ORGN **596.** Rapid, protecting-group free route to acyl pyrrolidines using imines as substrates in the aza-Cope rearrangement—Mannich cyclization. **H.A. Lindsay**, A. Oudeif, J.M. Reder, B. Yambrosic

ORGN **597.** Synthesis of 2-indolinones through microwave-assisted intramolecular transamidation derived from a multicomponent coupling cascade process. **A. Maddirala**, P.R. Andreana

ORGN **598.** Ring opening chemistry of epoxides with new carbon nucleophiles for the synthesis of novel γ-lactones and γ-lactams. **A. Kumar**

ORGN **599.** Toward the miniaturization of chemical library synthesis to the sub-micromole scale using functionalized high loading magnetic nanoparticles. **P.C. Kearney**, P.K. Maity, S. Faisal, P.R. Hanson

ORGN **600.** Ligand-controlled, tunable silver-catalyzed C–H amination. **J.M. Alderson**, A.M. Phelps, R. Scamp, N.S. Dolan, J.M. Schomaker

ORGN **601.** Asymmetric β hydroxylation and amidation of enals via N heterocyclic carbene catalysis. **C. Hosier**, N.A. White, T. Rovis

ORGN **602.** Solid phase catalysts for the synthesis of α-aryl carboxylic acids. **W.E. Brenzovich**, A. Denton, R. Kohinke, B.R. Craig, D. Moore

ORGN **603.** Synthesis of N-heterocycles via transition metal-catalyzed C-H activation. **K.E. Ruhl**, T. Hyster, T. Rovis

ORGN **604.** New catalytic methods for N-heterocycle synthesis by late transition metal-mediated C-H bond activation. **P. Kilaru**, P. Zhao

ORGN **605.** Substituted 5,6,11,12-tetradehydrodibenzo[a,e] cyclooctenes: Syntheses, properties, and DFT studies of substituted Sondheimer diynes. **F. Xu**, A. Orita, J. Otera

PHYS

Division of Physical Chemistry

E.L. Sibert, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical and Pharmaceutical Research honoring David Case *(see COMP, Mon, Tue)*

Electronic Structure Methods for Highly Polarizable Systems *(see COMP, Sun, Mon)*

Computational Design, Discovery and Optimization of Organic Semiconductor Materials *(see COMP, Sun, Mon)*

Quantum Chemistry *(see COMP, Sun, Mon, Tue, Wed)*

Molecular Mechanics: Force Field Development *(see COMP, Mon)*

Computational Chemistry In The Undergraduate Curriculum: What Is Working And How Do We Assess It? *(see CHED, Wed)*

SUNDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

New Particle Formation and Growth

M. Freedman, *Organizer*
D. Cziczo, *Organizer, Presiding*
J. Pierce, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **1.** Aerosol nucleation and growth in the CLOUD experiment at CERN. **J. Curtius**

8:45 PHYS **2.** Contribution of human related sources to indoor volatile organic compounds. **S. Liu**, R. Li, R. Wild, J. Krechmer, S. Thompson, C. Warneke, J.A. de Gouw, S.S. Brown, S. Miller, J.L. Jimenez, P. Ziemann

9:05 PHYS **3.** Global climate impact of sulpher-plume chemistry and particle formation. **J. Pierce**, R. Stevens

9:30 Intermission.

9:45 PHYS **4.** Mechanisms of formation and growth of particles in air. **B.J. Finlayson Pitts**

10:50 PHYS **5.** Detection of low-volatility gas-phase organic compounds from the OH-initiated oxidation of isoprene hydroxyhydroperoxide and their relevance to organic aerosol production. **J. Krechmer**, M. Coggan, J.B. Nowak, J. Kimmel, H. Stark, P. Massoli, J.T. Jayne, J.D. Crounse, T.B. Nguyen, P. Wennberg, J.H. Seinfeld, D.R. Worsnop, J.L. Jimenez, M. Canagaratna

10:25 PHYS **6.** Nanoparticle growth by carbonaceous matter. **M.V. Johnston**

11:10 PHYS **7.** Interplay between secondary organic aerosol chemistry, phase state, and growth dynamics. **R.A. Zaveri**, J. Shilling, A. Zelenyuk-Imre, J. Liu, J. Wilson, A. Laskin, B. Wang, J. Fast, R. Easter, J. Wang, C. Kuang, J.A. Thornton, A. Setyan, Q. Zhang, T.B. Onasch, D.R. Worsnop

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Carbon Star Outflows

L. J. Allamandola, T. J. Lee, *Organizers*
J. Oomens, *Presiding*

8:00 PHYS **8.** Lifecycle of cosmic carbon. **A. Tielens**

8:35 PHYS **9.** Molecular content of carbon-rich evolved stars and the carbon balance from observations at all wavelengths. **P. Chernicharo**

9:10 PHYS **10.** Formation of complex organics and carbonaceous grains in the outflow of carbon stars: A laboratory study. **F. Salama**

9:45 Intermission.

10:15 PHYS **11.** Synthesis of pure and N-substituted cyclic hydrocarbons (e.g. pyrimidine) via gas-phase ion-molecule reactions. **P.P. Bera,** R. Peverati, M.P. Head-Gordon, T.J. Lee

10:50 PHYS **12.** Computational rovibrational spectroscopy and applications to astrochemistry. **R.C. Fortenberry**, X. Huang, W. Morgan, R.A. Theis, T. Crawford, T.J. Lee

11:15 PHYS **13.** Multiple excited states of PANH anions using informed orbital descriptions. **M.L. Theis**, A. Candian, A. Tielens, T.J. Lee, R.C. Fortenberry

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Accurate Energies for Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
M. S. Gordon, *Presiding*

8:00 PHYS **14.** Potential energy surfaces for dynamics calculations. **D.G. Truhlar**

8:30 PHYS **15.** Strategies towards dynamic and non-dynamic electron correlation. **A.K. Wilson**

9:00 PHYS **16.** Dissecting the effect of morphology on the rates of singlet fission: Insights from theory. **A. Krylov**

9:20 PHYS **17.** Aerobic oxidation of methanol to formic acid on Au_8^-: Benchmark analysis based on completely renormalized coupled-cluster and density functional theory calculations. **P. Piecuch,** J.A. Hansen, M. Ehara

9:40 Intermission.

10:00 PHYS **18.** Complications in potential energy surfaces for molecules involving second row elements. **T.H. Dunning**

10:30 PHYS **19.** Dynamics of curved carbon π systems. **K.K. Baldridge**

11:00 PHYS **20.** Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters. **R.Q. Topper**, J.J. Biswakarma, V. Ciocoi

11:20 PHYS **21.** Analysis of changes in bonding patterns along reaction paths in terms of molecule-intrinsic quasi-atomic orbitals. **K. Ruedenberg**, A.C. West, M.W. Schmidt, M.S. Gordon

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid β: Structures and Molecular Interactions

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
J. E. Shea, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **22.** High resolution insights on the membrane mediated amyloid aggregation. **A. Ramamoorthy**

8:45 PHYS **23.** Modulation of molecular interactions of Alzheimer's Aβ peptide fibrils and oligomers with lipid membranes. F. Tofoleanu, B. Brooks, **N. Buchete**

9:25 PHYS **24.** Interaction of A-beta with model lipid membranes. **P.S. Cremer**

9:45 Intermission.

10:05 PHYS **25.** Determining the structural ensemble of intrinsically disordered disease peptides: Applications to Alzheimer's disease biology in solution and membrane. **T.L. Head-Gordon**

10:45 PHYS **26.** Revealing the interplay between amyloid-β and membranes through molecular simulations. **B. Strodel**

11:25 PHYS **27.** Structural studies of the membrane disruption pathways induced by β-amyloid peptides in Alzheimer's disease. **W. Qiang**, R.D. Akinlolu, M. Nam, N. Shu, D. Delgado

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Advances in Simulation Methodology

Cosponsored by COMP

A. E. Garcia, *Organizer*
G. Hummer, *Organizer, Presiding*

8:00 PHYS **28.** Sense and nonsense when performing and interpreting molecular dynamics simulations of biomolecular systems. **W. van Gunsteren**

8:35 PHYS **29.** Potential function as a variable: Advances in using simulations of multiple states to solve hard biomolecular problems. **M.R. Shirts**

9:10 PHYS **30.** TRAM: Optimal estimation of trajectory data from multiple thermodynamic states. **F. Noe**

9:45 PHYS **31.** Exact milestoning. **R. Elber**

10:20 PHYS **32.** Fluorescent proteins as pH sensors: Insights from constant pH molecular dynamics. **E.N. Laricheva**, C.L. Brooks

10:55 PHYS **33.** Molecular multipole models for complex biomolecules. **T. Ichiye**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
H. Jaeger, *Presiding*

8:00 PHYS **34.** Photoinduced proton-coupled electron transfer in solution: Quantum mechanical/molecular mechanical nonadiabatic dynamics. **S. Hammes-Schiffer**

8:40 PHYS **35.** Energy transfer in closely packed Si quantum dots: The role of surface defects. **S.V. Kilina**

9:20 PHYS **36.** Cheap models for electronic transitions and their application to lead-halide perovskites. **J. Parkhill**

9:40 Intermission.

10:00 PHYS **37.** Modeling artificial and natural light harvesting systems with DFT. **E. Jakubikova**

10:40 PHYS **38.** Photodissociation dynamics of phenol. **X. Xu**, J. Zheng, K. Yang, D.G. Truhlar

11:20 PHYS **39.** Computational photochemistry of thioanisole. **S.L. Li**, D.G. Truhlar

11:40 PHYS **40.** Time-dependent density functional theory study of the excited state energy landscape of gold phosphine thiolate complexes. **E.B. Guidez**, C.M. Aikens

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, *Organizer*
S. Link, K. A. Willets, *Organizers, Presiding*

8:00 PHYS **41.** Ultrafast photoelectron imaging microscopy of plasmonic nanoparticles. **D.J. Nesbitt**

8:35 PHYS **42.** Tuning the acoustic frequency of a gold nanodisk through its adhesion layer. **W. Chang**, F. Wen, D. Chakraborty, M. Su, Y. Zhang, B. Shuang, P.J. Nordlander, J. Sader, N.J. Halas, S. Link

8:55 PHYS **43.** Coherent plasmonics for ultrasensitive and single molecule sensing. **N.J. Halas**

9:30 PHYS **44.** Probing ground-state single-electron self-exchange across a molecule-metal interface and molecule-substrate electronic coupling by simultaneous spectroscopic and topographic Near-field SERS Imaging. Y. Wang, P. Sevinc, Y. He, **H. Lu**

9:50 PHYS **45.** Using STEM/EELS to probe energy transfer in plasmon-enhanced solar devices. **J.P. Camden**

10:25 PHYS **46.** Use of electron microscopy to probe quantum plasmonics, hot electrons and energy transport in hybrid nanoparticle/semiconductor systems. **C. Cherqui**

10:45 PHYS **47.** Cathodoluminescence-activated nano-imaging by resonant energy transfer. **N.S. Ginsberg**, C.G. Bischak, C. Hetherington, Z. Wang, J. Precht, D. Kaz, C. Stachelrodt, D. Schlom

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Recent Advances in Computational Methods

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 PHYS **48.** Self-interaction correction to density-functional approximations with unitary invariance. **M.R. Pederson**

8:35 PHYS **49.** Toward rational design of small molecule adsorption in open-site metal-organic frameworks with density functional theory. **J. Neaton**

9:05 PHYS **50.** New density functionals obtained by a genome-scale search approach to functional design. N. Mardirossian, **M.P. Head-Gordon**

9:35 PHYS **51.** Mechanism of C–H bond activation of C_2H_6 by iron(IV)–oxo sites in magnesium-diluted Fe_2(dobdc). **P. Verma**, K.D. Vogiatzis, N. Planas, J. Borycz, D. Xiao, J.R. Long, L. Gagliardi, D.G. Truhlar

‡ *Cooperative Cosponsorship*

9:55 Intermission.

10:15 PHYS **52.** Enantioselective adsorption in zeolites and metal-organic frameworks. R. Bueno-Perez, A. Martín-Calvo, P. Gómez-Alvarez, J. Gutiérrez-Sevillano, P. Merkling, T. Vlugt, T. van Erp, D. Dubbeldam, **S. Calero**

10:45 PHYS **53.** New computational tools for modeling metal-organic frameworks. **F. Paesani**

11:15 PHYS **54.** Computational materials design of co-polymers for organic electronics. **R.E. Larsen**, T.W. Kemper, S. Sides, P. Graf, D.C. Olson

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Dynamics

Sponsored by COMP, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Ice Nucleation

M. Freedman, *Organizer*
D. Cziczo, *Organizer, Presiding*
J. Lu, *Presiding*

1:30 PHYS **59.** Nucleation of ice: A molecular perspective. **V. Molinero**

2:10 PHYS **60.** Homogeneous freezing of single submicron to micron-sized water and hydrocarbon aerosol droplets levitated in a Bessel beam trap. **J.W. Lu**, M. Isenor, R. Signorell

2:30 PHYS **61.** Ice formation in ultracold cirrus. **E. Moyer**, K. Lamb, B. Clouser, L. Sarkozy, M. Bolot, O. Moehler, H. Saathoff, V. Ebert

2:55 PHYS **62.** Ice nucleation in clouds: Sensitivities to physicochemical IN properties and cloud microphysics. **B. Ervens**, G. Feingold

3:20 Intermission.

3:35 PHYS **63.** Atmospheric ice nucleating particles from the sea surface microlayer. **B. Murray**, T.W. Wilson, L. Ladino, P. Alpert, M. Breckels, I. Brooks, J.A. Huffman, C. Judd, W.P. Kilthau, R. Mason, G. McFiggans, L. Miller, J. Najera, E. Polishchuk, S. Rae, S. Corinne, M. Si, T. Whale, J. Wong, O. Wurl, J. Yakobi, J.P. Abbatt, J.Y. Aller, A.K. Bertram, D.A. Knopf

4:15 PHYS **64.** Contact-induced efflorescence of amorphous inorganic microparticles. **R.D. Davis**, S. Lance, J.A. Gordon, S.B. Ushijima, M. Tolbert

4:35 PHYS **65.** Studies of the abundance and compositions of organic ice nucleating particles in the atmosphere. **P.J. DeMott**, T.C. Hill, C.S. McCluskey, E.J. Levin, K.J. Suski, O. Laskina, Y. Tobo, D.B. Collins, C. Sultana, C. Lee, G. Cornwell, H. Al-Mashat, M. Santander, C.M. Beall, F. Malfatti, R. Mason, D. Pham, N.G. Swoboda-Colberg, V.H. Grassian, R. Moffet, A.K. Bertram, K.A. Prather, S. Kreidenweis

5:00 PHYS **66.** Atmospheric ice nucleation: Microspectroscopic imaging and characterization of individually identified ice nucleating particles. **D.A. Knopf**, P. Alpert, B. Wang, W.P. Kilthau, D. Bothe, R.E. O'Brien, S.T. Kelly, A. Laskin, M.K. Gilles, J.Y. Aller

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Carbon Star Outflows

L. J. Allamandola, T. J. Lee, *Organizers*
F. Salama, *Presiding*

1:30 PHYS **67.** Observations of organic molecules in carbon-rich proto-planetary nebulae and planetary nebulae. **E. Peeters**

2:05 PHYS **68.** Dust formation in carbon stars. **I. Cherchneff**

2:40 PHYS **69.** Ion chemistry of cyclic aromatics and interactions with polar molecules leading to the formation of complex organics in the gas phase and on ice grains. **M. El-Shall**

3:15 Intermission.

