

- ORGN **779.** Diastereoselective, site-selective, and enantiospecific synthesis of 1,3-amino alcohols via azallyl anion ring-opening of epoxides. P. Daniel
- ORGN **780.** Intramolecular pyridone / benzene [4+3] meta photocyclization. C. Stockdale, S.M. Sieburth
- ORGN **781.** Organocatalytic chiral oxygenations: anti 1,2-diols from α -oxyaldehydes and α,β,γ -trioxygenation of enals. G.A. Abeykoon, S. Chatterjee, J.S. Chen
- ORGN **782.** Functionalization of alkyl C-N bonds via nickel-catalyzed Suzuki-Miyaura cross-couplings. C. Basch, J. Plane, J. Liao
- ORGN **783.** Catalytic borylation of methane: A low barrier high throughput approach. S. Berritt, K.T. Smith, M. Gonzalez Moreiras, S. Ahn, M.R. Smith, M. Baik, D.J. Mindiola
- ORGN **784.** Z-selective cross metathesis with 3(E)-1,3-dienes. J. Cannon, S. Luo, K. Engle, B.L. Taylor, K.N. Houk, R.H. Grubbs

PHYS

Division of Physical Chemistry

G. Engel, Program Chair

OTHER SYMPOSIA OF INTEREST:

- Impacts of Nanotechnology & Single Molecule Spectroscopy in Biology & Medicine (see ANYL, Tue, Wed)
- Vibrational Nanospectroscopy for Chemical & Biochemical Analysis (see ANYL, Mon, Thu)
- Computational Study of Water (see COMP, Wed)
- Elucidating the Molecular-Level Interactions Between Biological Membranes & Engineered Nanomaterials (see COLL, Tue, Wed, Thu)
- Nanostructured Interfaces: From Fundamentals of Sensing & Catalysis to Applications (see COLL, Mon, Tue, Wed, Thu)
- Recent Advances in Modeling & Simulations of Synthetic Polymers & Biopolymers (see PMSE, Wed, Thu)

SUNDAY MORNING

Section A

- DoubleTree by Hilton Hotel Philadelphia Center City
Ormandy East
- Advanced Potential Energy Surfaces**
- Classical Simulation Models & Methods**
Cosponsored by COMP
C. Skylaris, Organizer
T. L. Head-Gordon, Organizer, Presiding
- 8:00 PHYS 8.** Beyond Born-Mayer: Improved models for short-range repulsion and atomic anisotropy in standard force field. J.R. Schmidt
- 8:30 PHYS 9.** Calibration of the AMOEBA Force Field Against ab Initio EDA Methods. J. Rackers, J.W. Ponder
- 9:00 PHYS 10.** Ongoing developments in the Drude polarizable force field for biomolecules. A.D. Mackerell

- 9:30 PHYS 11.** Efficient solutions of classical polarization using hybrid extended Lagrangian/self-consistent methods. A. Albaugh, T.L. Head-Gordon, O. Demerdash
- 9:50** Intermission.
- 10:00 PHYS 12.** Many-body potential energy surfaces with chemical and spectroscopic accuracy. F. Paesani, P. Bajaj, M. Riera, S. Straight
- 10:30 PHYS 13.** Polarizable multipole based nucleic acid force field. P. Ren, C. Zhang, C. Lv, J.W. Ponder
- 11:00 PHYS 14.** Many-body expansion for energy and forces for classical polarization and its parallel implementation. O. Demerdash

Section B

- DoubleTree by Hilton Hotel Philadelphia Center City
Aria A/B
- Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory**
- Proton & Electron Transfer Reactions in Natural & Artificial Systems**
Financially supported by Coherent

- J. M. Anna, A. Nitzan, Organizers
M. R. Wasielewski, Organizer, Presiding
- 8:00 PHYS 15.** How exciton-vibrational coherences control charge separation in the photosystem II reaction center. R. van Grondelle, V. Novoderezhkin, E. Romero, P. Maly
- 8:35 PHYS 16.** Probing and exploiting vibronic coupling in charge transfer processes in metal chromophores. M. Delor, I. Sazanovich, S. Archer, T. Keane, P.A. Scattergood, A.W. Parker, A.J. Meijer, M. Towrie, J.A. Weinstein
- 9:10 PHYS 17.** Role of frustration in electron transfer reactions confined within layered manganese dioxides. R. Remsing
- 9:30** Intermission.
- 9:50 PHYS 18.** Electrochemical and photoinduced proton-coupled electron transfer in energy conversion processes. S. Hammes-Schiffer
- 10:25 PHYS 19.** Photobasicity: Thermodynamics, kinetics, and possible applications. J. Dawlaty, E. Driscoll
- 11:00 Presentation by Sponsor - Coherent.**
- 11:10** Intermission.
- 11:20 PHYS 20.** Multithermal currents in charge transfer reaction networks. G. Craven, A. Nitzan
- 11:40 PHYS 21.** Photoinduced electron and energy transfer within supramolecular donor-acceptor peptide nanostructures under aqueous conditions. T.J. Magnanelli, A.M. Sanders, J.D. Tovar, A.E. Bragg

