conformational changes with two-dimensional infrared spectroscopy. **C.T. Kuhs**, A.T. Krummel

PHYS **506.** Time resolved resonance Raman spectroscopic and laser flash photolysis studies on typical significant stocks-shifted large π system. **L. Song-Bo**, M. Li, Z. Ruixue, D.L. Phillips

PHYS **507.** Withdrawn.

PHYS **508.** Anomalies of ice Ih in second-order many-body perturbation theory. **M. Salim**, S. Hirata

PHYS **509.** Withdrawn.

PHYS **510.** Microwave spectroscopy of 3,3,3-trifluoro-2-(trifluoromethyl)propanoic acid-formic acid complex. J. Thomas, **M.J. Carrillo**, A. Serrato, W. Jaeger, Y. Xu, W. Lin

PHYS **511.** Ultrafast extreme-ultraviolet reflection spectroscopy of electro-phonon dynamics in Germanium. **C. Kaplan**, P. Kraus, L.J. Borja, M.W. Zuerch, H. Chang, M.F. Jager, S. Cushing, D.M. Neumark, S.R. Leone

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

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PHYS **512.** Photoionization cross sections of three propargylic fuels. **M. Winfough**, G. Meloni

PHYS **513.** Simulating the chemistry of ionizing radiation in solids. **C.N. Shingledecker**, E. Herbst

PHYS **514.** Synthesis and photophysical characterization of bipyridyl hybrid oligomers: Examining mixed furan-thiophene systems using spectroscopy and DFT methods. **A.E. Steen**, S. Nguyen, T.L. Ellington, G.S. Tschumper, D.L. Watkins, N. Hammer

PHYS **515.** Modeling protein organization in thylakoid membrane stacks via a lattice gas model. **A. Rosnik**, P. Geissler

PHYS **516.** Quantum control of Yukawa interaction at nucleus. **Q. Wang**

PHYS **517.** Withdrawn.

PHYS **518.** Structural trends and reactivity of first-row transition metal cation-acetylene complexes revealed by probing their C-H stretching fundamentals. **A.D. Brathwaite**, S.A. Ferguson, T.B. Ward, R.S. Walters, M.A. Duncan

PHYS **519.** Nonadiabatic dynamics of $C(^3P) + SiH_4$ reaction. **A.H. Chang**

PHYS **520.** Preferential solvation of iodide anion in aqueous binary liquid mixtures. **Y. Al Hussain**, B.H. Milosavljevic

PHYS **521.** Rotational spectroscopic and theoretical studies of the perfluorobutyric acid--formic acid complex. J. Thomas, **A. Serrato**, M.J. Carrillo, W. Lin, W. Jaeger, Y. Xu

PHYS **522.** Molecular geometry and conformation analysis of the monomer and monohydrate of 4,4,4-trifluorobutyric acid. **A. Treviño**, W. Lin

PHYS **523.** Spatially extended active site: How distal residues contribute to catalysis in human phosphoglucose isomerase. **S.C. Begay**, P.J. Beuning, M.J. Ondrechen

PHYS **524.** Electronic structure and RRKM calculations on the reaction $CH_3OH_2^+ + CH_3OH$. **M. Rosi**, S. Falcinelli, N. Balucani, N. Faginas-Lago, C. Ceccarelli, D. Skouteris

PHYS **525.** Photophysical characterization of free-base triphenylcorrole reduced and oxidized tautomers. **G.N. Calvillo**, **C. Reed**, F. Kohl, S. Klein, A. Loogman, S. Lupercio, E.A. Alemán

PHYS **526.** Enthalpy relaxation below T_g in low molecular weight poly(dimethylsiloxane). **D. Eason**, A.D. Schwab

PHYS **527.** Role of ion-specific effects in DNA/ionene complexation. M. Seru nik, B. Zener, **B. Hribar Lee**

PHYS **528.** Effects of the anion nature of cationic polymethine dyes on the spectral-luminescent and photovoltaic properties of polymer-based photoconductive composites. A.A. Ishchenko, G. Bulavko, **N. Barashkov**, **T. Sakhno**

PHYS **529.** Investigation of relationship between the rate of converting leuco form of Indigo Carmine in its colored form and oxygen permeability of polymer films. **N. Barashkov**, I. Irgibayeva, **T. Sakhno**