3:45 PHYS **70.** Laboratory infrared spectroscopy of 'hard-to-get' ionized polyaromatics. **J. Oomens**

4:20 PHYS **71.** Carbonaceous dust and fullerenes in evolved stars. **J. Cami**

4:45 PHYS **72.** Quantum chemical studies of interstellar organic molecules: Formation mechanisms, spectroscopic signatures, and properties. **T.J. Lee**

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Gas-Phase Kinetics and Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
G. C. Schatz, *Presiding*

1:30 PHYS **73.** Mode-, bond- and stereo-selective bimolecular reactions. **K. Liu**

2:00 PHYS **74.** Sudden vector projection model: Mode specificity and bond selectivity made easy. **H. Guo**

2:30 PHYS **75.** Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering. **D. Babikov**

2:50 PHYS **76.** Sum over histories representation for chemical kinetics. **R.T. Skodje**

3:10 Intermission.

3:30 PHYS **77.** Resonances in chemical reactions. **X. Yang**

4:00 PHYS **78.** Reaction dynamics on ab initio potential energy surfaces. **J.M. Bowman**, Y. Wang, Z. Homayoon, R. Conte, P. Houston

4:30 PHYS **79.** Improved semiclassical tunneling. **A.F. Wagner**

4:50 PHYS **80.** Alkyl CH stretch vibrations as a probe local environment. **E.L. Sibert**, D.P. Tabor, N. Kidwell, J.C. Dean, T.S. Zwier

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid Precursor Protein, Origin of Amyloid β

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
M. T. Zanni, *Presiding*

1:30 PHYS **81.** Structure, dimerization, and cholesterol binding of the amyloid precursor protein transmembrane C99 domain and amyloidogenesis. **C.R. Sanders**

2:10 PHYS **82.** Impact of membrane composition on the structure, stability, and processing of the transmembrane domain of the amyloid precursor p. **L. Dominguez**, L. Foster, J.E. Straub, D. Thirumalai

2:50 PHYS **83.** Conformational changes induced by the A21G Flemish mutation in the amyloid precursor protein lead to increased Aβ secretion in Alzheimer's disease. **T. Tang**, Y. Hu, P. Kienlen-Campard, L. El Haylani, M. Decock, J. Van Hees, Z. Fu, J. Ocatve, S. Constantinescu, S.O. Smith

3:10 Intermission.

3:30 PHYS **84.** Titration of charged residues in the context of membrane bilayers; A constant pH molecular dynamics study. **A. Panahi**, C.L. Brooks

3:50 PHYS **85.** Dimerization of a transmembrane peptide from amyloid precursor protein. **S. Meredith**

4:30 PHYS **86.** Multiscale molecular dynamics simulations of transmembrane structures of amyloid precursor protein in biological membrane. **Y. Sugita**

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Classical and Quantum Descriptions of Protein Function

Cosponsored by COMP

G. Hummer, *Organizer*
A. E. Garcia, *Organizer, Presiding*

1:30 PHYS **87.** Proton-coupled electron transfer in soybean lipoxygenase: Hydrogen tunneling and conformational motions. **S. Hammes-Schiffer**

2:05 PHYS **88.** Activation mechanisms in RAF kinase dimers. **E. Rosta**

2:40 PHYS **89.** Ab initio QM/MM simulations point to an alternative mechanism for the AlkB catalyzed repair of 1-methyl adenine. D. Fang, **G.A. Cisneros**

3:15 PHYS **90.** Exploring water penetration in soluble proteins and ion pumps. **Q. Cui**

3:50 PHYS **91.** Withdrawn.

4:25 PHYS **92.** Theoretical analysis and modeling of rhodopsin's unusual kinetics of thermal reactions and its role in dim-light vision. Y. Guo, S. Sekharan, J. Liu, V.S. Batista, J.C. Tully, **E.C. Yan**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
S. W. Kilina, *Presiding*

1:30 PHYS **93.** Quantum simulation of coherent exciton dynamics in conjugated systems. **P.J. Rossky**

2:10 PHYS **94.** Electronic excitation of metal-organic frameworks. **H. Jaeger**

2:50 PHYS **95.** Auger relaxation of hot electrons in CdSe quantum dots using GFSH. **D. Trivedi**, L. Wang, O. Prezhdo

3:10 PHYS **96.** Nonlinear optical structural properties of room-temperature ionic liquids, calculated with the combined fragment molecular orbital and linear-response time-dependent density functional theory method (FMO/LR-TDDFT). **A.D. Findlater**, F. Zahariev, M.S. Gordon

3:30 Intermission.

3:50 PHYS **97.** Evolution of photoexcited states in extended molecular chromophores. **S. Tretiak**

4:30 PHYS **98.** Excited state dynamics at metal to semiconductor interfaces. **D. Kilin**

5:10 PHYS **99.** Excited states in large molecular systems by the combined quantum Monte Carlo/effective fragment molecular orbital method. **F. Zahariev**, A.D. Findlater, M.S. Gordon

5:30 PHYS **100.** Electronic structure study of CIGS solar cells by X-ray absorption spectroscopy: Experiment and theory. **C.P. Schwartz**, D. Nordlund, T. weng, K. Ramanathan, D. Sokaras, D. Prendergast, S. Christensen

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, D. J. Masiello, *Organizers*
K. A. Willets, *Organizer, Presiding*
J. P. Camden, *Presiding*

1:30 PHYS **101.** Quantum and molecular plasmonics. **P.J. Nordlander**

2:05 PHYS **102.** Single photon interactions with localized surface plasmons: Exploiting fano resonances to generate quantum beats. **N. Thakkar**, C. Cherqui, D.J. Masiello

2:25 PHYS **103.** Understanding heterogeneity in plasmonic metal oxide nanocrystals. **D.J. Milliron**, R. Johns, A. Agrawal, S.D. Lounis, D. Nordlund, H. Bechtel

3:00 PHYS **104.** Mid-infrared surface phonon polaritons in dolar Dielectrics: An alternative approach. **A.J. Giles**, J. Caldwell

3:20 PHYS **105.** Life and times of plasmonically-generated energetic electrons. **M. Moskovits**

3:55 PHYS **106.** Characterizing the generation of hot electrons by metal nanoparticles through their interaction with molecular-type electron acceptors. **A. Hoggard**, B. Foerster, D. Huang, W. Chang, S. Link

4:15 PHYS **107.** Towards nanophotonic and time-resolved spectroscopy of plasmonic systems. **I. Thomann**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Gas Separation & Gas Storage: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 PHYS **55.** Accurate first-principles force fields for high-throughput screening of gas uptake in metal-organic frameworks. J.G. McDaniel, S. Li, E. Tyllianakis, R. Snurr, **J.R. Schmidt**

2:00 PHYS **56.** First principles simulations in the study of metal-organic frameworks: From stability to activity. **N. Lopez**

2:30 PHYS **57.** Metal organic framework based catalyst for release of chemically stored nitric oxide. **R. Kumar**

3:00 PHYS **58.** Top-down generation and screening of metal-organic frameworks for gas storage and separation applications. D. Gomez-Gualdron, Y.J. Colon, Y. Chung, **R. Snurr**

3:30 Intermission.

3:50 PHYS **108.** Ab initio simulation of adsorption isotherms for gases and gas mixtures in porous media. **J. Sauer**

4:20 PHYS **109.** 2D crystalline zeolites, non-aluminosilicate molecular sieves, and metal organic frameworks. **M. Tsapatsis**

4:50 PHYS **110.** Developing a predictive, descriptor based approach for CO and NO adsorption to Fe, Co, Ni and Cu sites in zeolites. **F. Goeltl**, P. Mueller, I. Hermans, P. Sautet

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Embedding: QM/QM and QM/MM

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Methodology

Sponsored by COMP, Cosponsored by PHYS

MONDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Water & Organic Aerosol

D. Cziczo, M. Freedman, *Organizers*
R. Washenfelder, Q. Zhang, *Presiding*

8:00 PHYS **111.** Hydration state of methylglyoxal at the air-water interface. G.L. Richmond, **S. Wren**, B.P. Gordon, N. Valley, L. McWilliams

8:40 PHYS **112.** Direct and quantitative measurement of the surface tension of airborne microdroplets. **B.R. Bzdek**, R.M. Power, J.P. Reid

9:00 PHYS **113.** Calculated equilibrium constants for formation of peroxy radical/water complexes to elucidate radical inititated particle formation. **R.B. Shirts**, S. Kumbhani, E. Burrell, J.C. Hansen

9:20 Intermission.

9:35 PHYS **114.** Liquid/vapor interface of aqueous solutions relevant to tropospheric chemistry. **J.C. Hemminger**

10:15 PHYS **115.** Single scattering albedo studies of brown carbon formation in evaporating droplets. **M. Zauscher**, M.A. Symons, D.O. Dehaan

10:35 PHYS **116.** Air-water interface: As Influenced by ions, lipids, and electric fields. **H.C. Allen**

11:00 PHYS **117.** Redistribution of black carbon in aerosol particles undergoing liquid-liquid phase separation. **S. Brunamonti, U. Krieger, C. Marcolli**, T. Peter

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in the Diffuse Interstellar Medium

L. J. Allamandola, T. J. Lee, *Organizers*
J. Cami, *Presiding*

8:00 PHYS **118.** Carbon bearing molecules in interstellar clouds. **J. Krelowski**

8:35 PHYS **119.** Molecular laboratory astrophysics: About molecular transients and molecule formation under interstellar conditions. **H. Linnartz**

9:10 PHYS **120.** Carbon in the galaxy. **E. Roueff**

9:45 Intermission.

10:15 PHYS **121.** Low temperature formaton of polycyclic aromatic hydrocarbons in the Interstellar medium via bimolecular neutral-neutral reactions. **R. Kaiser**

10:50 PHYS **122.** Angle-resolved PEPICO imaging of the dissociative ionization of methyl azide and methylenimine using a tabletop high harmonic generation light source. W.K. Peters, **D.E. Couch**, C.W. Hogle, D. Beltran, P. Towstik, D.M. Jonas, H. Kapteyn, M.M. Murnane

11:15 PHYS **123.** Electronic excited states of interstellar species: Quantum chemical prediction of spectroscopic signatures using quartic force fields. **W.J. Morgan,** R.C. Fortenberry

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Enzyme Kinetics and Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
S. Hammes-Schiffer, *Presiding*

8:00 PHYS **124.** Tunneling and the role of barrier width in enzymatic C-H activation. **J.P. Klinman**

8:30 PHYS **125.** Theoretical studies of enzymatic reactions. **W. Thiel**

9:00 PHYS **126.** Role of dynamics in enzyme catalysis: Challenges in comparing calculations to measurements. **A. Kohen**

9:20 PHYS **127.** Quantum mechanical/molecular mechanical simulations of the hydride transfer reactions in quinone reductase 2. C.R. Reinhardt, **S. Bhattacharyay**

9:40 Intermission.

10:00 PHYS **128.** QM/MM excited state dynamics of complex systems. **U. Roethlisberger**

10:30 PHYS **129.** Understanding metalloenzyme catalysis with QM/MM free energy simulations. **Q. Cui**

11:00 PHYS **130.** Adaptive-partitioning QM/MM dynamics simulations of proton transfer. S. Pezeshki, **H. Lin**

11:20 PHYS **131.** Functional mode electron transfer theory. **H. Chen**

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

α-Synuclein, the Parkinson's Protein

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
G. L. Millhauser, *Presiding*

8:00 PHYS **132.** Structure of the toxic core of α-synuclein, the amyloid associated with Parkinson's disease. **D. Eisenberg**, J.A. Rodriguez, M. Ivanova, M. Sawaya, D. Cascio, F. Reyes, D. Shi, E. Guenther, L. Johnson, J. Hattne, S. Sangwan, B. Nannega, A. Brewster, M. Messerschmidt, S. Boutet, N. Sauter, T. Gonen

8:40 PHYS **133.** NMR approaches to uncovering the molecular basis of inhibition of alpha-synuclein aggregation by beta synuclein. **J. Baum**, M. Janowska, G. Moriarty, M. Olson, N. Sikka

9:20 PHYS **134.** Examining the folding landscape of α-synuclein using time-resolved FRET. **S.K. Hess**, J.C. Lee

9:40 Intermission.

10:00 PHYS **135.** Misfolding and membrane interaction of amyloidogenic proteins. **R. Langen**

10:40 PHYS **136.** Aggregation mechanism of amyloidogenic proteins involved in neurodegenerative disorders. **C. Stultz**

11:20 PHYS **137.** Amyloidogenic proteins A-beta, alpha-synuclein and Tau interact with and disrupt membranes via different mechanisms and exhibit cell-type dependent toxicity. **H. Lashuel**

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Membrane Proteins

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
E. Tajkhorshid, *Presiding*

8:00 PHYS **138.** Large-scale computer simulations of lipids: Coarse-grained simulations of complex mixed bilayers. **D.P. Tieleman**

8:35 PHYS **139.** Membrane proteins: From structure refinement and remodeling to functional mechanisms. **H. Zhou**

9:10 PHYS **140.** Specific protein-lipid interactions stabilize an active state of the beta 2 adrenergic receptor. **C. Neale**, H.D. Herce, R. Pomès, A.E. Garcia

9:45 PHYS **141.** Dynamics of dopamine transporter: Molecular simulations and comparison with LeuT dynamics. M.H. Cheng, **I. Bahar**

10:20 PHYS **142.** Channel rhodopsin: Structure vs. function relationships from molecular dynamics simulations. S.W. Rick, **M. VanGordon**, S.L. Rempe

10:55 PHYS **143.** Assembly and mechanistic details of drug translocation in MexAB-OprM efflux pump. C.A. Lopez, J. Phillips, B. Alexandrov, **G. Gnanakaran**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Excited States in Biology

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
L. V. Slipchenko, *Presiding*

8:00 PHYS **144.** Excitonic states in natural light-harvesting systems. **B. Mennucci**

8:40 PHYS **145.** Electronic progression during the photoisomerization of microbial and vertebrate light-sensing rhodopsins. H. Luk, S. Gozem, F. Melaccio, S. Rinaldi, **M. Olivucci**

9:20 PHYS **146.** Theoretical study of the electron transfer in DNA repair process of the cyclobutane pyrimidine dimer lesion. **L. Joubert-Doriol**, T. Domratcheva, M. Olivucci, A.F. Izmaylov

9:40 Intermission.

10:00 PHYS **147.** Insights into the role of excimers/exciplexes in the photophysics and photochemistry of DNA. **S. Matsika**

10:40 PHYS **148.** Excited-state electron transfer in fluorescent proteins. **A. Krylov**

11:20 PHYS **149.** Charge-transfer dynamics of light-harvesting systems in complex solvated environments. **B.M. Wong**, M. Oviedo

11:40 PHYS **150.** Spectroscopic properties of a cholesteric liquid glass platinum acetylide. **T.M. Cooper**, A.R. Burke, D.M. Krein, R.F. Ziolo, J.E. Haley, D.J. Stewart, S.L. Long, A.E. Bell

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
I. Thomann, *Presiding*

8:00 PHYS **151.** Shape and surface control of plasmonic particles. **C.J. Murphy**

8:35 PHYS **152.** Plasmonic properties of coupled gold nanostructures. C. Liow, A. Li, **S. Li**

8:55 PHYS **153.** Mechanisms of on-colloid nanoparticle growth. **J. Millstone**, P. Straney, L. Marbella

9:30 PHYS **154.** Probing G_{M3} and G_{M1} contents of HIV-1 and ebola virus-like particles through plasmon coupling microscopy. **A. Feizpour**, C. Silva, H. Akiyama, C.M. Miller, S. Gummuluru, B.M. Reinhard

9:50 PHYS **155.** Surface plasmon polaritons in chemically synthesized nanostructures. **G.V. Hartland**, P. Johns, M. Devadas, K. Yu

10:25 PHYS **156.** Understanding the STEM/EELS magneto-optical responses of aromatic plasmon-supporting metal oligomers. **N. Bigelow**, C. Cherqui, A. Vaschillo, H. Goldwyn, D.J. Masiello

10:45 PHYS **157.** Plasmon/exciton and plasmon/photonic mode interaction. **G.C. Schatz**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

The Materials Genome and DataMining

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 PHYS **158.** Materials project for accelerated materials design. **K. Persson**

8:30 PHYS **159.** Predictive materials discovery: Finding optimal zeolites for challenging separations and chemical conversions. **J.I. Siepmann**, P. Bai, M. Jeon, L. Ren, C. Knight, M.W. Deem, M. Tsapatsis

9:00 PHYS **160.** Recent applications of databases of crystal structures and experimental data for metal-organic framework materials. **D. Sholl**, X. Nie, T. Duerinck, K. Walton, D. Nazarian, J. Camp

9:30 PHYS **161.** Computational screening of MOFs with open metal sites for adsorption and catalysis applications. **K.D. Vogiatzis**, E. Haldoupis, J.I. Siepmann, L. Gagliardi

9:50 Intermission.