Section C

- DoubleTree by Hilton Hotel Philadelphia Center City
Concerto A/B
- Frontiers of Solar System Chemistry: Planets to Comets & Beyond**
- Missions, Observatories & Laboratory Needs**
R. L. Hudson, S. N. Milam, Organizers, Presiding
- 8:00** Introductory Remarks.
- 8:05 PHYS 22.** Laboratory and theoretical work applied to the inference of the chemical composition of the atmospheres of Titan and of other icy moons. A. Coustenis
- 8:40 PHYS 23.** Volatiles and isotopes, and the exploration of ancient and modern Martian habitability with the Curiosity rover. P.R. Mahaffy

- 9:15 PHYS 24.** Development of an extraterrestrial organic analyzer (EOA) for highly sensitive organic detection on a European kinetic penetrator. A.M. Stockton, Z. Duca, T. Cantrell, G. Tan, M. Van Enige, M. Dorn, M. Cato, S. Foreman, J. Kim, P. Putman, A. Butterworth, P. Turin, R.A. Mathies
- 9:35** Intermission.
- 9:50 PHYS 25.** Exploration of Pluto and the Kuiper Belt by New Horizons. H. Weaver
- 10:25 PHYS 26.** Recent advances in understanding the formation and distribution of complex organic material in the atmosphere of comets. A. Remijan, S.N. Milam, M. Cordiner
- 11:00 PHYS 27.** Observations of Titan with the James Webb Space Telescope. C. Nixon, R. Achterberg, M. Adamkovics, B. Bezard, G. Bjoraker, T. Cornet, A. Hayes, E. Lellouch, M. Lemmon, M. Lopez-Puertas, S. Rodriguez, C. Sotin, N. Teanby, E. Turtle, R. West

Section D

- DoubleTree by Hilton Hotel Philadelphia Center City
Assembly E
- Intrinsically Disordered Proteins: Structure, Function & Interactions**
J. Mittal, Organizer
N. Fawzi, Organizer, Presiding
- 8:00** Introductory Remarks.
- 8:05 PHYS 28.** Atomistic and coarse-grained modeling of histone cores and tails. G. Papoian
- 8:35 PHYS 29.** Structural biophysics of intrinsically disordered proteins. S.A. Showalter, E.B. Gibbs
- 9:05 PHYS 30.** Structural effects of phosphorylation and O-GlcNAcylation: phosphothreonine is a uniquely ordered amino acid, with a large disorder-to-order transition on threonine phosphorylation. N.J. Zondlo
- 9:35** Intermission.
- 9:55 PHYS 31.** Challenges of developing biomolecular force fields for the accurate simulation of both ordered and disordered states. S. Piana-Agostinetti, P. Robustelli, D. Tan, D.E. Shaw
- 10:25 PHYS 32.** Characterization of A β monomers with multiple force fields and high pressure NMR. C. Wang, D. Rosenman, N. Clemente, A.E. Garcia

- 10:55 PHYS 33.** Dynamic and structural characterization of intrinsically disordered peptides via molecular simulations. G.H. Zerze, S.M. Vaiana, J. Mittal
- 11:15 PHYS 34.** Elucidating the structure and dynamics of RNA polymerase II C-terminal domain in complex with cancer-linked FET protein assemblies. A. Janke, N. Fawzi

Section E

- DoubleTree by Hilton Hotel Philadelphia Center City
Assembly F
- Physical Chemistry Meets AMO**
M. C. Heaven, Organizer
K. Brown, Organizer, Presiding
- 8:00 PHYS 35.** Attosecond dynamics: A time resolved x-ray spectroscopic revolution. S.R. Leone
- 8:45 PHYS 36.** Optical multidimensional coherent spectroscopy of atomic vapors and quantum dots. S. Cundiff, T. Suzuki, D. Almeida, H. Li
- 9:30 PHYS 37.** Shape and Feshbach resonances of uracil. S. Matsika, M. Fennimore
- 10:00** Intermission.
- 10:15 PHYS 38.** Crossroads between chemical dynamics, molecular spectroscopy and condensed-matter physics. R. Krems
- 11:00 PHYS 39.** Novel spectroscopic use for the velocity mapped ion imaging technique: Doppler-imaged state spectroscopy for visualization of broadening and splitting in metastable Kr transitions. D.W. Chandler, J. Guzman, J.D. Stelll, L.M. Culberson

Section F

- DoubleTree by Hilton Hotel Philadelphia Center City
Maestro B
- Physical Chemistry of Atmospheric Processes**
- Halogen & Aerosol Chemistry**
E. C. Browne, P. Ziemann, Organizers, Presiding
- 8:00 PHYS 40.** First kinetic study of the reactions of BrHg⁺ with atmospherically abundant free radicals. Y. Jiao, T.S. Dibble
- 8:20 PHYS 41.** Chemistry at interfaces over tropical oceans. R. Volkamer, T. Koenig, Y. Miyazaki, B. Dix, E.C. Apel, R. Chiu, S. Wang, R. Sommariva, R. von Glasow
- 8:55 PHYS 42.** Chlorine-initiated oxidation of isoprene: Observation of secondary hydroxyl radical chemistry by a high resolution time-of-flight chemical ionization mass spectrometer. D. Wang, L. Hildebrandt Ruiz
- 9:15 PHYS 43.** Partitioning and activation of reactive chlorine during the WINTER C-130 aircraft campaign: implications for wintertime oxidant budgets. J.A. Thornton, F. Lopez-Hilfiker, B. Lee, J. Haskins, V. Shah, L. Jaegle, D.L. Fibiger, E. McDuffie, P. Veres, S.S. Brown, T. Sparks, C. Ebben, P. Wooldridge, R.C. Cohen, J. DiGangi, G.M. Wolfe, J. Dibb, J. Schroder, P. Campuzano-Jost, D.A. Day, J.L. Jimenez, A. Sullivan, H. Guo, R. Weber, A. Weinheimer, T. Campos
- 9:50 PHYS 44.** Multiphase chlorine chemistry in biomass burning emissions. A. Ahern, L. Goldberger, L. Jahn, L. Jahl, J.A. Thornton, R.C. Sullivan

10:10 Intermission.