PHYS **530.** Novel approaches to the development of biosensor by using systems of formulation and analytical techniques. **G. Ren**, Y. Lo, E.J. Parish, **H. Honda**, T. Wei

PHYS **531.** Tuning the structure and photophysics of a fluorous phthalocyanine platform. **C.M. Drain**, C. Farley

PHYS **532.** Using isothermal titration calorimetry to investigate dicationic alkylammonium bromide Gemini surfactants. M.L. McKim, B.K. Rich, P. Okoroji-Ohabor, S.J. Bachofer, **R.D. Sheardy**

PHYS **533.** Linking pH, temperature, ionic strength and conformation for the DNA i-motif. **T. Nguyen**, C. Fraire, A. Fernandes, M. Choi, **R.D. Sheardy**

PHYS **534.** Uncertainty and sensitivity analysis of the Marcus electron transfer rate model. **E.J. Alvarado**, D.D. Mendez, E.J. Morales-Butler, M. Cruz-Aponte

PHYS **535.** Tensor structured coupled cluster method. **R. Schutski**, G.E. Scuseria

PHYS **536.** Evaluation of VLE data from the TraPPE Force Field. **B.L. Eggimann**

PHYS **537.** DNA mutation and fluorescent label effects in surface-bound 25mer microarrays: Molecular simulation of bright mismatches. B. Rivard, **J.M. Stubbs**

PHYS **538.** Photochemical activity of layered potassium niobate in the redox processes. V. Shvalagin, G. Grodzyuk, N. Andryushina, V. Granchak, M. Skoryk, **T. Sakhno**, **N. Barashkov**

PHYS **539.** Investigation of the mechanism of fullerene and carbon nanotube formation by molecular dynamics simulation. **B. Amofah**, T.J. Fuhrer

PHYS **540.** Quantum chemical studies of ether formation with peroxide reagents. **K.T. Kuwata**, T. Truttmann

PHYS **541.** Investigation of organic radicals and intermediates via high-resolution infrared spectroscopy. **M.D. Schuder**, A. Kortyna, D.J. Nesbitt

THURSDAY MORNING

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Effects of Nanoconfinement & Local Asymmetry on Dynamics & Chemistry: Interfaces

J. Dawlaty, *Organizer*

A. V. Benderskii, *Organizer, Presiding*

8:00 PHYS **542.** Sum frequency generation spectra from density functional theory. **V.S. Batista**

8:40 PHYS **543.** Measuring orientation heterogeneity of heterogeneous catalysts using HD 2D SFG spectroscopy. **W. Xiong**, Z. Li, J. Wang, Y. Li

9:00 PHYS **544.** Heterodyne-detected sum frequency generation spectroscopy of aqueous interfaces. **S. Yamaguchi**

9:40 Intermission.

10:00 PHYS **545.** Chiral water structures in biological systems. M. McDermott, H. Vanselous, S. Sanders, **P.B. Petersen**

10:40 PHYS **546.** Water bending vibration: A closer look at the flip-flop of water molecules at charged interfaces. **C. Dutta**, M. Mammetkuliyev, A.V. Benderskii

11:00 PHYS **547.** Probing the surfaces of CdSe quantum dots using sum frequency generation. **B.R. Watson**, B. Doughty, T.R. Calhoun

11:20 PHYS **548.** Vibrational sum-frequency scattering spectroscopy reveals the detailed surface chemistry of biomaterials in aqueous solutions. **P.K. Johansson**, L. Schmüser, Y. Wang, D.G. Castner

11:40 PHYS **549.** Understanding catalytic selectivity via the absolute molecular orientation of adsorbed interfacial molecules. **B. Doughty**, S. Goverapet Srinivasan, S. Bryantsev, D. Lee, H. Lee, D.R. Salahub, Y. Ma, D.A. Lutterman

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Exciton Photodynamics: Hard Materials

D. S. Larsen, M. Olivucci, *Organizers*

K. Glusac, *Organizer, Presiding*

8:00 PHYS **550.** Photoexcited carriers recombination and trapping in spherical vs faceted TiO2 nanoparticles. **C. Di Valentin**, G. Fazio, L. Ferrighi, D. Selli

8:30 PHYS **551.** Withdrawn.