10:10 PHYS **162.** Material informatics in discovery of nanoporous materials for energy applications. **M. Haranczyk**

10:40 PHYS **163.** Prediction of high deliverable capacity metal-organic frameworks with an evolutionary algorithm. Y. Bao, R. Martin, C. Simon, M. Haranczyk, B. Smit, **M.W. Deem**

11:10 PHYS **164.** Materials genome in action: Finding a nanoporous material for methane storage. **C. Simon**, J. Kim, D. Gomez-Gualdron, J. Camp, Y. Chung, R. Martin, R. Mercado, M.W. Deem, D. Gunter, M. Haranczyk, D. Sholl, R. Snurr, B. Smit

11:30 PHYS **165.** Cheminformatics-inspired approaches for big materials data. **O. Isayev**, D. Fourches, E. Muratov, A. Tropsha

Molecular Mechanics

Force Field Development

Sponsored by COMP, Cosponsored by PHYS

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Correlation Methods & DFT

Sponsored by COMP, Cosponsored by PHYS

MONDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Aqueous Chemistry

D. Cziczo, M. Freedman, *Organizers*
D. O. Dehaan, M. D. Zauscher, *Presiding*

1:30 PHYS **166.** Aqueous-phase and organic-phase photochemistry of atmospheric organic compounds. **S.A. Nizkorodov**

2:10 PHYS **167.** Laboratory and field studies of brown carbon aerosol in the near-ultraviolet spectral region. **R. Washenfelder**, J. Flores, G. Adler, C. Brock, J. Lee, J. Laskin, A. Laskin, S.A. Nizkorodov, L. Segev, S.S. Brown, Y. Rudich

‡ *Cooperative Cosponsorship*

2:30 PHYS **168.** Formation and photochemical evolution of phenolic SOA in aqueous phase. **Q. Zhang**, L. Yu, J.D. Smith, C. Anastasio, A. Laskin, J. Laskin

2:55 PHYS **169.** Cloud and fog processing of atmospheric organic matter. **J.L. Collett**, A. Boris, M. Schurman, Y. Desyaterik

3:20 Intermission.

3:35 PHYS **170.** Aerosol organics: Formation and processing in the aqueous phase. **V. McNeill**

4:15 PHYS **171.** Multiphase atmospheric chemistry of pyruvic acid. **V. Vaida**, A. Monod, J. Doussin, A.E. Reed Harris, E. Griffith, J.A. Kroll, R.J. Rapf

4:40 PHYS **172.** Aqueous-phase aldehyde photooxidation in the presence of ammonium salts, amines, and SO_2: brown carbon formation. **D.O. Dehaan**, N.G. Jimenez, P.D. Wickremasinghe, K.D. Sharp

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Interstellar Clouds

L. J. Allamandola, T. J. Lee, *Organizers*
H. Linnartz, *Presiding*

1:30 PHYS **173.** Review of the molecular complexity of organic material in the gas-phase ISM. **S.N. Milam**

2:05 PHYS **174.** Global optimization and broadband analysis software for interstellar chemistry. S.L. Widicus Weaver, **L. Zou**, M. Rad, J. Sanders

2:40 PHYS **175.** Molecular line lists of carbon-containing molecules for exoplanets and other hot bodies. **J. Tennyson**

3:15 Intermission.

3:45 PHYS **176.** Observations of carbon in interstellar and circumstellar ices. **A. Boogert**

4:20 PHYS **177.** Reliable abundances of extra-terrestrial hydrocarbon ices: Interminable quest or end in sight? **R.L. Hudson**, P.A. Gerakines

4:45 PHYS **178.** Optical properties of titan hazeaAnalogs using photoacoustic and cavity ring-down spectroscopy. **M.S. Ugelow**, K.J. Zarzana, M.A. Tolbert

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Catalysis

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
C. T. Campbell, *Presiding*

1:30 PHYS **179.** Silica thin films: From crystals to glass in 2D. **H. Freund**

2:00 PHYS **180.** Doped metal clusters on oxides: Rationalization and design through the prism of chemical bonding. **A. Alexandrova**

2:30 PHYS **181.** Some recent developments in saddle point finding methods: Gradient squared minimization, solid state transitions, and temperature accelerated adaptive kinetic Monte Carlo. **G.A. Henkelman**

3:00 PHYS **182.** Catalysis with metal clusters anchored at the Zr6-based metal-organic framework NU-1000. **L. Gagliardi**, D.G. Truhlar, C.J. Cramer, J. Borycz, L. Fernandez, S. Tussupbayev

3:20 Intermission.

3:40 PHYS **183.** New approaches to simulating biological and molecular catalysts. **T.F. Miller**

4:10 PHYS **184.** Organometallic and organocatalytic reactions explored using the automated reaction route mapping method. **K. Morokuma**

4:40 PHYS **185.** Hydrazine decomposition in the gas phase and on an Iridium catalyst. **M.W. Schmidt**, M.S. Gordon

5:00 PHYS **186.** Density functional theory study of lithium ion battery anode materials: Ruthenium (IV) oxide, tin (IV) oxide, and tin (IV) sulfide. **B.R. Ramachandran**, A.S. Hassan, K. Moyer, T. Dixon, C.D. Wick

Section D

Colorado Convention Center
Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Islet Amyloid Polypeptide (IAPP) at the Water/Lipid Interface

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*
T. L. Head-Gordon, *Presiding*

1:30 PHYS **187.** Islet amyloid polypeptide: Membrane interactions and cytotoxicity. **D.P. Raleigh**

2:10 PHYS **188.** Aggregation and Orientation of amyloid proteins at lipid/water interfaces probed by chiral sum frequency generation spectroscopy. L. Fu, Z. Wang, D. Xiao, V.S. Batista, **E.C. Yan**

2:50 PHYS **189.** β-Sheet intermediate dictates the fiber formation kinetics of amylin from type 2 diabetes. **M.T. Zanni**

3:30 Intermission.

3:50 PHYS **190.** Islet amyloid and the shared molecular origins of membrane poration and cytotoxicity. **A. Miranker**

4:30 PHYS **191.** Exploring the free energy and conformational landscape of amyloidogenic peptides upon aggregation and amyloid formation. **R. Winter**

5:10 PHYS **192.** Protein folding and assembly on membrane-mimics in constant volume replica-exchange simulations. **Z.A. Levine, R.G. Mullen, J.E. Shea**

5:30 PHYS **193.** Structure of insulin at the air/water interface: monomers or dimers? **S. Mauri, T. Weidner**, H. Arnolds

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Molecular Machines

Cosponsored by COMP

A. E. Garcia, *Organizer*
G. Hummer, *Organizer, Presiding*

1:30 PHYS **194.** Modeling the function of molecular motors and other challenging biological systems. **A. Warshel**

2:05 PHYS **195.** Energy barriers and driving forces in tRNA translocation through the ribosome. **K. Grubmueller**, L.V. Bock, G.F. Schroder, I.I. Davydov, M.V. Rodnina, H. Stark, A.C. Vaiana, N. Fischer, C. Blau

2:40 PHYS **196.** Simulating conformational changes of the ribosome. **K. Sanbonmatsu**

3:15 PHYS **197.** Unraveling the mystery of ATP hydrolysis in actin filaments. **G.A. Voth**

3:50 PHYS **198.** Specificity, mechanism, and membrane organization of ATP synthases. **J. Faraldo-Gomez**

4:25 PHYS **199.** Visualizing complex functional motions of membrane transporters using advanced simulation and free energy techniques. **E. Tajkhorshid**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Multiple Chromophores

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
A. F. Izmaylov, *Presiding*

1:30 PHYS **200.** Ab initio exciton model for nonadiabatic dynamics of multichromophoric systems on GPUs. A. Sisto, D.R. Glowacki, **T.J. Martinez**

2:10 PHYS **201.** New electronic structure methods for describing excited states in multichromophore and other large systems. **J.M. Herbert**, X. Zhang, A.F. Morrison

2:50 PHYS **202.** Charge transfer-like excitations in solution: A critical assessment of TDDFT/continuum models. **C.A. Guido**, D. Jacquemin, C. Adamo, B. Mennucci

3:10 PHYS **203.** Modeling protein - chromophore electrostatic interactions with multiple electronic states: Diabatic population matrix approach. J.W. Park, **Y.M. Rhee**

3:30 Intermission.

3:50 PHYS **204.** Vibronic interactions in bi- and multi-chromophores. **L.V. Slipchenko**

4:30 PHYS **205.** Accurate simulation of exciton dynamics for hundreds to tens of thousands of chromophores: Theoretical methods and acceleration by general-purpose graphics processing units (GPGPU). **A. Aspuru-Guzik**

5:10 PHYS **206.** Photoexcited energy transfer in a weakly coupled dimer. L. Alfonso Hernandez, **T. Nelson**, S. Tretiak, S. Fernandez-Alberti

5:30 PHYS **207.** Theoretical investigation of singlet fission in quinoidal bithiophenes. **A. Chien**, A. Molina, T.G. Goodson, P.M. Zimmerman

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
P. K. Jain, *Presiding*

1:30 PHYS **208.** Mechanistic study of serum albumin interaction with therapeutic nanoparticles. **C.F. Landes**, S. Dominguez-Medina, L. Kisley, S. Link

2:05 PHYS **209.** Biological targeting of plasmonic nanoparticles improves cellular imaging via the enhanced scattering in the aggregates formed. **M. Aioub**, B. Kang, M. Mackey, M.A. El-Sayed

2:25 PHYS **210.** Probing single metal-semiconductor heterostructures for visible light photocatalysis. **N. Fang**, B. Dong, F. Zhao

3:00 PHYS **211.** Triplet-state mediated super-resolution imaging of fluorescently-labeled gold nanorods. **K. Blythe**, K.A. Willets

3:20 PHYS **212.** Plasmon-enhanced fluorescent protein emission: A new paradigm for improved single-molecule bio-imaging. **J.S. Biteen**

3:55 PHYS **213.** Superstudies of plasmonically mediated emission: Beyond the Gaussian point-spread function. **E.J. Titus**, K.A. Willets

4:15 PHYS **214.** Energy conversion within a single nanocavity structure. **T.W. Odom**

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Gas Separation & Gas Storage: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 PHYS **215.** Experimental and theoretical approach to the study of CO_2 adsorption in an extensive family of metal-organic frameworks. **W.L. Queen**, E.D. Bloch, J.S. Lee, J.D. Howe, J.A. Mason, M.I. Gonzalez, M.R. Hudson, K. Lee, S.J. Teat, J. Neaton, B. Smit, J.R. Long, C.M. Brown

2:00 PHYS **216.** Engineering metal organic framework materials for optimum methane storage. **T. Yildirim**

2:30 PHYS **217.** Computational screening of MOFs for gas separations. **S. Keskin**

3:00 PHYS **218.** Parasitic energy: A potential building block for the prediction of CCS materials. **J. Huck**, L. Joos, R. Mercado, L. Lin, A. Berger, A. Bhown, K.U. Reuter, B. Smit

3:20 Intermission.

3:40 PHYS **221.** Small molecule adsorption in metal organic frameworks with open meal sites. **B. Vlaisavljevich**, R. Mercado, L. Lin, K. Lee, J. Huck, B. Smit

4:00 PHYS **220.** Robust metal-organic frameworks: rational design and gas storage. **D. Feng**, H. Zhou

4:30 PHYS **219.** Gas separations in metal-organic frameworks. T.M. McDonald, E.D. Bloch, Z.R. Herm, J.A. Mason, B.M. Wiers, M.T. Kapelewski, M.I. Gonzalez, J. Oktawiec, G. Barin, D. Gygi, W. Queen, **J.R. Long**

WCC Rising Stars Awards Symposium

Sponsored by WCC, Cosponsored by BIOT, COLL, GEOC, INOR, ORGN, PHYS, PMSE and PROF

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

Electronic Structure Methods for Highly Polarizable Systems

Excitons

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Methodology

Sponsored by COMP, Cosponsored by PHYS

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E.L. Sibert, Organizer

8:00 - 10:00

32, 43, 88, 113, 175, 196, 205, 212. See previous listings.

PHYS**222.** Discovery and Innovation of inorganic graphene analogs by computations. **Z. Chen**

286, 316, 324, 376, 405, 409, 463, 483, 519, 532, 557, 580. See subsequent listings.

TUESDAY MORNING

Section B

Colorado Convention Center
Room 607

PHYS Award Symposium

E. L. Sibert, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PHYS **223. Award Address** (Peter Debye Award in Physical Chemistry sponsored by E. I. du Pont de Nemours & Co.). Single molecule biophysical chemistry: Life at the single molecule level. **S. Xie**

8:35 PHYS **224. Award Address** (Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by ExxonMobil Research and Engineering). Dynamics of polar solvation. **M. Maroncelli**

9:05 PHYS **225. Award Address** (Francis P. Garvan–John M. Olin Medal sponsored by the Francis P. Garvan–John M. Olin Medal Endowment). Theoretical development and modeling across the periodic table: Toward accurate and inaccurate energetic prediction. **A.K. Wilson**

9:35 PHYS **226. Award Address** (ACS Award in Theoretical Chemistry sponsored by the ACS). Fragmentation: A route to accurate calculations on large molecular systems. **M.S. Gordon**

10:05 PHYS **227. Address Award** (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation). Bringing bioelectricity to light. **A.E. Cohen**

10:35 Intermission.

10:55 PHYS **228. Award Address** (Ahmed Zewail Award in Ultrafast Science and Technology sponsored by the Ahmed Zewail Endowment Fund established by Newport). Multidimensional electronic and vibrational spectroscopy of molecules using attosecond X-ray pulses and quantum light. **S. Mukamel**

11:25 PHYS **229. Award Address** (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). Mapping atomic motions with ultrabright electrons: The chemists' gedanken experiment enters the lab frame. **R. Miller**

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Organic Aerosol

D. Cziczo, M. Freedman, *Organizers*

N. Riemer, J. Surratt, *Presiding*

1:30 PHYS **230.** Sources, properties, aging, and anthropogenic influences on OA and SOA over the Southeast US and the Amazon during SOAS, DC3, SEAC4RS, and GoAmazon. **J.L. Jimenez**

2:10 PHYS **231.** Isoprene-derived SOA formation across mulitiple sites in the southeastern U.S.: Implications for air quality and human health. **J.D. Surratt, S. Budisulistiorini, W. Rattanavaraha,** Y. Lin, X. Li, M. Arashiro, A. Gold, Z. Zhang, S. Shaw, P. Croteau, M. Canagaratna, E. Knipping, S. Bairai, R.L. Tanner, M. Riva, T.P. Riedel, K. Chu

2:35 PHYS **232.** Gas-phase vs. aqueous-phase aging of secondary organic aerosol. **J.H. Kroll**, J. Hunter, K. Daumit, A.J. Carrasquillo

3:00 PHYS **233.** Influence of particle phase and viscosity on the heterogeneous OH-initiated oxidation of organic aerosol. **J.F. Davies**, K.R. Wilson

3:20 Intermission.