10:30 **PHYS 45.** Volatility means not having to say you're sticky. N.M. Donahue

11:05 **PHYS 46.** Atmospheric conditions governing aerosol particle phase organic reaction. M. Kalberer

11:40 **PHYS 47.** Processing of ambient aerosol upon transport to the indoor environment in Philadelphia winter. A. Johnson, M. Waring, P.F. DeCarlo

Modeling Water & Solvation in Biochemistry: Developments & Applications

Sponsored by COMP, Cosponsored by PHYS

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Sponsored by COMP, Cosponsored by PHYS and POLY

Quantum Mechanics

Sponsored by COMP, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

DoubleTree by Hilton Hotel Philadelphia Center City
Ormandy East

Advanced Potential Energy Surfaces

Classical Simulation Methods & Software

Cosponsored by COMP

T. L. Head-Gordon, C. Sklyaris, *Organizers*
A. MacKerrel, *Presiding*

1:00 **PHYS 48.** Fast tree method for multipolar electrostatic interactions. H.A. Boateng

1:30 **PHYS 49.** Molecular dynamics calculations with very large time steps on advanced potential energy surfaces. M.E. Tuckerman

2:00 **PHYS 50.** Lessons learned in building polarizable and fixed-charge water models. L. Wang

2:30 **PHYS 51.** Improving free energy calculations with non-Boltzmann Bennett reweighting using QM and AMOEBA. F.C. Pickard, G. Koenig, A.C. Simmonett, Y. Shao, B. Brooks

2:50 Intermission.

3:00 **PHYS 52.** Improving the accuracy of dispersion interactions through Lennard-Jones lattice summation. E.R. Lindahl

3:30 **PHYS 53.** Polarizable QM/MD simulations with the AMOEBA. J.A. Piquemal

4:00 **PHYS 54.** Multipolar electrostatics performance within domain decomposition. I. Todorov, H.A. Boateng

Technical program information known at press time.

The official technical program for the 252nd ACS National Meeting is available at:
www.acs.org/Philadelphia2016

‡ Cooperative Cosponsorship

Section B

DoubleTree by Hilton Hotel Philadelphia Center City
Ormandy West

Advances in Biological Imaging

J. S. Biteen, L. J. Webb, *Organizers*

A. B. Hummon, *Organizer, Presiding*

1:00 **PHYS 55.** IR MALDESI: A novel molecular microscopy tissue imaging strategy. D.C. Muddiman

1:40 **PHYS 56.** Advances in ambient ionization mass spectrometry for molecular imaging of biological tissues. L. Schiavinato Eberlin

2:20 **PHYS 57.** Cell-by-cell profiling of metabolic activity in the developing embryo. P. Nemes, R. Onjiko, E. Portero, S.A. Moody

3:00 Intermission.

3:20 **PHYS 58.** Illuminating tumor types: the road to precision medicine. R. Heeren

4:00 **PHYS 59.** Advancing our understanding of biology with imaging secondary ion mass spectrometry (SIMS). L. Gamble

4:40 **PHYS 60.** Characterization of theranostic nanoparticles by scanning transmission and energy filtered electron microscopies. M.A. Aronova, A.A. Sousa, R.D. Leapman

Section C

DoubleTree by Hilton Hotel Philadelphia Center City
Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

J. M. Anna, N. Nitzan, M. R. Wasielewski, *Organizers*

S. T. Roberts, *Presiding*

1:00 **PHYS 61.** Capturing intermediates of molecular solar fuels catalyzed by femto- and nanosecond mid-IR spectroscopy. L. Hammarstrom, R. Lomoth, S. Ott

1:35 **PHYS 62.** Ultrafast structural dynamics of transition metal complexes and oxides for solar energy conversion. L.X. Chen, D.K. Hayes, R. Hadt, J. Hong, M.L. Shelby, N. Jackson, M.S. Kelley

2:10 **PHYS 63.** Understanding electron dynamics in mixed metal oxide catalysts showing high selectivity for photo-electrochemical CO₂ reduction to acetate. L. Baker

2:30 Intermission.

2:45 **PHYS 64.** Carrier-specific dynamics in hybrid perovskite photovoltaics probed with transient XUV spectroscopy. J. Vura-Weis, M. Lin, M.A. Verkamp, E.S. Ryland, K. Benke

3:20 **PHYS 65.** Bulk carrier dynamics in organo-halide perovskites without growing bulk crystals through surface passivation. J.B. Asbury

3:55 Intermission.