8:50 PHYS **552.** Withdrawn.

9:20 PHYS **553.** Ultrafast transient absorption spectroscopy investigation of photoinduced dynamics in donor-acceptor core-shell nanostructures for organic photovoltaics. **J. Strain**, T.M. Abeywickrama, H.P. Rathnayake, J. Liu

9:40 Intermission.

10:00 PHYS **554.** Role of interfaces on hybrid perovskite photocarrier dynamics. **D.S. Ginger**

10:30 PHYS **555.** Bulk carrier dynamics in nanocrystalline organo-halide perovskites through surface passivation. R. Stewart, **J.B. Asbury**

11:00 PHYS **556.** Direct charge transfer at organic semiconductor/metal interfaces. **W. Xiong**, Y. Li, B. Xiang

11:20 PHYS **557.** Excitation dynamics in nanoscale materials for solar energy harvesting: Time-domain ab initio studies. **O.V. Prezhdo**

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Solutions to the Energy Problem

C. J. Murphy, *Organizer*

P. K. Jain, *Organizer, Presiding*

8:00 PHYS **558.** Aluminum plasmonics: From new chemistry to new applications. **N.J. Halas**

8:35 PHYS **559.** Imaging acoustic-to-plasmonic vibrational dynamics with ultrafast electron microscopy. **D.J. Flannigan**, V.E. Ferry, D.T. Valley

8:55 PHYS **560.** Shine down - cut the cord. T. Tumkur, X. Yang, W. Wang, B. Jiang, X. Zhang, Y. Wei, S. Bahauddin, H. Robatjazi, B. Cerjan, C. Doiron, X. Liu, P. Wray, L. Vayssieres, N.J. Halas, P.J. Nordlander, **I. Thomann**

9:30 PHYS **561.** Impact of dopant choice on the optical response and near-field enhancement of doped indium oxide nanocrystals. **R.W. Johns**, D.J. Milliron

9:50 Intermission.

10:05 PHYS **562.** Withdrawn.

10:40 PHYS **563.** Strong coupling of localised surface plasmons to light-harvesting complexes from bacteria and plants. A. Tsargorodska, M. Cartron, G. Kodali, L. Dutton, C. Hunter, P. Torma, **G.J. Leggett**

11:00 PHYS **564.** Device applications of metafilms. **M. Brongersma**

11:35 PHYS **565.** Gas phase catalytic cycle of hydrogen production from water using small Mo-oxide cluster anions. **M. Ray**, A. Saha, C. Jarrold, K. Raghavachari

Section F

Parc 55 San Francisco

Stockton

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Radiation Chemistry of Europa's Surface

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

L. M. Ziurys, *Presiding*

8:00 PHYS **566.** Coupled surface-atmosphere chemical production of oxidants in the solar system. **S.K. Atreya**

8:45 PHYS **567.** Carbon dioxide chemistry at low temperatures. **R. Hodyss**, S. Piao, M.L. Cable, M.J. Malaska

9:30 PHYS **568.** Primary phosphorus sources within extraterrestrial ices. **M.A. Pasek**

10:15 PHYS **569.** Investigating the formation of alkylphosphonic acids in phosphine ices. **A.M. Turner**, R. Kaiser

10:45 PHYS **570.** Synthesis of di-depsipeptides under possible solar system environments. **E.T. Parker**, J.G. Forsythe, F.M. Fernandez

11:15 PHYS **571.** Infrared matrix isolation spectroscopy of photochemical products of acetylene and nitrogen in argon matrices. **B.T. Genest**, P.D. Cooper

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

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THURSDAY AFTERNOON

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Solutions for Medicine

P. K. Jain, *Organizer*

C. J. Murphy, *Organizer, Presiding*

1:30 PHYS **572.** Photothermal therapy of cancer in cells and in different animals using gold nano-rods: A progress report. **M.A. El-Sayed**

2:05 PHYS **573.** Single-Molecule super-resolution study of distance-dependent plasmonic fluorescence enhancement and emission mislocalization. **B. Fu**, J.S. Biteen

2:25 PHYS **574.** Plasmonic biosensors for resource-limited settings. **S. Singamaneni**

3:00 PHYS **575.** Nonlinear and ultrafast spectroscopy of gold-silver-gold core-shell-shell nanoparticles. **L.H. Haber**, T.E. Karam, R.R. Kumal, H. Smith, R.A. Khoury, B. Kruger, J. Ranasinghe, Z. Zhang

3:20 Intermission.