3:35 PHYS **234.** On the surface chemistry of secondary organic aerosol particles. **F. Geiger**

4:00 PHYS **235.** LIfetime of photosensizer triplet states in model troposheric aerosol. **E. Woods**, M. Barthold, J. Wan, M. Tigue

4:20 PHYS **236.** Organic aerosol composition and aging in the atmosphere: How to fit laboratory experiments, field data, and modeling together. **C.L. Heald**, Q. Chen

4:45 PHYS **237.** On the connection of organic aerosol ageing to viscosity. **F.A. Houle**, W. Hinsberg, K.R. Wilson

5:05 PHYS **238.** Oxidation flow reactors for the study of atmospheric chemistry systematically examined by modeling. **Z. Peng**, D.A. Day, A.M. Ortega, W. Hu, B.B. Palm, R. Li, K. Tsigaridis, J.A. de Gouw, W.H. Brune, J.L. Jimenez

Section B

Colorado Convention Center

Room 607

Ahmed Zewail Prize in Molecular Sciences

R. van Daalen, *Organizer*

D. C. Clary, *Presiding*

2:00 Introductory Remarks.

2:10 PHYS **239.** Chemical adventures using the unified principles of homogeneous and heterogeneous catalysis. **J.M. Thomas**

3:00 PHYS **240.** 4D electron microscopy: Developments and applications. **A.H. Zewail**

3:50 Intermission.

4:10 PHYS **241.** Catalytic chemistry: a subtle blend of voids and single sites. **M. Che**

4:45 PHYS **242.** Solution metallic catalysis on the nanoscale. **M.A. El-Sayed**

5:20 PHYS **243.** From single sites to nanostructured assemblies: Designing tools for high-precision chemical transformations. **T. Maschmeyer**

5:55 Concluding Remarks.

Section C

Colorado Convention Center

Room 503

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of O2

A. Co, D. A. Scherson, *Organizers*

J. M. Feliu, U. S. Ozkan, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS **244.** Bi adatoms at the surface of Pt single crystals. **J.M. Feliu**

2:15 PHYS **245.** Impurity effects on the oxygen reduction reaction (ORR). A. Jacob Jebaraj, N. Georgescu, **D. Scherson**

2:35 PHYS **246.** Effect of nitrogen functionalization on stability and performance of carbon-supported PtRu electrocatalysts in acid and alkaline media. **S. Pylypenko**, P. Joghee, K. Wood, A.R. Corpuz, J. Christ, G. Bender, R. O'Hayre

2:55 PHYS **247.** Galvanic displacement of Pt on nanoporous copper: An alternative synthetic route for obtaining robust and reliable oxygen reduction and alcohol oxidation catalysts. E. Coleman, H. Choi, K. Walz, **A. Co**

3:15 Intermission.

3:35 PHYS **248.** Tuning of perovskite oxides electrocatalytic activity for water oxidation and oxygen reduction. **K.J. Stevenson**, T. Mefford, W. Hardin, K.P. Johnston

4:15 PHYS **249.** Development of oxide-based materials for oxygen reduction and oxygen evolution reactions. **P.B. Atanassov**, A. Serov, I. Matanovic, A. Roy, N. Andersen

4:55 PHYS **250.** Theoretical investigation of water oxidation processes on small pure and Ca-doped MnO_x complexes. **K. Weerawardene**, C.M. Aikens

Section D

Colorado Convention Center

Room 504

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Prions and Beyond

Cosponsored by COLL and COMP

J. C. Lee, J. E. Straub, *Organizers*

D. P. Raleigh, *Presiding*

1:30 PHYS **251.** Surprising new structure for the cellular prion protein, and how this structure may influence membrane processes and prion disease. **G.L. Millhauser**

2:10 PHYS **252.** Influence of induced polarization on amyloid peptide misfolding in different solution environment. **J.A. Lemkul**

2:50 PHYS **253.** Role of cofactor molecules in encoding mammalian prion infectivity. **S. Supattapone**

3:30 Intermission.

3:50 PHYS **254.** Curli: Functional bacterial amyloid fibers. **C. Reichhardt**, D.M. Rice, J. Uang, L. Cegelski

4:10 PHYS **255.** Membrane microdomain composition may temporally modulate or determine protein function. H. Jang, A.L. Gillman, J. Lee, S. Ramachandran, F. Teran Arce, B. Kagan, R. Lal, **R. Nussinov**

4:50 PHYS **256.** What can theory and computations teach us about protein aggregation? **D. Thirumalai**

5:30 Closing Remarks.

Section F

Colorado Convention Center

Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*

K. A. Lopata, *Presiding*

1:30 PHYS **257.** Excited electronic states: Solvent effects and dynamics. **M.S. Gordon**, F. Zahariev, K. Keipert, Y. Harabuchi

2:10 PHYS **258.** Relativistic variational density functional theory of electronic excited states. **F.A. Evangelista**, W.D. Derricotte, P. Verma

2:50 PHYS **259.** Photoelectron spectra and photoelectron angular distributions from ab initio electronic structure methods. **S. Gozem**, A. Krylov

3:10 Intermission.

3:30 PHYS **260.** Potential energy surfaces for excited electronic states. **R. Dawes**

4:10 PHYS **261.** New developments in complete active space spin-flip methods for ground and excited states of large molecules with strong electron correlations. N. Mayhall, **M.P. Head-Gordon**

4:50 PHYS **262.** Time-resolved spectroscopy: A challenge for time-dependent density functional theory. **K. Luo**, J.I. Fuks, E. Sandoval, N. Maitra

5:10 PHYS **263.** Capturing geometric phase effects by mixed quantum-classical methods. **R. Gherib**, I.G. Ryabinkin, A.F. Izmaylov

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Sponsored by COMP, Cosponsored by PHYS

Quantum Chemistry

Applications

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING

Section A

Colorado Convention Center

Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Heterogeneous Chemistry, Sea Spray, Mineral Dust, and Black Carbon

D. Cziczo, M. Freedman, *Organizers*

J. G. Navea, E. Woods, *Presiding*

8:00 PHYS **264.** Water uptake and heterogeneous chemistry of model and authentic sea spray aerosol particles. **V.H. Grassian**

8:40 PHYS **265.** Transformations of nitrogen oxides at the troposphere-soil interface. **J.D. Raff**

9:05 PHYS **266.** Optical properties of mineral dust components and mixtures. **D. Veghte**, J. Moore, L. Jensen, M. Freedman

9:25 Intermission.

9:40 PHYS **267.** Determination of near UV absorption crossSections of surface-adsorbed H_2O and heterogeneous nucleation of H_2O on fused silica surfaces. **L. Zhu**

10:00 PHYS **268.** From the particle scale to the global scale: Quantifying black carbon climate impacts using a stochastic particle-resolved model. **N. Riemer**

10:25 PHYS **269.** Comparative photochemistry of nitric acid chemisorbed on different components of tropospheric particulate matter. **J.G. Navea**

10:45 PHYS **270.** Probing the impacts of aerosol sources on cloud microphysics and precipitation through in situ measurements of aerosol chemical mixing state. **K.A. Prather**

Section B

Colorado Convention Center

Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Interstellar Clouds

L. J. Allamandola, T. J. Lee, *Organizers*

S. N. Milam, *Presiding*

8:00 PHYS **271.** Organic molecules in ices and their release Into the gas phase. **E. Fayolle**, K. Oberg, R.T. Garrod, E.F. van Dishoeck, M. Rajappan, M. Bertin, C. Romanzin, J. Fillion

8:35 PHYS **272.** Ice chemistry in interstellar dense molecular clouds, protostellar disks, and comet. **S.A. Sandford**

9:10 PHYS **273.** Like a fly and the fire — polycyclic aromatic hydrocarbons (PAHs) in icy environments: A historical perspective. **M.S. Gudipati**

9:45 Intermission.

10:15 PHYS **274.** Theoretical studies of interstellar ice chemistry involving polycyclic aromatic hydrocarbons and other compounds. **D.E. Woon**

10:50 PHYS **275.** Formation of aromatic heterocycles from the UV-photoirradiation of aromatic hydrocarbons in ices. **C.K. Materese**, M. Nuevo, S.A. Sandford

11:15 PHYS **276.** Infrared spectroscopic properties of polycyclic aromatic nitrogen heterocycles (PANHs): The acridine series. **A.L. Mattioda**, J. Bregman, C. Bauschlicher, A. Ricca, D. Hudgins, L.J. Allamandola

Section C

Colorado Convention Center

Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Properties and Processes in Solvated Systems

Cosponsored by COMP

J. Gao, B. C. Garrett, *Organizers*

B. Mennucci, *Organizer, Presiding*

8:00 PHYS **277.** 25 years of SM*x* models: Quantum and classical continuum solvation. **C.J. Cramer**, D.G. Truhlar

8:30 PHYS **278.** Protein aggregation, collapse, and disorder: Model systems. **B.M. Pettitt**, D. Karandur

9:00 PHYS **279.** BioEFP: Effective fragment potential method for biological systems. **L.V. Slipchenko**

9:20 PHYS **280.** Role of solvent structure on the rate of ion-pairing. **M.D. Baer,** C.J. Mundy, G.K. Schenter

9:40 Intermission.

10:00 PHYS **281.** Quantum-classical path integral: A rigorous methodology. **N. Makri**

10:30 PHYS **282.** Structure, properties, excited states and reactivity of complex systems in solution: Putting together the pieces. **G. Scalmani**, M.J. Frisch

‡ *Cooperative Cosponsorship*

11:00 PHYS **283.** How reliable are calculations of absorption spectra of solvated molecules with CC theory and PCM? **M. Caricato**

11:20 PHYS **284.** Continuum solvation calculations of solvatochromic shifts: Recent advances and perspectives. **A.V. Marenich**, C.J. Cramer, D.G. Truhlar, G. Scalmani, M.J. Frisch

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrochemical Formation of Semiconductors

D. A. Scherson, *Organizer*
A. Co, *Organizer, Presiding*
S. Maldonado, *Presiding*

8:00 PHYS **285.** Investigations into the electrochemical formation of germanene. **J.L. Stickney**, M. Ledina, J. Jung

8:40 PHYS **286.** Electrocatalytic crystallization of covalent inorganic semiconductors. **S. Maldonado**

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of H2O and H2

A. Co, *Organizer*
D. A. Scherson, *Organizer, Presiding*
S. Maldonado, *Presiding*

10:00 PHYS **287.** Withdrawn.

10:40 PHYS **288.** Graphene oxide-promoted hydrogen and oxygen evolution. **N. Wu**

11:00 PHYS **289.** Electrocatalytic hydrogen production performed by model protein scaffolds. **H.S. Shafaat**, J.W. Slater, A.C. Manesis, S.L. Cirino, H.A. Monaco

11:20 PHYS **290.** Electrocatalytic water oxidation by iminium ions. **K. Glusac**

11:40 PHYS **291.** Electrocatalytic water oxidation on model cobalt oxide dimer and cubane complexes. **A. Fernando**, C.M. Aikens

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Modeling of Macromolecular Structure and Function

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*
M. Chu-Moyer, *Presiding*

8:00 PHYS **292.** Integrative structural biology. **A. Sali**

8:35 PHYS **293.** Unveiling the function of macromolecular assemblies using integrative dynamic modeling. **M. Dal Peraro**

9:10 PHYS **294.** Introducing molecular flexibility in Monte Carlo simulations of many-protein systems. V. Prytkova, M. Heyden, J.A. Freites, **D.J. Tobias**

9:45 PHYS **295.** Building toy models of proteins using co-evolutionary information. **R.R. Cheng**, M. Raghunathan, J.N. Onuchic

10:20 PHYS **296.** Atomistic and coarse-grained simulations of histones, Nuclesomes and DNA. **G. Papoian**, D. Winogradoff, H. Zhao, I. Echeverria, Y. Dalal

10:55 PHYS **297.** Relative resolution: A hybrid strategy for molecular modeling. **A. Chaimovich**, K. Kremer, C. Peter

11:30 PHYS **298.** Beyond Hofmeister: Interactions between ions and proteins in water. **P. Jungwirth**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*
F. A. Evangelista, *Presiding*

8:00 PHYS **299.** Understanding photochemistry and photoelectron spectra with highly correlated electronic structure methods based on coupled-cluster theory. **P. Piecuch**, J.A. Hansen, N.P. Bauman

8:40 PHYS **300.** Electronic structure methods for high-energy excited states. **X. Li, P. Lestrange**, D.B. Williams-Young, J.J. Goings

9:20 PHYS **301.** Linear response time-dependent complex generalized Hartree-Fock for frustrated spin systems. **J.J. Goings**, D.B. Williams-Young, F. Ding, M.J. Frisch, X. Li

9:40 PHYS **302.** Graphical processing unit acceleration of "two-step" complete active space configuration interaction (CASCI) methods. **B. Fales**, B. Levine

10:00 Intermission.

10:20 PHYS **303.** Above-ionization excited states with non-Hermitian time-dependent density functional theory. **K.A. Lopata**

11:00 PHYS **304.** Caution when using real-time TDDFT: Two-electron Rabi oscillations and peak-shifting. **C. Isborn**, M. Provorse, B. Habenicht

11:40 PHYS **305.** Charge transfer and other non-linear electron dynamics: the problem of detuning in TDDFT. **J.I. Fuks**, K. Luo, E. Sandoval, N. Maitra

12:00 PHYS **306.** Experimental perspective on the electronic structure and dynamics of higher-lying electronic states. **C.G. Elles**, C.L. Ward, A.L. Houk, T.J. Quincy

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

S. Link, K. A. Willets, *Organizers*
D. J. Masiello, *Organizer, Presiding*
J. S. Biteen, *Presiding*

8:30 PHYS **307.** Probing the mechanistic of charge transfer from optically excited plasmonic metal nanoparticles to adsorbates leading to chemical transformations. **S. Linic**

9:05 PHYS **308.** Electrochemistry on plasmonic nanoparticle electrodes. **A. Wilson**, K.A. Willets

9:25 PHYS **309.** Collective behavior in the solid-state elucidated by plasmonic spectroscopy. **P.K. Jain**

10:00 PHYS **310.** Single-particle absorption spectroscopy of plasmonic nanostructures. **M. Yorulmaz**, S. Nizzero, W. Chang, L. Wang, S. Link

10:20 PHYS **311.** Atomistic simulations of surface-enhanced spectroscopies. **L. Jensen**

10:55 PHYS **312.** Design and optimization of plasmonic crystals for surface enhanced Raman spectroscopy using the finite-difference time-domain method. **R. Petit**, J.M. Montgomery

11:15 PHYS **313.** Electron microscopy and spectroscopy of plasmonic alloys. **E. Ringe**, S.M. Collins, C.J. DeSantis, S.E. Skrabalak, P.A. Midgley

Section H

Colorado Convention Center
Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Catalysis and Materials for Catalysis: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

8:00 PHYS **314.** Global energy and emissions reduction potential of new materials development. **C. Tway**, E.G. Rightor, J. Liu, C. Han, M. McAdon, J. Goss, K. Andrews

8:30 PHYS **315.** Thermodynamics and kinetics of elementary reaction steps on late transition metal catalysts, and using them to search for better catalysts. **C.T. Campbell**

9:00 PHYS **316.** Tailored mesoscale gold alloy materials for energy- and resource-efficient catalysis. **M.L. Personick**, B. Zugic, C.M. Friend

9:20 Intermission.

9:40 PHYS **317.** Impact of location and concentration of acid sites in zeolites for acid catalyzed reactions in condensed phase. **J.A. Lercher**

10:10 PHYS **318.** Harnessing polymorphism for the rational design of new nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility. F. Trousselet, L. Bouessel du Bourg, **F. Coudert**

10:30 PHYS **319.** Material descriptor of oxygen vacancy formation energies in wide band gap oxides. **A. Deml, A. Holder**, R. O'Hayre, C. Musgrave, V. Stevanovic

Quantum Chemistry

Quantum Dynamics & Monte Carlo Simulations

Sponsored by COMP, Cosponsored by PHYS

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Sponsored by CHED, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Gas Phase Atmospheric Chemistry

D. Cziczo, M. Freedman, *Organizers*
K. T. Kuwata, C. Womack, *Presiding*

1:30 PHYS **320.** Photochemical and multiphase sources of isoprene derived secondary organic aerosol. **J.A. Thornton**, B. Lee, C. Gaston, E. D'Ambro, F. Lopez-Hilfiker, J. Liu, J. Shilling, C. Mohr, T.P. Riedel, Z. Zhang, A. Gold, J. Surratt, W. Hu, D. Day, P. Campuzano-Jost, B. Palm, J.L. Jimenez, N. Ng, L. Xu

2:10 PHYS **321.** Atmospheric chemistry in the southeast U.S. **J. de Gouw, C. Warneke, M. Trainer**

2:35 PHYS **322.** Uncertainties in global atmospheric composition due to uncertainties in inorganic and organic rate constants. **M.J. Evans**, B. Newsome

3:00 Intermission.