4:05 **PHYS 66.** Accessing triplet states for exciton fission and fusion in organic semiconductors. C.J. Bardeen

4:40 **PHYS 67.** Controlling charge recombination in conjugated block-copolymer photovoltaics by chemical design of their covalent linkage. C. Grieco, M.P. Aplan, A. Rimshaw, Y. Lee, T. Le, E.D. Gomez, J.B. Asbury

Section D

DoubleTree by Hilton Hotel Philadelphia Center City
Concerto A/B

Frontiers of Solar System Chemistry: Planets to Comets & Beyond

Chemistry, Moons & Small Bodies: Ice & Rock

S. N. Milam, *Organizer*

R. L. Hudson, *Organizer, Presiding*

M. J. Loeffler, *Presiding*

1:00 **PHYS 68.** Chemical and isotopic diversity of cometary volatiles: A window on evolutionary processes from the interstellar medium to icy planetesimals. M.J. Mumma

1:35 **PHYS 69.** Chemical origin of the colors of objects in the outer solar system and the Kuiper belt object-Jupiter Trojan connection. M. Brown

2:10 **PHYS 70.** Implications of recent measurements of the photodissociation of N₂, O₂, CO, and CO₂ in the windowless region of the vacuum ultraviolet (VUV) on cometary, planetary, and interstellar chemistry. K. Liu, Y.C. Chang, C. Ng, W.M. Jackson

2:30 Intermission.

2:45 **PHYS 71.** Compositions in the Pluto system as Investigated by New Horizons. W. Grundy, D. Cruikshank, C. Olkin, S. Stern, K. Ennico-Smith, L. Young, H. Weaver

3:20 **PHYS 72.** PAHs, Dust and ice in the solar system. A.L. Mattioda, G. Cruz-Diaz

3:55 **PHYS 73.** Methanol photolysis in the production of organic matter during solar system formation. S.L. Widicus Weaver, M. McCabe, C. Powers, S. Zinga

Section E

DoubleTree by Hilton Hotel Philadelphia Center City
Assembly E

Intrinsically Disordered Proteins: Structure, Function & Interactions

N. Fawzi, J. Mittal, *Organizers*

S. A. Showalter, *Presiding*

1:00 **PHYS 74.** All-atom models for intrinsically disordered proteins: Structure, dynamics and experimental interpretation. W. Zheng, G. Zerze, A. Borgia, M. Borgia, H. Hofmann, B. Schuler, J. Mittal, R.B. Best

1:30 **PHYS 75.** Post-translational modifications and membrane composition influence the interaction of huntingtin with lipid membranes. J.A. Legleiter, M. Chaibva, X. Gao

2:00 **PHYS 76.** Characterizing the free energy landscape of intrinsically disordered proteins by metadynamics simulation and experiments. D. Granata, G. Zerze, J. Mittal, M. Vendruscolo, A. Laio

2:30 Intermission.

2:50 **PHYS 77.** Ramachandran map analysis of the monomeric Aβ1-40 and Aβ1-42 peptides by solution NMR reveals very similar random coil distributions. J. Roche, A. Bax

3:20 **PHYS 78.** Characterizing disorder to order transitions in proteins. C. Stultz

3:50 **PHYS 79.** Computational methods and models for intrinsically disordered peptides. T.L. Head-Gordon

Section F

DoubleTree by Hilton Hotel Philadelphia Center City
Assembly F

Physical Chemistry Meets AMO

K. Brown, M. C. Heaven, *Organizers*

B. Odom, *Presiding*

1:00 **PHYS 80.** Ultracold molecular assembler. K. Ni

1:45 **PHYS 81.** Ultracold molecules and chemistry. R. Cote

2:30 **PHYS 82.** Towards state-resolved ultracold chemical reactions with KRb molecules. Y. Liu, Y. Chen, M. Hu

3:00 Intermission.

3:15 **PHYS 83.** Towards quantum-state-resolved charged-neutral chemistry. E.R. Hudson

4:00 **PHYS 84.** AMO methods for precise studies of chemical reactions. S. Willitsch

Section G

DoubleTree by Hilton Hotel Philadelphia Center City
Maestro A

Physical Chemistry of Atmospheric Processes

Aerosol Chemistry

P. Ziemann, *Organizer*

E. C. Browne, *Organizer, Presiding*

J. Thornton, *Presiding*

1:00 **PHYS 85.** Organic photosensitizer chemistry in atmospheric aerosols: New insights from laboratory and modeling studies. V.F. McNeill, W.G. Tsui, Y. Rao

1:35 **PHYS 86.** Enrichment of organic matter and carbohydrates in nascent sea spray aerosol. T. Jayaratne, R. Cochran, C. Lee, C. Sultana, K. Moore, C. Cappa, T. Bertram, K.A. Prather, V.H. Grassian, E.A. Stone

2:10 **PHYS 87.** Marine atmospheric particle chemical composition in the Arctic. K.A. Pratt, R. Kirpes, M. Gunsch, A.P. Ault, B. Alexander, T. Barrett, R.J. Sheesley, A. Laskin, B. Wang, S. China

2:45 Intermission.