3:35 PHYS **576.** Manipulating light-matter interactions in bioprogrammable crystals. **C.A. Mirkin**

4:10 PHYS **577.** Plasmonics at the cluster limit: Dielectric sensing with DNA-stabilized silver clusters. **S.M. Copp**, D. Schultz, S. Swasey, A. Faris, E. Gwinn

4:30 PHYS **578.** DNA-Encapsulated silver cluster chromophores. **J.T. Petty**, R. Dickson, T. Yeh

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Mechanisms & Molecular Simulations

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POLY

Division of Polymer Chemistry

C. Lipscomb, *T. White and T. Epps, Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Materials, Devices, and Switches (see *ORGN,* Tue, Wed, Thu)

Peptides, Proteins & Amino Acids (see *ORGN,* Tue, Wed)

Polymers under Deformation (see *PMSE,* Tue, Wed)

SOCIAL EVENTS:

Reception, 5:00 PM: Tue

Reception, 5:30 PM: Wed

Breakfast, 7:30 AM: Tue

Luncheon, 12:00 PM: Sun

SUNDAY MORNING

Section A

Moscone Center

120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

A. M. Alb, P. S. Majumdar, *Presiding*

8:00 POLY **1.** Design of experiments based approach to investigate the adhesion of latex paints over alkyd surfaces. **P.S. Majumdar**, J. Sweeney, C. Kozak, S.A. Carpenter, S. Eberly, W. Howell, L.C. Fioravanti, A.M. Piwowar

8:20 POLY **2.** Measurement and control of migrating species on water-borne coatings surfaces. **J. Bohling**, J. Gallagher, A. Gong, K. David, B. Cooper

8:40 POLY **3.** Mussel inspired coatings based on tannic acid and polyamines. **I. Yilgor**, E. Yilgor, C. Kosak

9:00 POLY **4.** Withdrawn.

9:20 POLY **5.** Macromolecular characterization of biopolymers as alternative depressants for iron ore flotation. **A.M. Alb**

9:40 POLY **6.** Shape memory polymers from amino acid-based poly(ester urea)s. **G.I. Peterson**, E.P. Childers, J. Yu, H. Li, A. Dobrynin, M. Becker

10:00 POLY **7.** Withdrawn.

10:20 POLY **8.** Effect of monomer sequence on the properties of hyperbranched copolymers. **Y. Shi**, H. Gao

10:40 POLY **9.** Synthesis and characterization of new high temperature multigraft copolymer superelastomer: Polyisoprene-graft-polybenzofulvene. **H. Wang**, W. Wang, W. Lu, X. Lu, N. Kang, J.W. Mays

11:00 POLY **10.** Tunable photonic nanocomposite film formed by gelation of self-assembled block copolymer. **Y. Huang**, Y. Zheng, J. Pribyl, B.C. Benicewicz

11:20 POLY **11.** Topology transformation of rotaxane-linked star/linear ABC terpolymer: Synthesis and characterization. **H. Sato**, D. Aoki, T. Takata

11:40 POLY **12.** Visualizing randomness: Synthesis and imaging of statistical and segmented colloidal copolymers. **N.G. Pavlopoulos**, J. Pyun

Section B

Moscone Center

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Next Generation Smart Materials

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Y. C. Simon, *Organizer*

E. B. Berda, J. Foster, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **13.** Antisense gene regulation with non-cationic polymer carriers. **K. Zhang**

8:35 POLY **14.** Sulfur-free RAFT, sequence-controlled methacrylic multiblockcopolymers via emulsion polymerization. **D.M. Haddleton**, A. Anastasaki, N. Engelis, V. Nikolaou, G. Nurumbetov

9:05 POLY **15.** Precision functional polyethylene-based polymers via acyclic Diene Metathesis (ADMET). **K.B. Wagener**, M.H. Bell, H. Li, T.W. Gaines

9:35 Intermission.