3:15 PHYS **323.** Relative abundances of gas phase amines and ammonia in the ambient atmosphere. **J. Murphy**, T.C. Vandenboer, G. Wentworth, M. Markovic, P. Gregoire

3:40 PHYS **324.** Probing the composition of atmospheric interfaces through measurement of trace gas reactive uptake and product yields. **T.H. Bertram**, O.S. Ryder, N. Campbell

4:05 PHYS **325.** Heterogeneous chemistry of nitrogen oxides: Results from recent field studies. **S.S. Brown**

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

Organic Molecules in Dense Clouds and Star and Planet Forming Regions

L. J. Allamandola, T. J. Lee, *Organizers*
E. Peeters, *Presiding*

1:30 PHYS **326.** Complex organic molecules in star-forming regions: Sweet results from ALMA. **E.F. van Dishoeck**

2:05 PHYS **327.** Polycyclic aromatic hydrocarbons as catalysts for interstellar molecular hydrogen formation. **L. Hornekaer**

2:40 PHYS **328.** Modeling grain surface chemistry in dense molecular clouds. **H. Cuppen**, L. Karssemeijer

3:15 Intermission.

3:45 PHYS **329.** Formation of complex organic molecules in protoplanetary disks. **T. Millar**

4:20 PHYS **330.** Time-domain terahertz spectroscopy of polycyclic aromatic hydrocarbons. **M.A. Allodi**, P. Carroll, S. Ioppolo, B.A. McGuire, G.A. Blake

4:45 PHYS **331.** Tackling the theoretical anharmonic infrared spectra of polycyclic aromatic hydrocarbons. **C. Mackie**, A. Candian, X. Huang, T.J. Lee, A. Tielens

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Nonadiabatic Dynamics

Cosponsored by COMP

J. Gao, B. C. Garrett, B. Mennucci, *Organizers*
X. Li, *Presiding*

1:30 PHYS **332.** Beyond the Born-Oppenheimer approximation: Construction of accurate multicomponent wave function using explicitly-correlated and projection-based methods. **A. Chakraborty**

2:00 PHYS **333.** Directly correlating electronic and vibrational motions with multidimensional coherent spectroscopies. **M.H. Khalil**

2:30 PHYS **334.** Approximate time-dependent diabatic states computed using a measure driven tessallation technique for use in on-the-fly quantum dynamics methods. **S.S. Iyengar**

3:00 PHYS **335.** Avoiding the Born-Oppenheimer separation between electrons and protons in wavefunction and density functional theory calculations. **S. Hammes-Schiffer**

3:20 Intermission.

3:40 PHYS **336.** Surface hopping and spectroscopy. **J.E. Subotnik, A.S. Petit**

4:10 PHYS **337.** Novel approaches to nonadiabatic molecular dynamics. **O.V. Prezhdo**

4:40 PHYS **338.** Time-dependent electronic and nuclear potentials that exactly capture electron-ion coupling. **N. Maitra**

5:00 PHYS **339.** Time-derivative coupling scheme for accurate electronic state transition probabilities in nonadiabatic molecular dynamics. **G. Meek, B. Levine**

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

In Situ Characterization

A. Co, D. A. Scherson, *Organizers*
C. L. Korzeniewski, D. Scherson, *Presiding*

1:30 PHYS **340.** Vibrational spectroscopy and 2D correlation analysis applied to probe structure in ionomer membrane materials. **C.L. Korzeniewski**, T. Zhang

2:10 PHYS **341.** Operando X-ray studies of electrocatalysis for energy conversion. **D. Friebel**

2:50 Intermission.

3:10 PHYS **342.** Irrelevance of CO poisoning in methanol oxidation on PtRu electrocatalysts: A re-visit of the bifunctional mechanism. **Y. Tong**

3:50 PHYS **343.** In operando optical studies of solid oxide fuel cells operating with biogas: heterogeneous surface chemistry vs. electrochemical oxidation. **R.A. Walker**, J. Kirtley, J. Owrutsky, D.A. Steinhurst

Section E

Colorado Convention Center

Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Folding and Aggregation

Cosponsored by COMP

A. E. Garcia, G. Hummer, *Organizers*

R. Nussinov, *Presiding*

1:30 PHYS **344.** Accurate atomistic simulations of intrinsically disordered proteins. **R.B. Best**, W. Zheng, J. Mittal

2:05 PHYS **345.** Regulation and aggregation of intrinsically disordered peptides. **J.E. Shea**

2:40 PHYS **346.** Multiscale and multiresolution simulations of aggregation in polyglutamine containing block copolymers. **R.V. Pappu**

3:15 PHYS **347.** Spontaneous formation of oligomers and fibrils in large scale molecular dynamics simulations of peptides. **C.K. Hall**, M. Cheon, D.C. Latshaw, I. Chang

3:50 PHYS **348.** Alzheimer's disease: Aggregation of WT and protective Aβ peptides, free or in the presence of inhibitors and under shear flow by all-atom and coarse-grained simulations. J. Nasica-Labouze, P. Nguyen, B. Tarus, F. Sterpone, M. Chiricotto, O. Berthoumieu, P. Faller, A. Doig, S. Melchionna, **P. Derreumaux**

4:25 PHYS **349.** Protein folding and recognition in the cell — an in silico approach. **M.S. Cheung**

Section F

Colorado Convention Center

Room 505

Modeling Excited States of Complex Systems

Electronic Structure

Cosponsored by COMP

B. G. Levine, S. A. Varganov, *Organizers*

J. I. Fuks, *Presiding*

1:30 PHYS **350.** Modeling excited states with multireference quantum chemical methods. **L. Gagliardi**, R. Carlson, D.G. Truhlar, K. Vogiatzis

2:10 PHYS **351.** Single- and multireference quantum chemical methods for nonadiabatic molecular dynamics. **H. Lischka**, M. Barbatti

2:50 PHYS **352.** Low valency in rare earth diatomics. **G. Schoendorff**, A.K. Wilson

3:10 Intermission.

3:30 PHYS **353.** Active space decomposition. **T. Shiozaki**

4:10 PHYS **354.** Representation of adiabatic potential energy surfaces coupled by conical intersections and their use in describing nonadiabatic processes. **D.R. Yarkony**, X. Zhu, J. Dillon, C. Malbon

4:50 PHYS **355.** Electronic structure of diatomic rare earth species. **C. South**, G. Schoendorff, A.K. Wilson

5:10 PHYS **356.** Size-inconsistency effects in transition moments for quasi-degenerate variational perturbation theory and averaged coupled-pair functional theory. **K. Dwelle**, R.J. Cave

Section G

Colorado Convention Center

Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, K. A. Willets, *Organizers*

S. Link, *Organizer, Presiding*

R. R. Frontiera, *Presiding*

1:30 PHYS **357.** Raman scattering in time and frequency on a nantenna and its molecular load. **V.A. Apkarian**

2:05 PHYS **358.** Photoluminescence quantum yield of strongly coupled gold plasmonic molecule. **D. Huang**, C. Byers, L. Wang, A. Hoggard, B. Hoener, W. Chang, C.F. Landes, S. Link

2:25 PHYS **359.** Plasmons and intraband transitions. **P. Guyot-Sionnest**

3:00 PHYS **360.** Electron dynamics in gold nanoparticles under strong laser fields. **J. Powell**, A. Rudenko, C.M. Sorensen

3:20 PHYS **361.** Controlling and probing spatially dependent plasmonic field effect and charge transfer dynamics using single quantum dot modified AFM tips. **T. Lian**

3:55 PHYS **362.** Strong coupling between individual plasmonic metal nanostructures and quantum dots. **M. Pelton**

Section H

Colorado Convention Center

Room 607

Design of Materials and Chemical Processes: The Genomic Approach

Catalysis and Materials for Catalysis: Experiments & Calculations

L. Gagliardi, B. Smit, *Organizers, Presiding*

1:30 PHYS **363.** Computational design of highly selective transition metal catalysts encapsulated by metal-organic frameworks for butane oxidation to 1-butanol. S. Dix, **R. Getman**

2:00 PHYS **364.** Metal–organic frameworks as highly functional catalytic arrays. **O.K. Farha**

2:30 PHYS **365.** Metal-organic framework materials for solar energy applications. **W. Lin**

3:00 PHYS **366.** Performance descriptors for the design of solar energy materials. **A. Walsh**

3:20 Intermission.

3:40 PHYS **367.** Withdrawn.

4:10 PHYS **368.** In silico prediction of emergent catalysts. **D.G. Vlachos**

4:40 PHYS **369.** Impact of MOF topology upon solvent organization, dynamics, and solution phase stability. **A.E. Clark**, W. Queen, X. Yang

Quantum Chemistry

Applications

Sponsored by COMP, Cosponsored by PHYS

Computational Chemistry in the Undergraduate Curriculum: What is Working and How Do We Assess It?

Sponsored by CHED, Cosponsored by PHYS

WEDNESDAY EVENING

Section G

Colorado Convention Center

Hall C

Physical Chemistry Poster Session

E. L. Sibert, *Organizer*

6:30 - 9:30

PHYS **370.** Quantum numerical control for particles at matter surface. **Q. Wang**

PHYS **371.** Scaled quantum mechanical scale factors for vibrational calculations using alternate polarized and augmented basis sets with the B3LYP density functional calculation model. **W.B. Collier**, C.R. Legler, N.R. Brown, R.A. Dunbar, M.D. Harness, K. Nguyen, O.O. Oyewole

PHYS **372.** Calculating the infrared spectra of the eigenion using anharmonic vibrational theory. **B. Thomsen**, K. Yagi, Y. Sugita

PHYS **373.** Theory and efficient computation of vibrational difference spectra. **T. Joutsuka**, A. Morita

PHYS **374.** Diabatic states of a delta function model. **T. Middlemas**, R.J. Cave

PHYS **375.** Lifetimes of vibrational states of XY ions (X=Li, Na; Y=Be, Mg) calculated using the CCSDT potential energy and dipole moment curves. **D.K. Barnes**, D. Fedorov, S.A. Varganov

PHYS **376.** Probing vibrational-electronic interactions of a sensitizing dye at the TiO_2 surface using heterodyne detected doubly resonant sum-frequency generation spectroscopy. **C.C. Rich**, M. Mattson, A.T. Krummel

PHYS **377.** Time-resolved infrared spectrocopy of [FeFe]-hydrogenase model compounds. **R. Meyer**, A. Zhandosova, E.J. Heilweil, C.J. Stromberg

PHYS **378.** Statistically weight averaged vibrational spectrum over molecular fragments for studying the amide I vibration of sphingomyelin bilayer. **K. Yagi**, P. Li, K. Shirota, T. Kobayashi, Y. Sugita

PHYS **379.** Structural and energetic properties of lanthanide trihalides via DFT and ab initio approaches. **R.J. Weber**, G. Schoendorff, A.K. Wilson

PHYS **380.** Ferrocene - ozone reactions: A matrix-isolation and DFT study. **R.W. Kugel**, L. Pinelo, B.S. Ault

PHYS **381.** Mechanistic investigations of siderophore complexation via density functional theory. M.F. Skaro, M.S. Hughey, **J.L. Sonnenberg**

PHYS **382.** Theoretical phase diagram for Fe_3O_4 (111) surfaces using a DFT + *U*(Fe) approach. **X. Huang**, S. Ramadugu, S.E. Mason

PHYS **383.** DFT and ab initio composite method investigations of oxygen fluorides and related hydrides. **Z.H. Alsunaidi**, A.K. Wilson

PHYS **384.** Effect of choline chloride on secondary structure conformation for two small peptides: A circular dichroism study. **M. Giordano**, M. Vermeuel, P. Gupta, D. Léon, M.R. Bunagan

PHYS **385.** Deconstructing solvent organization in confined nanoporous materials: Implications for separation. **C. Wang**, A.E. Clark

PHYS **386.** Crystallographic characterization of three furan-substituted benzimidazoles and calculation of C-H/π and π/π interaction energies. D.K. Geiger, **C. Geiger**

PHYS **387.** Quantum electronic kinetics from an atom-centered bath model. **T. Nguyen**, S. Blau, T. Markovich, J. Parkhill

PHYS **388.** Impact of resonance stabilization on H-atom shift isomerization and ring closure reactions. **K. Wang**, S. Villano, A.M. Dean

PHYS **389.** Sodium dodecyl sulfate monomers induce XAO peptide polyproline II to -helix transition. **Z. Hong,** D. Krishnan Achary, S.A. Asher

PHYS **390.** Multishells vs. gradient-alloyed shells on core quantum dots: Ensemble and single particle optical properties. **P. Bajwa**, F. Gao, B.O. Omogo, C.D. Heyes

PHYS **391.** Physicochemical investigation of ionic liquid mixtures. **M.T. Clough**, J. Gräsvik, P. Hunt, H. Niedermeyer, T. Welton

PHYS **392.** Antibunching in small clusters of quantum dots. **J.Q. Geisenhoff**, K.J. Whitcomb, D. Ryan, M.P. Gelfand, A.K. Van Orden

PHYS **393.** Modification method of natural zeolite by ultrasonic and sodium chloride. **W. Qun**, Y. Zhichao, G. Mingkun, X. He, C. Bin, C. Shuang

PHYS **394.** Understanding nanoconfined hydrogen: first ever quantum free-energy profiles of diffusion of hydrogen and the importance of condensed phase environment in sII clathrate hydrate. **A. Powers**, O. Marsalek, L. Ulivi, M.E. Tuckerman, Z. Bacic

PHYS **395.** Solution dynamics of group 8 metal pentacarbonyls in fluorinated benzene solvents. **C.P. Baryiames,** A. Devanny, C. Laperle

PHYS **396.** Solution dynamics of osmium pentacarbonyl in alcohol solvents. **C. Laperle, A. Devanny**

PHYS **397.** Surface thermodynamics and vesicle formation of decanoic acid. **B. Kessenich**, R. Rapf, R.J. Perkins, V. Vaida

PHYS **398.** Molecular dynamics simulation of ion transports through liquid-liquid interface. **N. Kikkawa**, A. Morita, L. Wang

PHYS **399.** Raman spectroscopic study of graphene photochlorination dynamics in the gas phase and in solution. **K.Z. Rinaldi**, N. Patel, S. Ramrattan, A. Crowther

PHYS **400.** Decomposing hydrogen bond dynamics into multiscale components: Understanding the hydrophobic effect. **T. Zhou**, A.E. Clark

PHYS **401.** Diabatic electronic population matrix and its utilization in simulating electronically excited state dynamics. **J. Park**, Y.M. Rhee

PHYS **402.** Decoherence in nonadiabatic dynamics from an approximate mixed quantum-classical Poisson bracket mapping equation formalism. **H. Kim,** Y.M. Rhee

PHYS **403.** Interdomain dynamics of chloroplast signal recognition particle proteins studied by time-resolved single-molecule FRET. **D. Baucom**, F. Gao, P. Patel, A. Kight, R. Goforth, R. Henry, C. Heyes

PHYS **404.** Molecular dynamics to study energy transduction in the ATP powered translocation of PcrA along DNA. **R.B. Davidson**, M. McCullagh

PHYS **405.** Two-photon spectroscopy, dynamics, and quantum yields of a photochromic molecular switch. **A.L. Houk**, C.G. Elles