3:05 **PHYS 88.** Atmospheric processing and novel source identification of aerosols over Antarctica. M. Giordano, L. Kalnajs, A. Johnson, J.D. Goetz, S. Davis, T. Deshler, P.F. DeCarlo

3:40 **PHYS 89.** Sea spray aerosol – it's not just salt: Molecular characterization, hygroscopicity and heterogeneous reactivity of the organic and biological components. V.H. Grassian

4:15 **PHYS 90.** Constraining the importance of nocturnal chemistry to particle nitrate production in the San Joaquin Valley. C. Cappa, G. Prabhakar, X. Zhang, C. Parworth, Q. Zhang, D. Young, H. Kim, S. Pusede, R.C. Cohen, L. Ziemba, A. Beyersdorf, J.B. Nowak, T. Bertram

Modeling Water & Solvation in Biochemistry: Developments & Applications

Sponsored by COMP, Cosponsored by PHYS

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Sponsored by COMP, Cosponsored by PHYS and POLY

MONDAY MORNING

Section A

DoubleTree by Hilton Hotel Philadelphia Center City

Ormandy East

Advanced Potential Energy Surfaces

QM with MM

Cosponsored by COMP

T. L. Head-Gordon, C. Skylaris, *Organizers*

Y. Shao, *Presiding*

8:00 PHYS 91. Density functional theory for non-covalent interactions: Recent advances and implications for QM/MM. M.P. Head-Gordon

8:30 PHYS 92. BioEFP: polarizable embedding in biological systems. L.V. Slipchenko

9:00 PHYS 93. Modeling of electrostatics and polarization effects in embedded systems within quantum chemical approaches. B. Mennucci

9:30 PHYS 94. How do extended Lagrangian schemes perform for classical polarizable force fields and density functional theory? V. Vitale, A. Albaugh, J. Dziedzic, T.L. Head-Gordon, C. Skylaris

9:50 Intermission.

10:10 PHYS 95. Implementation and assessment of the AMOEBA water model for fully polarizable QM/MM calculations. Y. Mao, Y. Shao, T.L. Head-Gordon, M.P. Head-Gordon

10:30 PHYS 96. DFTB3: recent developments. Q. Cui

11:00 PHYS 97. How carbohydrate-active enzymes work. Insights from QM/MM metadynamics simulations. L. Raich, J. Iglesias-Fernández, A. Ardévol, C. Rovira Virgili

11:30 PHYS 98. Polarizable QM/MM based on the AMOEBA force field and linear-scaling DFT. J. Dziedzic, Y. Mao, Y. Shao, M.P. Head-Gordon, T.L. Head-Gordon, C. Skylaris

Section B

DoubleTree by Hilton Hotel Philadelphia Center City

Ormandy West

Advances in Biological Imaging

J. S. Biteen, A. B. Hummon, *Organizers*

L. J. Webb, *Organizer, Presiding*

8:00 PHYS 99. Nanoscience approaches to heterogeneity in biological systems. P.S. Weiss

8:40 PHYS 100. Plasmonic views of lipid membranes on gold nanorods. J.H. Hafner, J. Matthews, C. Payne, S. Demmers, G. Isakson, C. Shirazinejad

9:20 Intermission.

9:40 PHYS 101. Terminal alkynes as Raman probes of α -Synuclein amyloid formation. J.D. Flynn, J.C. Lee

10:00 PHYS 102. Label-free super-resolution microscopy. R.R. Frontiera

10:40 PHYS 103. Fast relaxation imaging of protein structure, stability, and folding in biomaterial environments with variable crowding. L. Kisley, P.V. Braun, M. Gruebele, D.E. Leckband

Section C

DoubleTree by Hilton Hotel Philadelphia Center City

Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

J. M. Anna, A. Nitzan, M. R. Wasielewski, *Organizers*

J. Vura-Weis, *Presiding*

8:00 PHYS 104. Designer nanocrystal materials for photovoltaics. C.R. Kagan, D. Straus, E. Goodwin, E.A. Gaulding, S. Oh, C.B. Murray

8:35 PHYS 105. Two birds with one stone: Tailoring singlet fission for both triplet yield and exciton diffusion length. T. Zhu, Y. Wan, G. Zhi, J.C. Johnson, L. Huang

8:55 Intermission.

9:10 PHYS 106. Enabling singlet fission by controlling intramolecular charge transfer in π -stacked covalent terylene diimide dimers. M.R. Wasielewski, E. Margulies, C.E. Miller, Y. Wu, L. Ma, R. Young, G. Schatz

9:45 PHYS 107. Singlet Fission in isolated molecular dimers and in amorphous thin films. S.E. Bradforth

10:20 Intermission.

10:30 PHYS 108. Dynamics at the donor/acceptor interface in organic solar cells. J.E. Bredas

11:05 PHYS 109. Utilizing singlet fission materials to repack solar energy. A.K. Le, J.A. Bender, R. Pandey, A.P. Moon, S.T. Roberts

11:40 PHYS 110. Withdrawn.

Section D

DoubleTree by Hilton Hotel Philadelphia Center City

Assembly E

Intrinsically Disordered Proteins: Structure, Function & Interactions

N. Fawzi, J. Mittal, *Organizers*

R. B. Best, *Presiding*

8:00 PHYS 111. Regulation of intrinsically disordered peptides. J.E. Shea

8:30 PHYS 112. Experimental assessment of the conformational distribution of a disordered peptide. F. Gai

9:00 PHYS 113. Sequence determinants of the phase behavior of intrinsically disordered proteins. R.V. Pappu

9:30 Intermission.