9:45 POLY **16.** One-pot synthesis of responsive polymers with highly branched structures. **H. Gao**, Y. Shi, X. Cao

10:15 POLY **17.** Shape memory in self-healing polymers: Synchronized physico-chemical events. Y. Yang, C.C. Hornat, **M.W. Urban**

10:45 POLY **18.** Host-guest chemistry to control polymeric architecture and conformation. **H.W. Gibson**, T. Price, H. Wessels, Z. Bear

Section C

Moscone Center

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Polymeric Materials for Performance & Sustainability

Biobased Polymers

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

J. M. McCollum, *Presiding*

8:00 Introductory Remarks.

8:10 POLY **19.** Molecular dynamics simulation of cellulose nanofibrils used to modify polymer gels. **Y. Sliozberg**, S. Coleman, H. Dong, J. Snyder, A. West, T. Chantawansri

8:40 POLY **20.** Mechanophore activation at the crosslinked epoxy-nanocellulose interface: Insight from density functional theory and molecular dynamics simulations. **K.S. Khare**, F.R. Phelan

9:10 POLY **21.** Ductile polyacrylonitrile fibers with high cellulose nanocrystals loading. **H. Chang**, J. Luo, H.c. Liu, A. Bakhtiary Davijani, P. Wang, G. Lolov, R. Dwyer, S. Kumar

9:30 Intermission.

9:45 POLY **22.** New and unexpected properties from polycyanurate networks prepared from bio-based monomers. **A.J. Guenthner**, B.G. Harvey, A.P. Chafin, M.C. Davis, J. Zavala, K. Lamison, J. Reams, M.D. Ford, K. Ghiassi, T.J. Groshens, J.M. Mabry

10:15 POLY **23.** Styrene-free soybean oil-based thermosets and their natural fiber composites. **W. Liu**, R. Qiu

10:35 POLY **24.** Synthesis and properties of new cross-linked bio-based aliphatic polycarbonates. **P. Durand**

10:55 POLY **25.** Transient networking in glucarodilactone-containing polyesters. **L.M. Lillie**, W.B. Tolman, T.M. Reineke

Section D

Moscone Center

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Separation of Macromolecules & Particulates

Cosponsored by ANYL, COLL and PMSE

Financially supported by PSS Polymer Standards Service GmbH, The Dow Chemical Company, Tosoh Bioscience LLC, Wyatt Technology

S. V. Orski, Y. Wang, *Organizers*

W. Gao, X. M. Liu, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **26.** Theoretical perspective on the separation mechanism of complex polymers by interaction chromatography. **Y. Wang**

8:45 POLY **27.** Polymer microstructure analysis by HPLC. **D. Lee**, S. Qiu, J. Munro, C. Li Pi Shan, T. Huang, R. Cong

9:15 POLY **28.** Separation and characterization of living and dead chains in polystyrene synthesized by ATRP. **T. Chang**

9:45 Intermission.

9:55 POLY **29.** Understanding of aqueous oligomers formed during emulsion polymerization and their interfacial behavior via LC-MS. **T. Zhang**, B. McCulloch, W. Gao, R. Even

10:25 POLY **30.** Copolymer structure elucidation by multidimensional techniques with focus on UPLC x ESI-TOF-MS. **J. Falkenhagen**

10:55 POLY **31.** Application of different chromatographic techniques to characterize chemical and molar mass heterogeneity in graft copolymers. R. Leinweber, P. Montag, J. Preis, **W. Radke**

11:25 POLY **32.** Large-scale separation and purification of block copolymers via selective and competitive adsorption on silica. **C.Y. Ryu**

Section E

Moscone Center

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Incorporating Polymer Science into the Classroom

Undergraduate Curriculum

Cosponsored by CHED, MPPG‡ and PMSE

K. A. Cavicchi, S. E. Morgan, *Organizers*, *Presiding*

8:00 POLY **33.** Green synthesis of renewable triblock polymers in the organic chemistry laboratory: Not your typical white solid. **J.E. Wissinger**

8:25 POLY **34.** Undergraduate polymer synthesis developed for lecture and laboratory experiments. **P.J. Costanzo**

8:50 POLY **35.** Integration of polymerization kinetics in polymer, physical chemistry, and chemical engineering courses. **A. Guymon**

9:15 Intermission.

9:30 POLY **36.** Polymer physical structure labs at Allegheny College. **R.M. Van Horn**

‡ *Cooperative Cosponsorship*