PHYS **406.** Global potential energy surfaces of O_4 and dynamics of high-energy O_2-O_2 collision-induced energy transfer and dissociation. **Y. Paukku**, Z. Varga, W. Lin, R. Meana-Pañeda, J. Bender, G.V. Candler, D.G. Truhlar

PHYS **407.** Time-dependent excited-state molecular dynamics of photofragmentation of gas-phase tris(isopropylcyclopentadienyl) lanthanum complexes. **Y. Han**, Q. Meng, P.S. May, M.T. Berry, D. Kilin

PHYS **408.** Structural characterization of supported noble metal nanocatalyst from atomistic simulations. **S. Xiong**, R. Diwan, Y. Li

PHYS **409.** Investigating the efficient conversion of unsaturated acids to olefins over acid catalysts. **T.J. Evans**, J.M. Clark, C. Mukarakate, M.M. Yung, M.R. Nimlos, D.J. Robichaud

PHYS **410.** First principles treatment of photoluminescence linewidth in semiconductors. **D.J. Vogel**, D. Kilin

PHYS **411.** Investigating the best type of gold and platinum bimetallic nanoparticle catalyst for alcohol oxidation reactions. A. Earle, **J.M. Petroski**

PHYS **412.** Laser-assisted nickel liquid phase deposition on surface of dielectrics and semiconductors. **E. Khairullina**, S. Araslanova, S. Safonov

PHYS **413.** Reaction kinetics of NO and NO_2 with pyrite. **H.M. Bevsek**

PHYS **414.** Probing the mechanism of DNA duplex formation in sequences with consecutive versus alternating purines and pyrimidines using stopped flow kinetics experiments. **S.P. Carney**, R. Stratil, A. Deckert

PHYS **415.** Monitoring internal temperatures and kinetics in nitrogen- and oxygen-containing plasma systems. **E. Sutor**, J. Blechle, E.R. Fisher

PHYS **416.** Effects of organic matter on polycyclic aromatic hydrocarbon photolysis kinetics in ice and at ice surfaces. **P. Malley**, T. Kahan

PHYS **417.** Dissociation processes of deprotonated nucleobases: Astrobiological implications. **C.A. Cole**, Z. Wang, T.P. Snow, V.M. Bierbaum

PHYS **418.** Carbon chains in low-mass young stellar objects. **O.H. Wilkins**, D.M. Graninger, K. Oberg

‡ *Cooperative Cosponsorship*

PHYS **419.** Formation mechanism of interstellar PANH cations: Experimental and computational studies. **Z. Wang**, V.M. Bierbaum, C.A. Cole, T.P. Snow

PHYS **420.** Spectral characteristics and lightfastness of fluorescent dyes absorbed on nanoparticles of aerosil dispersed in polymer matrix. **N. Barashkov, S. Sheshenia, T. Sakhno**, V. Granchak, S. Kuchmii, I. Irgibayeva

PHYS **421.** Investigation of two alternative methods of introducing fluorescent dyes in the Au nanoparticles-polysiloxane composites. **N. Barashkov**, I. Irgibayeva, A. Aldongarov, A. Mantel, A. Ishchenko, T. Sakhno

PHYS **422.** Electron and nuclear dynamics in gold and silver nanoparticles. **R.D. Senanayake**, C.M. Aikens

PHYS **423.** Electrochemical fabrication of CdSe/TiO_2 nanotubes for photoelectrocatalytical water splitting application. **F. de Souza Lucas**, M. Sant'anna, R.G. Freitas, L.H. Mascaro, E.C. Pereira

PHYS **424.** Pseudo-direct bandgap transitions in silicon nanocrystals: Effect on optoelectronics and thermoelectrics. V. Singh, Y. Yu, **Q. Sun**, B. Korgel, P. Nagpal

PHYS **425.** Work function modification of various electrodes by deposition of carbon nanotubes via aerosol jet printing. **C.A. Jordan**, R.S. Aga, E. Kreit, C.M. Bartsch, E.M. Heckman, R.S. Aga

PHYS **426.** Temperature dependent solubility of gold nanoparticle suspensions. **J. Powell**, K. Bayliff, E. Herman, C.M. Sorensen

PHYS **427.** Doping of wide-bandgap titanium-dioxide nanotubes: Optical, electronic and magnetic properties. **Y. Ding**, Y. Alivov, V. Singh, P. Nagpal

PHYS **428.** Computational studies of pathways toward the growth of small boron and boron-carbon nanomaterials. **D.C. Woods**, A.L. Dibble, J.R. Rocha

PHYS **429.** Withdrawn.

PHYS **430.** Quantitative SERS-based detection using Ag–Fe3O4 nanocomposites with an internal reference. **P.B. Joshi., Y. Zhou**, T. Ozkaya, P. Zhang

PHYS **431.** Singlet oxygen generation under NIR and light visible light excitation of Chlorin e6 on the surface of fluorescent polymer coated $NaYF_4$ upconversion nanoparticles. **P.B. Joshi**, P. Zhang

PHYS **432.** Novel approach to modeling the absorption spectra and colloidal stability of few- and single-chirality single walled carbon nanotubes. **K.C. Tvrdy**, K. Prescott, K. Rosenthal

PHYS **433.** Withdrawn.

PHYS **434.** Preparation of metal oxide substrates for surface-enhanced Raman scattering. B. Li, C. Weng, C. Yang, C. Lin, **S. Lee**

PHYS **435.** Spin-forbidden transitions between electronic states of the active site of rubredoxin. **G. dePolo**, D. Kaliakin, S.A. Varganov

PHYS **436.** Charge transfer complexes and photochemistry of ozone with n-butylferrocene and ferrocene: A UV-Vis matrix isolation study. **L. Pinelo**, R. Kugel, B.S. Ault

PHYS **437.** Engineering long range ferromagnetism in 2D transition metal dichalcogenide WSe_2. **C. Gil**, A. Pham, S. Li

PHYS **438.** Structure and bonding of metal complexes containing possible hepatitis C inhibitors. **R.M. Drazenovic**, D.N. Ward, P.J. Smith, J.L. Sonnenberg

PHYS **439.** Interaction of niobium-containing chloride melts with niobium metal. M.V. Chernyshov, **I.B. Polovov**, V.A. Volkovich, O.I. Rebrin

PHYS **440.** Organic nanowire waveguide exciton-polariton nanolaser and its photonic application. **Q. Liao**

PHYS **441.** Triplet states of pyrazine. **R. Bendiak**, R.J. Cave

PHYS **442.** Effect of reaction environment on atmospheric photochemistry of pyruvic acid. **A.E. Reed Harris**, B. Ervens, R.K. Shoemaker, J.A. Kroll, R.J. Rapf, E.C. Griffith, A. Monod, J. Doussin, V. Vaida

PHYS **443.** Kirkwood-Buff derived force field for esters. **G. Pallewela**, P.E. Smith

PHYS **444.** Stabilization of a Cl—Cl– anion pair in the gas phase: Ab initio microsolvation study. **A.S. Ivanov, G. Frenking**, A.I. Boldyrev

PHYS **445.** Detecting organic nitrates using thermal dissociation cavity ringdown spectrometry. **N. Keehan**, B. Ayres, J.L. Fry

PHYS **446.** Rotational and hyperfine analysis of the $E2\Pi_{1/2}$ state of TaO. **T.D. Varberg**, C.R. Christopher, S.Y. Lee, F.B. Gwandu, A.J. Matsumoto, B.J. Knurr, T.K. Mahle, Z.W. Morrow

PHYS **447.** Metal-mediated proton transfer in maleic acid and implications for enzyme catalysis. **M.T. Ruggiero**, T.M. Korter

PHYS **448.** Combined photoelectron spectroscopy and ab initio studies of pure, carbon-doped, and transition-metal-doped boron clusters. **I.A. Popov**, W. Li, Z.A. Piazza, R. Pal, V.F. Popov, K.V. Bozhenko, I.Černušák, X.C. Zeng, A.I. Boldyrev, L. Wang

PHYS **449.** Raman spectra of EDAB and Its analogs in various solvents. **S. Farmer, M.L. Fetterolf**, G. Rowe

PHYS **450.** QM/MM simulations reveal the involvement of excimers in the photophysics of adenine based oligonucleotides. **V.A. Spata**, S. Matsika

PHYS **451.** TiO_2 mediated photooxidation of squalene: A kinetic and mechanistic study. **M.L. Kaak**, J.A. Ganske

PHYS **452.** Is ketene an intermediate in the addition of imines to azlactone to form a β-lactam? **C. Kordes**, P. Willoughby, J. Scanlon

PHYS **453.** Aerosol formation initiated by nucleation of radical- water complexes. **E. Burrell**, S. Kumbhani, R.B. Shirts, J.C. Hansen, L. Hansen

PHYS **454.** Drinking water disinfection by a low-voltage pulsed electric field device. P. Hung, **Y. LI,** O. LEE, K. LAM, S. Kwan, J. Kwan, K.L. Yeung

PHYS **455.** Experimental and computational investigation of the dissociation pathways of first generation protonated nitrile-terminated PPI dendrimer. **W.D. Price**

PHYS **456.** Photophysical properties and electronic structure of strongly coupled hydroporphyrin dyads with extended near-infrared absorption. **H. Kang**, N.N. Esemoto, J.R. Diers, D.M. Niedzwiedzki, J.A. Greco, J. Akhigbe, Z. Yu, C. Pancholi, G.V. Bhagavathy, J.K. Nguyen, R.R. Birge, C.R. Kirmaier, D.F. Bocian, M. Ptaszek, D. Holten

PHYS **457.** Investigation of the hygroscopicity of glycine and lysine aerosols and their mixtures with Na_2SO_4. **J.P. Darr**, P. Morales, S. Gottuso, A. Johnson

PHYS **458.** Docking studies of binding of *Plasmodium falciparum* plasmepsin II to normal and sickle hemoglobin. **S.C. Marguet**, V.F. Waingeh

PHYS **459.** Correlation consistent composite approach (ccCA): Application to organics and beyond. **A. Morris**, A. Wilson

PHYS **460.** Charge-transfer in fullerene: Molecular cluster co-crystals. **N. Patel**, K.Z. Rinaldi, E. O'Brien, X. Roy, A. Crowther

PHYS **461.** Raman spectroscopic study of solvent-mediated electron-transfer chemical doping of graphene. **J. Karten**, B. Janicek, A. Crowther

PHYS **462.** Rapid scan electron paramagnetic resonance improves sensitivity relative to conventional methods. **G.R. Eaton**, S. Eaton, M. Tseytlin, R. Quine, G. Rinard, D. Mitchell, J. Biller, Z. Yu, Y. Shi

PHYS **463.** Photon and water mediated sulfur oxide and acid chemistry in planetary atmospheres. **J.A. Kroll**, V. Vaida

PHYS **464.** Theoretical analysis on the methods to derive surface molecular orientation by sum frequency generation spectroscopy. **A. Morita**, T. Ishihara, K. Saito, T. Ishiyama, L. Wang

PHYS **465.** Thermodynamics of uranium in gallium-aluminum based liquid alloys. **V.A. Volkovich**, D.S. Maltsev, L.F. Yamshchikov, I.B. Polovov, A.G. Osipenko

PHYS **466.** Thermodynamic modeling and experimental verification of f-elements separation employing Ga-Sn eutectic alloys. S.Y. Melchakov, D.S. Maltsev, **V.A. Volkovich**, L.F. Yamshchikov, D.G. Lisienko, M.A. Rusakov

PHYS **467.** Thermodynamic properties of lanthanum in alloys based on gallium-aluminum eutectic mixture. A.V. Shchetinskiy, A.S. Dedyukhin, **V.A. Volkovich**, L.F. Yamshchikov, A.G. Osipenko

PHYS **468.** Characterization of aqueous metal-pyrazole complexes. **A.K. Huff**, G. Turcios, S. Miller

PHYS **469.** Photodissociation of cis- and trans-CH_3ONO: Is conformation destiny? **J. Lantis**, M. Birndorf, J.A. Bartz

PHYS **470.** Photodissociation of t-butyl nitrite: Steric influences on vector correlations. **M. Birndorf**, J. Lantis, J.A. Bartz

PHYS **471.** Effects of large water box on anatase thin film surface: A computational analysis on changing electronic properties. **S.J. Jensen**, D. Kilin

PHYS **472.** Influence of various solvents on the physical properties of materials for organic electronic devices. **A. Foote**, R. Aga, E. Niwemukiza

PHYS **473.** BOMD study of M+(tryptamine)$(H_2O)_n$ cluster ions. P.E. Hoerner, **J. Beck**, M.P. Gaigeot

PHYS **474.** Spectroscopic study of the effects of local environment and deuteration on the structure of trimethylamine N-oxide (TMAO). **L. McNamara**, D.N. Reinemann, H.U. Valle, J.C. Prather, P.L. Reves, D.H. Magers, T.K. Hollis, G.S. Tschumper, N. Hammer

PHYS **475.** Thermal decomposition of iron dithiocarbamates. J.C. Becca, **J.F. Fuller**

PHYS **476.** Enzymatic activation of nitric oxide. **J.C. Pearson**, A.K. Wilson

PHYS **477.** Characterizing novel solid-state reaction intermediates using advanced in situ X-ray diffraction techniques. **C. Benson**, J. Cox, I. Walton, J.B. Benedict

PHYS **478.** Withdrawn.

PHYS **479.** Withdrawn.

PHYS **480.** Spectroscopic characterization of free-base bis(arylethynyl)porphyrins bearing *p*-hydroxyphenyl substituents. **K.K. Evens**, K.E. Splan

PHYS **481.** Fingerprinting molecular structure via photoinization out of Rydberg states and microwave Rayleigh scattering. **R.D. Oster**, S. Purohit, S. Atkins, F. Rudakov

PHYS **482.** Impact of basis set completeness on computed dissociation energies of transition metal complexes. **J. Plascencia**, A.K. Wilson

PHYS **483.** On the B800-850 LH2 antenna complex of the purple sulfur bacterium *Allochromatium vinosum*. **A. Kell**, M. Jassas, K. Hacking, R.J. Cogdell, R. Jankowiak

PHYS **484.** Comments on the optical lineshape function: Application to transient hole burned spectra of bacterial reaction centers. **A. Kell**, M. Reppert, T.O. Pruitt, D. Sanchez, R. Jankowiak

PHYS **485.** Critical assessment of the low-temperature optical spectra of the CP47 antenna protein complex of Photosystem II: Revised structural assignments. **J. Chen**, A. Kell, T. Reinot, M. Jassas, R. Jankowiak

PHYS **486.** Heat capacity of oxygen atoms at high temperatures. **L. Biolsi**

PHYS **487.** Membrane catalyzed aggregation of amylin using 2D IR spectroscopy. **K. Rich**, M.T. Zanni

PHYS **488.** Ab initio approaches for accurate predictions of lanthanide thermochemistry. **C.C. Peterson**, A.K. Wilson

PHYS **489.** Evaluation of charge density analysis methods. **C.C. Jeffrey, M.J. Carlson, A.K. Wilson**

PHYS **490.** Electron transfer rate modulation in a compact Re(I) donor-acceptor complex. **Y. Yue**, T. Grusenmeyer, M. Zheng, P. Zhang, R.H. Schmehl, D.N. Beratan, I.V. Rubtsov

PHYS **491.** Study of low temperature oxidation reactions of 2-methylfuran using synchrotron photoionization mass spectrometry. **A.R. Smith**, G. Meloni

PHYS **492.** Gas-phase acidities of nitrated azole species from the extended kinetic method. **C.M. Nichols**, W. Old, W.C. Lineberger, V.M. Bierbaum

PHYS **493.** Modeling stopped-flow data for nucleic acid duplex formation reactions. **A. Deckert**, J. Sikora, B. Rauzan

PHYS **494.** DSC and rheological study of supercooled ethylene glycol-water mixture. **S. Kim**, R. Fore, E. Kook, B.H. Milosavljevic