9:50 PHYS 114. Liquid structure of elastin. R. Pomes

10:20 PHYS 115. Elastin and beyond: New peptide polymers that display aqueous coacervation behavior. A. Chilkoti

10:50 PHYS 116. Towards reliable atomistic simulation of disordered protein ensembles. J. Chen

Section E

DoubleTree by Hilton Hotel Philadelphia Center City

Assembly F

Physical Chemistry Meets AMO

K. Brown, M. C. Heaven, *Organizers*

E. R. Hudson, *Presiding*

8:00 PHYS 117. Probabilistic rotational state preparation of a single molecular ion through consecutive partial projection measurements. M. Drewsen

8:45 PHYS 118. Direct laser cooling and trapping of polar molecules. D. McCarron, M. Steinecker, Y. Zhu, E. Norrgard, D. DeMille

9:30 Intermission.

9:45 PHYS 119. Adding trapped molecules to the quantum toolkit. B. Odom

10:30 PHYS 120. Effect of conical intersections on chemical reactivity of ultracold molecules in optical potential. S. Kotochigova

Section F

DoubleTree by Hilton Hotel Philadelphia Center City

Maestro A

Physical Chemistry of Atmospheric Processes

Characterization of Emissions

E. C. Browne, P. Ziemann, *Organizers*

C. Cappa, E. A. Stone, *Presiding*

8:00 PHYS 121. Mass spectral characterization of aerosol emissions from South Asian combustion sources. J.D. Goetz, M. Giordano, C. Stockwell, T. Christian, P. Bhawe, P. Praveen, A. Panday, T. Jayarathne, E.A. Stone, R. Yokelson, P.F. DeCarlo

8:20 PHYS 122. Measurements of volatile organic compounds in the atmosphere using a novel H₂O⁺ time-of-flight chemical ionization mass spectrometry instrument. J. de Gouw, A. Koss, B. Yuan, M. Coggon, K. Sekimoto, P. Veres, J.M. Roberts, B. Lerner, J. Gilman, C. Warneke

8:55 PHYS 123. Following emissions from non-traditional oil and gas development through their impact on tropospheric ozone. E.V. Fischer, D. Farmer, I.B. Pollack, A. Abeleira, J. Lindsaas, Z. Tzompa Sosa, J. Zaragoza, E. Emerson, F. Flocke, J.R. Roscioli, S.C. Herndon

9:30 PHYS 124. Sources of secondary organic aerosol in the Front Range of Colorado. R. Bahreini, K.K. Vu, J. Dingle, R. Ahmadov, S. McKeen, E.C. Apel, T.L. Campos, C. Cantrell, F. Flocke, A. Fried, J. Gilman, S.C. Herndon, A.H. Hills, R.S. Hornbrook, G. Huey, L. Kaser, B. Lerner, R. Mauldin, D.D. Montzka, J.B. Nowak, D. Richter, J. Roscioli, S. Shertz, M. Stell, D. Tanner, G.S. Tyndall, J. Walega, P. Weibring, A. Weinheimer

10:05 Intermission.

10:25 PHYS 125. VOC emissions from gasoline vehicles: high time resolution VOC profiles and implications for future fleet emissions and pollutant formation. G. Drozd, Y. Zhao, B. Frodin, R. Saleh, G. Saliba, H. Maldonado, S. Sardar, A. Robinson, A. Goldstein

10:45 PHYS 126. Studies of the selective transfer of biological species from the ocean to the atmosphere. K.A. Prather

11:20 PHYS 127. Emission and chemical transformation of marine volatile organic compounds. T.H. Bertram, M. Kim, M. Zuerb

Section G

DoubleTree by Hilton Hotel Philadelphia Center City

Maestro B

Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications

M. Sfeir, G. Wang, j. Zheng, *Organizers*

R. Jin, *Organizer, Presiding*

8:00 PHYS 128. Magic-size semiconductor nanoclusters in the (II-VI)₁₃ and (II-VI)₃₄ families. Y. Zhou, Y. Wang, F. Wang, W.E. Buhro

8:35 PHYS 129. Nanoscale building blocks in solid-state chemistry. X. Roy

9:10 Intermission.

9:25 PHYS 130. Periodicities in atomically precise gold nanoclusters. C. Zeng, R. Jin

9:45 PHYS 131. Atomically precise doping and size control of silver nanoclusters. O.M. Bakr

10:20 PHYS 132. Role of magic-sized clusters in the growth of InP quantum dots. B.M. Cossairt, D. Gary

10:55 PHYS 133. Gold nanoclusters for the highly chemoselective hydrogenation of nitrobenzaldehyde. G. Li

Modeling Water & Solvation in Biochemistry: Developments & Applications

Sponsored by COMP, Cosponsored by PHYS

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Sponsored by COMP, Cosponsored by PHYS and POLY

Pioneering Single Molecule Detection under Ambient, Aqueous Conditions: A Tribute to Richard Keller

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Quantum Mechanics

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QM/MM Simulation of Chemical & Biochemical Reaction Pathways: Recent Developments & Applications

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MONDAY AFTERNOON

Section A

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy East

Advanced Potential Energy Surfaces

Excited State Surfaces & Spectroscopy

Cosponsored by COMPT

T. L. Head-Gordon, *Organizer*

C. Skylaris, *Organizer, Presiding*

1:00 PHYS 134. Fragment-based models for calculating accurate potential energy surfaces and spectroscopic properties of large molecules and nanoscale systems. K. Raghavachari

1:30 PHYS 135. Spin-flip time-dependent density functional theory for exploring excited-state potential energy surfaces. X. Zhang, J. Herbert

2:30 PHYS 136. Ground and excited state ab initio molecular dynamics using graphical processing units. T.J. Martinez

2:30 PHYS 137. Excited-state dynamics of mPlum fluorescent protein. S. Faraji, A. Krylov

2:50 Intermission.