PHYS **495.** Using kinetic models to understand H atom reactions in solid parahydrogen. **F.M. Mutunga**, D.T. Anderson

PHYS **496.** Evaluation of a novel nontraditional processing aid for the pulp and paper industry. **C. Kirwan**, R. Hamm, B. Wilson, L. Bava

PHYS **497.** Template and model sets of protein structures. **I. Anishchanka**, P. Kundrotas, A. Tuzikov, I. Vakser

PHYS **498.** Overcoming costly sampling simulations using non-Boltzmann Bennet's acceptance ratio method to generate potentials of mean force. P.S. Hudson, **F.L. Kearns**, S. Boresch, H.L. Woodcock

PHYS **499.** Development of bacteriochlorophyll a potential energy surface by quantum chemical calculations. **C. Kim**, Y.M. Rhee

PHYS **500.** Environmental effect on excited energy transfer in photosynthetic light harvesting complex: Comparing Poisson bracket mapping equation and reduced hierarchical equation of motion. **W. Lee**

PHYS **501.** Evaluation of defoamer chemistries for brown stock washing. **R. Hamm**, C. Kirwan, B. Wilson, L. Bava

PHYS **502.** DsDNA-assisted dissolution of tungsten (IV) disulfide in aqueous solution. **M. Simmons,** X. Xu, W. Zhao

PHYS **503.** Computational study of the reduction by 2-propanol of acetophenone in supercritical 2-propanol. **D.B. Lawson**

PHYS **504.** Electron transmission in molecular electronics: A computational study. **B. Topham**

PHYS **505.** Effect of substitution on the rate of benzyloxyl radical generation through a 1,2-Hydrogen atom shift: A computational study. **D.J. Van Hoomissen**, S. Vyas

PHYS **506.** Computational studies of inhibitor binding to human immunodeficiency virus, Type 2 (HIV-2) protease. **R. Summay**, V.F. Waingeh

PHYS **507.** Solid phase microextraction with polystyrene- poly(dimethylsiloxane) block copolymers. **A. Schlaus**

PHYS **508.** Mixed polarization vibrational sum frequency generation spectra of organic semiconducting thin films. **P.M. Kearns**, A.M. Massari

PHYS **509.** Stochastic approach to reaction diffusion modeling of the fragmentation processes during heterogeneous oxidation of organic aerosol. **A.A. Wiegel**, K.R. Wilson, W. Hinsberg, F.A. Houle

PHYS **510.** Characterization of a real-time tfor isoprene epoxydiols-derived secondary organic aerosol (IEPOX-SOA) from aerosol mass spectrometer measurements. **W. Hu**, P. Campuzano-Jost, B. Palm, D. Day, A. Ortega, P. Hayes, Q. Chen, M. Kuwata, Y. Liu, S. Simoes de Sa, S.T. Martin, M. Hu, S. Budisulistiorini, J. Surratt, K. Docherty, G. Isaacman, A. Goldstein, J. Clair, J.D. Crounse, P. Wennberg, J. Jimenez

PHYS **511.** Water vapor enhancement of peroxy radical reactions. **S. Kumbhani**, T. Cline, M. Killian, J. Clark, L. Hansen, R.B. Shirts, D. Robichaud, J.C. Hansen

PHYS **512.** Kinetics of acid-catalyzed dehydration of aerosol cyclic hemiacetals formed from the OH radical-initiated reaction of *n*-pentadecane. **A.P. Ranney**, P. Ziemann

PHYS **513.** Heterogeneous oxidation of liquid and solid alkanes by OH in the presence and absence of NO or SO_x. **N.K. Richards-Henderson**, M.D. Ward, A. Goldstein, K.R. Wilson

PHYS **514.** Investigating index of refraction trends in ammonium sulfate and glyoxal reactions. **M. Symons**, M.D. Zauscher, M.M. Galloway, D.O. Dehaan

PHYS **515.** Determination of N-containing conjugated brown carbon products In glycolaldehyde, methylamine, and glycine reaction mixtures. **T. Kress**

PHYS **516.** Measurements of in-situ SOA formation and chemistry using an oxidation flow reactor. **B.B. Palm**, P. Campuzano-Jost, D. Day, W. Hu, A.M. Ortega, S.S. de Sá, R. Seco, J. Park, A. Guenther, S. Kim, J. Brito, F. Wurm, P. Artaxo, R. Thalman, J. Wang, L. Kaser, W. Jud, T. Karl, A. Hansel, J. Fry, S.S. Brown, D. Draper, K.J. Zarzana, W.P. Dubé, N. Wagner, L. Hacker, A. Kiendler-Scharr, L. Yee, G. Isaacman, A. Goldstein, R. Souza, A. Manzi, O. Vega, J. Tota, M. Newburn, M. Alexander, S.T. Martin, W. Brune, J.L. Jimenez

PHYS **517.** SOA derived from isoprene epoxydiols: Insights into formation, aging and distribution over the continental US from the DC3 and SEAC4RS campaigns. **P. Campuzano Jost**, B.B. Palm, D. Day, W. Hu, A.M. Ortega, J. Jimenez, J. Liao, K.D. Froyd, I. Pollack, J. Peischl, T.B. Ryerson, J. Clair, J.D. Crounse, P. Wennberg, T. Mikoviny, A. Wisthaler, L. Ziemba, B.E. Anderson

PHYS **518.** Depositional ice nucleation on NX illite and mixtures of NX lilite with organic acids. **K.M. Primm, M. Tolbert**, G. Schill

PHYS **519.** Does the reaction of HO_2 with NO produce $HONO_2$ and HOONO? **L.A. Mertens**, H.M. Allen, M. Okumura, S.P. Sander

PHYS **520.** Gas/particle partitioning of organic acids during the southern oxidant and aerosol study (SOAS): Measurements and modeling. **S. Thompson**, L. Yatavelli, H. Stark, J. Kimmel, W. Hu, B.B. Palm, P. Campuzano-Jost, D. Day, G. Isaacman, A. Goldstein, R. Holzinger, A. Khan, F. Lopez-Hilfiker, C. Mohr, J.A. Thornton, J.T. Jayne, D.R. Worsnop, J.L. Jimenez

PHYS **521.** Reactions of resonantly-stabilized free radicals that impact molecular weight growth kinetics. **K. Wang**, S. Villano, A.M. Dean

PHYS **522.** Hydration of Krypton in dilute and concentrated solutions. **M. Chaudhari**, S.L. Rempe, D. Sabo, L.R. Pratt

PHYS **523.** Theoretical and experimental studies on the radical-radical reaction: $NO_2 + N_2H_3$. **G.L. Vaghjiani**, H. Sun, S.D. Chambreau, A. Schenk, C.K. Law

PHYS **524.** Estimation of quantum effects in atomic solids using quantum trajectory dynamics with dissipation. **B. Gu**, V. Rassolov, S. Garashchuk

PHYS **525.** Characterizing the effects of noncovalent interactions on hydrated azabenzene clusters: Charge localization and charge transfer. **J.T. Kelly**, K.H. Bowen, G.S. Tschumper, N. Hammer

PHYS **526.** Intrinsic bonding patterns via localized orbitals. **J. Duchimaza**, A. West, M.W. Schmidt, M.S. Gordon, K. Ruedenberg

PHYS **527.** Origins of long timescales in solvation dynamics of nanoconfined liquids. **J. Harvey**, W. Thompson

PHYS **528.** Magnetic stability and relaxation in single-molecule magnets: Insights from new stochastic theories. **D. Packwood**, K. Reaves, F. Federici Canova, I. Hamada, H. Katzgraber, W. Teizer

PHYS **529.** Multireference diagnostic criteria for 4d transition-metal-containing molecules. **J. Wang**, S. Manivasagam, A.K. Wilson

PHYS **530.** In search of an intrinsic chemical bond. **A. Morgenstern**, T. Wilson, T. Jones, J. Miorelli, M. Eberhart

PHYS **531.** Density functional theory study of the reduction of substituted quinones by lumiflavin. **E. Song**, C.R. Reinhardt, S. Bhattacharyay

PHYS **532.** First-principles interpretation of ultrafast time-resolved core-level spectroscopies investigating photo-induced charge transfer. **S. Pemmaraju**, S. Neppl, K. Siefermann, D. Prendergast, O. Gessner

PHYS **533.** Hydrocarbon structure impacts on the fumarate addition mechanism: Perspectives on the biodegradation susceptibility of fuels from electronic structure calculations. **V.S. Bharadwaj**, S. Vyas, S. Villano, C.M. Maupin, A.M. Dean

PHYS **534.** Intramolecular oxygen bond rearrangement reactions studied with density functional theory: Thermodynamics vs. kinetics. **F.X. Vazquez**

PHYS **535.** Creating transferrable multiscale models from all-atom data. **M. McCullagh**

PHYS **536.** Molecular polarizability as a descriptor of molecular conductance. **S. K. S. Mazinani**, R. Vatan, T. Pilarisetty, J.L. Palma, V. Mujica

PHYS **537.** Modeling electron transfer through hydrogen bonding. **M. Wimmer**, R. Vatan, T. Pilarisetty, V. Mujica, J.L. Palma

PHYS **538.** Raft environments assist the aggregation of the transmembrane region of Amyloid Precursor Protein. **N. Miyashita**, F. Ogushi, Y. Sugita

PHYS **539.** Influence of sequence and lipid type on membrane perturbation by human and rat amyloid β-peptide (1-42). **A. Brown**, D.R. Bevan

PHYS **540.** Light chain internalizes into human cardiomyocytes in a Dynamin-independent way. Amyloid fibrils recruit soluble protein in media and accelerate its internalization. **M. Marin-Argany**, M. Ramirez-Alvarado

PHYS **541.** Revisiting Thioflavin T as fibrilization sensor: What is actually probed? **J. Breffke**, M. Maroncelli

PHYS **542.** Contributions of collision-induced dissociation to collision crossSections measured using the crossSectional areas by Fourier transform ion cyclotron resonance (CRAFTI) approach. **C. Harper**, D.V. Dearden

PHYS **543.** Theoretical study of the two-photon circular dichroism of molecular structures simulating aromatic amino acids residues in proteins with secondary structures. **Y.K. Vesga Prada**, M. Higgs, C. Diaz, F. Hernandez

PHYS **544.** Analyzing small DNA constructs via chromophore model within the point dipole approximation. **P.G. Romano**

PHYS **545.** Octa-coordination and the hydrated Ba^{2+}(aq) ion. M. Chaudhari, **S.L. Rempe,** M. Soniat

PHYS **546.** Inferring latent states and force estimates via hierarchical Dirichlet process modeling in single particle tracking experiments. **C.P. Calderon**

PHYS **547.** Structure-activity and conformational-activity relationships of inhibitor of κB kinase-β. **M. Jones**, A.K. Wilson

PHYS **548.** New insight into the FMO antenna protein: Hole burning and modeling study. **A. Kell**, K. Acharya, M. Jassas, T. Reinot, J. Tang, R. Jankowiak

PHYS **549.** Computational study of folding thermodynamics and mechanism of Trp-cage mutants with RSFF2. **C. Zhou,** F. Jiang, Y. Wu

PHYS **550.** Engineering Aspects of Titania Nanotube Synthesis. **S.A. Ferdousi**, K.L. Yeung

PHYS **551.** Natural boundary condition for hydrodynamic transport is the slip boundary condition for all molecule sizes and all solvents. **S.R. Aragon**

PHYS **552.** Docking of protein models. **P. Kundrotas**, I. Anishchenko, A. Tuzikov, I. Vakser

PHYS **553.** Solvent effects on azobenzene photodynamics with spin-flip time-dependent density functional theory and effective fragment potential methods. **K. Keipert**, Y. Harabuchi, M.S. Gordon

PHYS **554.** Controlling the reactivity of large molecules by remote protonation of a side-group. J. Ditkovich, D. Pines, **E. Pines**

PHYS **555.** Bond energy orbitals: The concept and some applications. E.A. Boudreaux

THURSDAY MORNING

Section A

Colorado Convention Center
Room 501

Atmospheric Chemistry: Transformations of Matter in the Troposphere

Gas Phase Atmospheric Chemistry

D. Cziczo, M. Freedman, *Organizers*
T. H. Bertram, J. Murphy, *Presiding*

8:00 PHYS **556.** Reactions of atmospheric peroxy radicals studied by synchrotron VUV multiplexed photoionization mass spectrometry. L.G. Dodson, L. Shen, J. Savee, D.L. Osborn, N.C. Eddingsaas, S.P. Sander, C.A. Taatjes, F.J. Grieman, **M. Okumura**

8:40 PHYS **557.** Observation of the simplest criegee intermediate, CH_2OO, in the gas-phase ozonolysis of ethylene. **C. Womack**, M. Martin-Drumel, R. Field, M. McCarthy

9:00 PHYS **558.** Comprehensive theoretical mechanism for the Criegee intermediate-sulfur dioxide reaction. **K.T. Kuwata**, E.J. Guinn, M.R. Hermes, J.A. Fernandez

9:20 Intermission.

9:35 PHYS **559.** Ozone repsonses to climate change and NO_x reductions. **R.C. Cohen**

10:15 PHYS **560.** New 'bond and photons' paradigm for the tropospheric ozone budget. **P.M. Edwards**, M.J. Evans

10:35 PHYS **561.** How does nighttime oxidation of biogenic VOCs impact daytime ozone? **J. Mao**, J. Li, L. Horowitz, V. Naik, F. Paulot, M. Lin, I. Pollack, T.B. Ryerson, P.M. Edwards, K. Min, S.S. Brown, M. Graus, C. Warneke, J. Gilman, B. Lerner, A. Neuman, J.B. Nowak, P. Veres, J. Roberts, F. Lope-Hilfiker, B. Lee, J.A. Thornton, J. Kaiser, F. Keutsch, G.M. Wolfe, T.F. Hanisco, K. Wells, D. Millet, B. Henderson, K. Aikin, J. de Gouw

11:00 PHYS **562.** Novel method to estimate and evaluate OH rate constants for atmospherically relevant VOCs. **R.T. Lidster**, J.F. Hamilton, A.C. Lewis, M.J. Evans, A.R. Rickard, D.E. Heard, L.K. Whalley, D.R. Cryer, J.C. Young

11:20 Concluding Remarks.

Section B

Colorado Convention Center
Room 502

Carbon in the Galaxy: The Formation of Complex Organics from the Outflow of Carbon Stars & Their Evolution

PAH-Related Processes

L. J. Allamandola, T. J. Lee, *Organizers*
H. Cuppen, *Presiding*

8:00 PHYS **563.** Organic molecules in protoplanetary disks: Probes of planet formation and chemical evolution. **J. Najita**

8:35 PHYS **564.** Gas phase ion chemistry of complex organic species. **V.M. Bierbaum**, C.A. Cole, Z. Wang, T.P. Snow

9:10 PHYS **565.** Tying interstellar PAH emission spectra and (photo)chemistry to local physical conditions in the emission zones. **C. Boersma**

9:45 Intermission.

10:15 PHYS **566.** Dehydrogenation of PAHs: First steps towards fullerenes in the ISM. **P. Castellanos Nash**, J. Zhen, A. Candian, H. Linnartz, A. Tielens

10:50 PHYS **567.** Photochemical model of the top down formation of fullerenes in the interstellar medium. **O. Berne**, J. Montillaud, C. Joblin

11:25 PHYS **568.** Anharmonic bands in the 3-μm region of acenes: A combined experimental and theoretical study. **A. Petrignani**, E. Maltseva, A. Candian, A. Tielens, J. Oomens, W. Buma

Section C

Colorado Convention Center
Room 503

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Macromolecular Dynamics

Cosponsored by COMP

J. Gao, B. Mennucci, *Organizers*
B. C. Garrett, *Organizer, Presiding*

8:00 PHYS **569.** Computationally guided design and optimization of inhibitors of macrophage migration inhibitory factor. **W.L. Jorgensen**, D.J. Cole, M.J. Robertson

8:30 PHYS **570.** Multiscale characterization of macromolecular dynamics. **C. Clementi**

9:00 PHYS **571.** Dynamic effects in dihydrofolate reductase catalysis. **R.K. Allemann**, L. Luk, J. Loveridge

9:30 PHYS **572.** Advancing ab initio molecular dynamics via multiple-timestep methods. **R. Steele**

9:50 Intermission.

10:10 PHYS **573.** Toward a molecular theory of early and late events in monomer to amyloid fibril formation. **J.E. Straub**

10:40 PHYS **574.** Large spatiotemporal-scale quantum molecular dynamics simulations: A divide-conquer-recombine approach. **A. Nakano**, R.K. Kalia, K. Nomura, K. Shimamura, F. Shimojo, P. Vashishta

11:10 PHYS **575.** Sorbate dynamics in hierarchical porous materials. **J.I. Siepmann**, P. Bai, E. Haldoupis, M. Tsapatsis

11:30 PHYS **576.** Molecular dynamics simulations of ion transport in carbon nanotubes. **K.L. Shuford**, O. Samoylova, E. Calixte

Section D

Colorado Convention Center
Room 504

Physical Electrochemistry of Electrocatalytic Processes

Electrocatalysis of CO_2

D. A. Scherson, *Organizer*
A. Co, *Organizer, Presiding*
A. R. Asthagiri, *Presiding*

8:30 PHYS **577.** Understanding CO_2 electroreduction on Cu electrodes through first-principles modeling. **A.R. Asthagiri**

9:10 PHYS **578.** Extended π-attraction σ-repulsion model for carbon monoxide adsorbed on platinum-ruthenium-osmium-iridium quaternary alloys. **N. Dimakis**, N.E. Navarro, E.S. Smotkin

9:30 PHYS **579.** Charge-state dependent electrocatalytic activity of discretely charged, atomically-precise $Au_{25}(SR)_{18}^{q}$ nanoclusters (q = -1, 0, +1). **D. Kauffman**, D. Alfonso, C. Matranga, X. Deng, P. Ohodnicki, R. Siva, R. Jin

9:50 PHYS **580.** Investing the electroreduction pathway of carbon dioxide using surface enhanced Raman spectroscopy. J. Billy, E. Coleman, K. Muhlenkamp, **A. Co**

10:10 PHYS **581.** Pyridine-catalyzed CO_2 reduction on p-GaP photoelectrodes: First-principles investigation of possible reaction mechanisms. **M. Lessio**, C. Riplinger, A.B. Muñoz-García, E.A. Carter

Section E

Colorado Convention Center
Room 507

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Dynamics in Function and Inhibitor Design

Cosponsored by COMP

G. Hummer, *Organizer*
A. E. Garcia, *Organizer, Presiding*

8:00 PHYS **582.** Predicting drug-target binding kinetics through enhanced sampling simulations. **F. Gervasio**

‡ *Cooperative Cosponsorship*

8:35 PHYS **583.** Activation and drug design of a muscarinic G-protein coupled receptor. **Y. Miao**, J.A. McCammon

9:10 PHYS **584.** Prediction of mechanically hot spots in protein-protein interactions using perturbation response scanning method. **H. Abdizadeh**, A. Atilgan, C. Atilgan

9:45 PHYS **585.** Nucleotide-dependent interaction of K-Ras4B hypervariable region with Ras active site. T.S. Chavan, H. Jang, L. Khavrutskii, V. Gaponenko, N.I. Tarasova, **R. Nussinov**

10:20 PHYS **586.** Elucidating protein function and dynamics through molecular simulations and Markov state modeling: Allostery through conformational selection. **R.E. Amaro**, R. Malmstrom, S.S. Taylor, A. Kornev

10:55 PHYS **587.** Folding kinetics and local dynamics of the 60 nucleotide rRNA GTPase center RNA. M.J. Rau, **K.B. Hall**

Section F

Colorado Convention Center
Room 505

Modeling Excited States of Complex Systems

Nonadiabatic Effects

B. G. Levine, *Organizer*
S. A. Varganov, *Organizer, Presiding*

8:00 PHYS **588.** Excited state dynamics at complex interfaces: time-domain ab initio studies. **O.V. Prezhdo**

8:40 PHYS **589.** Geometric phase effects in non-adiabatic dynamics near two-state conical intersections. **A.F. Izmaylov**

9:20 PHYS **590.** PYXAID program: a tool for modeling excited state dynamics in complex systems. **A.V. Akimov**, O.V. Prezhdo

9:40 PHYS **591.** Self-trapping of excitons, violation of condon approximation, and efficient fluorescence in conjugated cycloparaphenylenes. **L. Adamska**, J. Liu, S. Fernandez-Alberti, R. Jasti, S.K. Doorn, S. Tretiak

10:00 Intermission.

10:20 PHYS **592.** Current view of surface hopping. **J.E. Subotnik**, B.R. Landry

11:00 PHYS **593.** Multidimensional effects in nonadiabatic statistical theories of spin-forbidden kinetics. **A. Jasper**

11:40 PHYS **594.** Semiclassical Monte-Carlo: A first principles approach to nonadiabatic molecular dynamics. **A. White**, V. Gorshkov, R. Wang, S. Tretiak, D. Mozyrsky

12:00 PHYS **595.** Modeling nonadiabatic photodynamics in aqueous environments with the ab initio multiple spawning and effective fragment potential methods. **K. Keipert**, S.R. Pruitt, M.S. Gordon

Section G

Colorado Convention Center
Room 506

Probing Nano-Plasmonic Phenomena at the Single Molecule, Single Electron, & Single Photon Level

D. J. Masiello, *Organizer*
S. Link, K. A. Willets, *Organizers, Presiding*

8:30 PHYS **596.** Single molecule chemistry probed by SERS and TERS at the nanometer length scale and picosecond time scale. **R.P. Van Duyne**

9:05 PHYS **597.** Optical characterization of pinholes in passivation layers on electrode surfaces. **K. Marchuk**, C. Renault, A.J. Bard, K.A. Willets

9:25 PHYS **598.** Plasmonic application in imaging at the single cancer cell level. **M.A. El-Sayed**

10:00 PHYS **599.** Withdrawn.

10:20 PHYS **600.** Probing magneto-plasmonic phenomena at the single nanostructure level. **K.L. Knappenberger**

10:55 PHYS **601.** Following plasmonically-enhanced chemical reactions with ultrafast Raman spectroscopies. **R.R. Frontiera**

POLY

Division of Polymer Chemistry

M. Jeffries-El, D. Boday and T. White, *Program Chairs*

SOCIAL EVENTS:

POLY Luncheon, 12:30 PM: Sun
POLY Luncheon, 12:30 PM: Mon
POLY Reception, 5:30 PM: Tue
POLY Breakfast, 7:30 AM: Tue
POLY Reception, 5:30 PM: Wed

BUSINESS MEETINGS:

POLY Programming Committee Meeting (Lunch), 12:00 PM: Tue

SUNDAY MORNING

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Cosponsored by PMSE‡

Y. C. Simon, *Organizer*
E. B. Berda, J. Foster, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **1.** Poly(phthalaldehydes) as stimuli-responsive, depolymerizable materials that are capable of providing amplified responses. **A.M. DiLauro**, S.T. Phillips

9:05 POLY **2.** Making "smarter" heparin-mimicking polymers. **N. Ayres, Y. Huang, Q. Chai**

9:35 POLY **3.** Nucleobase hydrogen bonding in polymers as a source of intelligence. **T.E. Long, K. Zhang**, M. Aiba, S. Cheng, W.D. Chiang

10:05 Intermission.

10:15 POLY **4.** Poly(phosphoester)s: From adhesives to stealth polymers. **F. Wurm**

10:45 POLY **5.** Light-degradable polymers: amplification strategies, response to new wavelengths, and application to a clinical challenge. J. Olejniczak, C. Carling, V. Nguyen Huu, A. Garcia, J. Luo, K. Zhang, **A. Almutairi**

11:15 POLY **6.** Folding single polymer chains. **C. Barner-Kowollik**, J. Willenbacher, O. Altintas

11:45 Concluding Remarks.

Section B

Sheraton Denver Downtown Hotel
Governor's Square 12

Putting Renewable Polymers to Work

D. Boday, E. C. Hagberg, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 POLY **7.** Poly(β-methyl δ-valerolactone) as a scalable and renewable soft segment for aliphatic polyester block polymers. **M.A. Hillmyer**

8:35 POLY **8.** Commercialization of triglyceride-based thermoplastic elastomers for polymer modified asphalt pavements: Where the (bio)rubber meets the road. **E.W. Cochran**, R. Williams, N. Hernandez, M. Yan, A. Hohmann, M.J. Forrester

9:05 POLY **9.** Conversion of agricultural residues into value-added products. **H. Cheng**, A. Biswas

9:35 Intermission.

9:50 POLY **10.** Synthesis and functional properties of renewable polymers. **R.M. Waymouth**, X. Zhang, B. Timothy, A.J. Ingram, K. Chung, W. Ho, J. Hedrick

10:20 POLY **11.** Design and synthesis of eumelanin-inspired polymers derived from vanillin. **T.L. Nelson**, R.P. Hopson, S. Selvaraju, N. Sachinthani

10:40 POLY **12.** Thiol-ene films derived from phenolic acids. G. Yang, H. Tesefay, **M.L. Robertson**

11:10 POLY **13.** Glass transition dynamics of biobased *poly*(ethylene 2,5-furandicarboxylate). **A. Codou**, N. Guigo, M. Moncel, L. Martino, J. Van Berkel, E. De Jong, N. Sbirrazzuoli

Section C

Sheraton Denver Downtown Hotel
Governor's Square 14

Celebrating the Fifth Year Anniversary of Polymer Chemistry (RSC)

Financially supported by Royal Society of Chemistry

D. M. Haddleton, B. S. Sumerlin, W. You, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 POLY **14.** Nature's functionality on synthetic polymers — zwitterions and inverse zwitteirons. **T. Emrick**

9:10 POLY **15.** Mimicry of photosynthesis: for the synthesis of well-defined polymers. S. Shanmugam, J. Xu, **C. Boyer**

9:40 POLY **16.** New methodology for controlled supramolecular polymerization. **X. Zhang**

10:10 Intermission.

10:30 POLY **17.** Sequential one-pot organocatalytic polymerization of epoxides and cyclic esters/carbonates. **J. Zhao**, D. Pahovnik, Y. Gnanou, N. Hadjichristidis

11:00 POLY **18.** Building smart materials from poly(2-vinyl-4,4-dimethylazlactone) scaffolds. **A.B. Lowe**

11:30 POLY **19.** Self-immolative polymersomes for high-efficiency triggered release and programmed enzymatic reactions. **G. Liu**, X. Wang, S. Liu

Section D

Sheraton Denver Downtown Hotel
Governor's Square 9

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
A. Carlmark, F. Horkay, *Presiding*

8:00 POLY **20.** Cartilage: architecture and function. **F. Horkay**, P.J. Basser

8:20 POLY **21.** Drug-functionalized cell-penetrating peptides for enhanced delivery and binding in myotonic dystrophy type 1 treatment. **Y. Bai**, L. Nguyen, Z. Song, J. Cheng, S.C. Zimmerman

8:40 POLY **22.** Novel biodegradable, biocompatible and biofunctional block copolymer scaffolds for tissue engineering applications. **P.P. Smith**, A.L. Rightler, B.K. McConnell, F. Zhang, S.O. Streubel, S. Lu, D. Price, S.G. Boyes

9:00 POLY **23.** Protein:polymer conjugates via graft-*from* ring-opening metathesis polymerization. **S.A. Isarov**, J.K. Pokorski

9:20 POLY **24.** Polylactic acid composite with natural fibers in food packaging. **S. Sedaghat**

9:40 POLY **25.** N-heterocyclic carbenes in the organopolymerization of N-substitued N-carboxy-anhydrides to polypeptoid. **I. Falivene**, M. Alghamdi, L. Cavallo

10:00 POLY **26.** Surface-initiated ring opening polymerization of carbonates and siloxanes from cellulose surfaces. S. Pendergraph, G. Klein, M.K. Johansson, **A. Carlmark**

10:20 POLY **27.** Optimizing photo-CuAAC polymerization kinetic for dental restorative materials. **H. Song**, A.D. Baranek, M. McBride, T. Gong, A. Flores, J.W. Stansbury, C.J. Kloxin, C. Bowman

10:40 POLY **28.** Chemical modification reactions of polysaccharides studied in real time by light scattering and viscometry-based methods. V.C. Spier, **A.M. Alb**

11:00 POLY **29.** Radiolabeled polymers to probe the enhanced permeability and retention effect. **M.C. Parrott**

11:20 POLY **30.** Investigating polymerization reactions with thermography: Differentiating between bulk effects, thermal diffusion and oxygen inhibition. **C. Wappl**, R. Geier, H. Freiszmuth, C. Slugovc, G. Gescheidt

11:40 POLY **31.** High performance hydrogels based on melt-assembled networks of sphere-forming block copolymers. **J. Lewis**, T.S. Bailey

12:00 POLY **32.** Smart polymers for on-demand drug delivery. Y. Zhang, K. Cai, **J. Cheng**

Section E

Sheraton Denver Downtown Hotel
Directors Row I

Macromolecular and Nanoparticle Separation Science

Cosponsored by ANYL and PMSE

Financially supported by The Dow Chemical Company, Wyatt Technology, Tosoh BioScience, Waters, NIST

K. Beers, A. K. Brewer, W. Gao, A. M. Striegel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 POLY **33.** Size exclusion chromatography/gel permeation chromatography – a blessing and curse of science and technology of synthetic polymers. **D. Berek**

9:15 POLY **34.** Industrial polymer analysis using a solvent elimination IR detector. **R. Allen**, S. Moyses, N. Jestel

9:45 POLY **35.** Is SEC-Raman a feasible way of measuring copolymer chemical heterogeneity? **A.M. Striegel**, L. Pitkanen, A.A. Urbas

10:15 Intermission.

10:30 POLY **36.** Probing serum phase oligomer in acrylic emulsion polymerization process by GPC-RI/MS. **T. Zhang**, W. Gao, R. Even, D. Kline

11:00 POLY **37.** Characterization of novel high temperature thermoplastic elastomers polybenzofulvene-block-polyisoprene-block-polybenzofulvene. **J.W. Mays**, W. Wang, T. White, N. Kang, K. Hong, R. Schlegel, M. Beiner, K. Williams, S.P. Gido

11:30 POLY **38.** Ultrahigh performance size exclusion chromatography of synthetic polymers. **M. Janco**, J.N. Alexander, E.S. Bouvier, D. Morrison

12:00 POLY **39.** Advanced polymer chromatography: Method development tools for SEC polymer analysis. **D. Morrison**, M. O'Leary

SUNDAY AFTERNOON

Section A

Sheraton Denver Downtown Hotel
Directors Row E

Next Generation Smart Materials

Bio-inspired and Biomimetic Systems

Cosponsored by PMSE‡

E. B. Berda, Y. C. Simon, *Organizers*
J. Foster, *Organizer, Presiding*
N. Zacharia, *Presiding*

1:30 Introductory Remarks.

1:35 POLY **40.** Progress towards the efficient synthesis of polymers with precisely defined mass, sequence, and stereochemistry. J. Barnes, D. Ehrlich, F. Leibfarth, T.F. Jamison, **J.A. Johnson**

2:05 POLY **41.** Programed block copolymers: At the end it is always good to be smart. **E.B. Coughlin**

2:35 POLY **42.** Tunable solid state fluorescent materials for supramolecular encryption. X. Hou, C. Ke, **J.F. Stoddart**

3:05 Intermission.

3:25 POLY **43.** Dynamic-covalent nanoparticles and self-healing hydrogels. S. Mukherjee, C.C. Deng, W. Brooks, M. Hill, **B.S. Sumerlin**

3:55 POLY **44.** Chirality-selected phase behavior in ionic polypeptide complexes. **M.V. Tirrell**