3:10 PHYS 138. Smoothing out excited-state dynamics: Dynamically weighted multiconfigurational self-consistent field. W.J. Glover

3:30 PHYS 139. Autoionizing resonances as gateway states for electron-attachment induced chemistry. K.B. Bravaya

4:00 PHYS 140. Role of excited states in determining the electronic structure and reactivity of complex molecular systems. S. Xantheas

Section B

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy West

Advances in Biological Imaging

J. S. Biteen, L. J. Webb, *Organizers*

A. B. Hummon, *Organizer, Presiding*

1:00 PHYS 141. MALDI mass spectrometric imaging (MSI) of endogenous signaling molecules in biological systems. L. Li

1:40 PHYS 142. Is the site of influenza virus assembly and budding enriched with cholesterol and sphingolipids? M.L. Kraft, A.N. Yeager, P.K. Weber, J. Zimmerberg

2:20 PHYS 143. Spatial metabolomics: Molecular annotation, visualization, and interpretation. T. Alexandrov

3:00 Intermission.

Technical program information known at press time.

The official technical program for the 252nd ACS National Meeting is available at:

www.acs.org/Philadelphia2016

‡ Cooperative Cosponsorship

3:20 PHYS 144. Tunable fluidic device for modeling the invasive tumor microenvironment in a colon carcinoma three dimensional tumor model. E. Weaver, A.B. Hummon, P. Zorlutuna

4:00 PHYS 145. Single-molecule fluorescence probes interaction between individual nanoparticles and proteins. D. Wang, D.K. Schwartz

Section C

DoubleTree by Hilton Hotel Philadelphia
Center City

Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

A. Nitzan, M. R. Wasielewski, *Organizers*

J. M. Anna, *Organizer, Presiding*

1:00 PHYS 146. Two-dimensional electronic spectroscopy of light-harvesting complexes. T.C. Jansen, R. Tempelaar

1:35 PHYS 147. Coarse-grained simulation of long range exciton dynamics in aggregates of light harvesting 2 (LH₂) complexes of purple bacteria. S. Jiang

2:10 PHYS 148. Chromophore specific spectral density of the Fenna-Matthews-Olson complex from dynamics simulations with first-principle quantum chemistry data. Y.M. Rhee, C.W. Kim

2:30 Intermission.

2:45 PHYS 149. Coherence in ultrafast chemistry. G.D. Scholes

3:20 PHYS 150. Electronic-Vibrational multidimensional spectroscopy to elucidate the origin of coherences in photosynthetic systems. E. Harel

3:55 Intermission.

4:05 PHYS 151. Elucidating the nanoscale dynamics of photo-induced phase separation in mixed halide hybrid perovskites. C.G. Bischak, D. Limmer, N.S. Ginsberg

4:40 PHYS 152. Probing dynamics of delocalization and energy transfer in Rhodobacter sphaeroides using two-dimensional electronic spectroscopy. S.C. Massey, P.D. Dahlberg, P. Ting, S. Soltan, C. Hunter, G.S. Engel

Section D

DoubleTree by Hilton Hotel Philadelphia
Center City

Concerto A/B

Frontiers of Solar System Chemistry: Planets to Comets & Beyond Chemistry, Ices & Icy Worlds

R. L. Hudson, S. N. Milam, *Organizers, Presiding*

1:00 PHYS 153. Radiation chemistry of cometary and planetary ices with in situ mass spectrometry. B.L. Henderson, M.S. Gudipati

1:35 PHYS 154. Radiation chemistry on the surfaces of ocean worlds of the outer solar system. K. Hand

2:10 PHYS 155. Radiation-induced production of near-surface volatiles on simulated Europa's surface. M.S. Gudipati, B.L. Henderson, B. Fleury, N. Rivas

2:30 PHYS 156. Application of tunable vacuum ultraviolet (VUV) light for the isomer-specific detection of complex organic molecules formed via interaction of ionizing radiation with simple and mixed astrophysical ice analogues. M. Abplanalp, R. Kaiser

2:50 Intermission.

3:05 PHYS 157. Space weathering effects on Europa and other Jovian satellites. C. Hibbitts, C. Paranicas

3:40 PHYS 158. New laboratory measurements of solid methanol at temperatures relevant to interstellar and outer solar system environments. P.A. Gerakines, T. Tway, R.F. Ferrante, R.L. Hudson

4:00 PHYS 159. Rotational spectroscopy of O(D) insertion reaction products for astrochemistry. B. Hays, M. McCabe, N. Wehres, S. Zinga, C. Powers, L. Zou, B.A. DePrince, J. Laas, S.L. Widicus Weaver

Section E

DoubleTree by Hilton Hotel Philadelphia
Center City

Assembly E

Intrinsically Disordered Proteins: Structure, Function & Interactions

N. Fawzi, J. Mittal, *Organizers*

R. V. Pappu, *Presiding*

1:00 PHYS 160. Chiral sum frequency generation spectroscopy for probing aggregation and orientation of amyloid proteins at lipid/water interface. E.C. Yan, L. Fu, V.S. Batista, D. Xiao

1:30 PHYS 161. IDPs on the brain: The role of disordered proteins and their interactions in brain function and dysfunction. D. Eliezer

2:00 PHYS 162. Illuminating the denatured state ensemble: Direct observation of chain compaction. D.P. Raleigh, I. Peran, J. Zou, Kathuria, C.L. Simmerling, C.R. Matthews, O. Bilse

2:30 Intermission.

2:50 PHYS 163. Triggers of alpha-synuclein aggregation and inhibition in Parkinson's disease. J. Baum, M. Janowska, M. Olson, T. Atieh, A. Nunes, G. Moriarty

3:20 PHYS 164. Fibril formation by intrinsically disordered peptides and proteins: Structural insights from solid state NMR. R. Tycko

3:50 PHYS 165. Unveiling dark matter in biology. D. Libich, V. Tugarinov, A. Ceccon, G.M. Clore

Section F

DoubleTree by Hilton Hotel Philadelphia
Center City

Assembly F

Physical Chemistry Meets AMO

K. Brown, *Organizer*

M. C. Heaven, *Organizer, Presiding*

1:00 PHYS 166. Cold and controlled complex molecules for studies of chemical reactivities and dynamics. J. Küpper

1:45 PHYS 167. Cold controlled reactions between molecular ions and molecular radicals. H. Lewandowski

2:30 PHYS 168. Ion-atom hybrid trap within a Fabry-Perot cavity: Cold interaction studies. J. Saraladevi, T. Ray, S. Dutta, S. Rangwala

3:00 Intermission.

3:15 PHYS 169. Ion-molecule reactions below 1 K: The H₂⁺+H₂ = H₃⁺+H reaction at low temperature. F. Merkt, J. Deiglmayr, P. Allmendinger, O. Schullian, K. Hoeveler

4:00 PHYS 170. Characterising cold ion-molecules reactions in Coulomb crystals. B. Heazlewood

Section G

DoubleTree by Hilton Hotel Philadelphia
Center City

Maestro A

Physical Chemistry of Atmospheric Processes

Fundamental Studies of Gas-Phase Processes

E. C. Browne, P. Ziemann, *Organizers*

N. M. Donahue, D. Heard, *Presiding*

1:00 PHYS 171. Gas phase reaction of CH₂O₂ radicals with OH studied over the 292 – 526 K temperature range. C. Yan, S. Kocovska, L.N. Krasnoperov

1:20 PHYS 172. Using computation to clarify the atmospheric reactivity of the vinyl hydroperoxide. K.T. Kuwata

1:40 PHYS 173. Investigations on the formation of organic nitrates in alkene oxidation. G.S. Tyndall, J.D. Crounse, A. Teng, P. Wennberg, F.F. Østerstrom, J.J. Orlando

2:15 PHYS 174. Low pressure yields of stabilized Criegee intermediates produced from ozonolysis of trans-2-butene and 2,3-dimethyl-2-butene. M. Campos-Pineda, J. Zhang

2:35 PHYS 175. Exploring uncharted regions of atmospheric reaction pathways. M.I. Lester

3:10 Intermission.

3:25 PHYS 176. Thermochemistry and kinetic modeling for OH addition to propene and O₂ association to the CH₂(OH)C⁺HCH₃ adduct. J.W. Bozzelli, S. Snitsiriwat

3:45 PHYS 177. Full-dimensional model of ozone forming reaction: Absolute value of recombination rate coefficient, its pressure and temperature dependencies. A. Teplukhin, D. Babikov

4:05 PHYS 178. Are spectroscopic arcanae relevant to geochemistry? R. Field, S. Ono, A. Hull

4:40 PHYS 179. Finding unexpected photolysis pathways in atmospheric chemistry. A.W. Hull, S. Ono, R. Field

Section H

DoubleTree by Hilton Hotel Philadelphia
Center City

Maestro B

Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications

R. Jin, M. Steir, G. Wang, *Organizers*

J. Zheng, *Organizer, Presiding*

1:00 PHYS 180. Spooling electrochemiluminescence spectroscopy for Au nanoclusters. Z. Ding, M. Hesari, M.S. Workentin

1:35 PHYS 181. Electrogenerated chemiluminescence from aqueous soluble Au nanoclusters under ambient conditions. G. Wang, T. Wang, D. Wang, J. Padelford, J. Jiang

2:10 PHYS **182**. PbS Colloidal nanocrystal linewidths are strongly influenced by multiple emissive states. J.R. Caram, S. Bertram, H. Utzat, M.G. Bawendi

2:30 Intermission.

2:50 PHYS **183**. Ultrafast dynamics of thiolate-protected gold nanoclusters. M. Pettersson

3:25 PHYS **184**. Molecular-like carrier dynamics in bulk-like Au₃₆ nanoclusters. M. Sfeir, M. Zhou, K. Appavoo, R. Jin

4:00 PHYS **185**. Single atom doping alters the ultrafast electron dynamics of M₁Au₂₄(SR)₁₈ (M=Pd, Pt) nanoclusters. M. Zhou, H. Qian, M. Sfeir, K. Nobusada, R. Jin

Modeling Water & Solvation in Biochemistry: Developments & Applications

Sponsored by COMP, Cosponsored by PHYS

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

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Pioneering Single Molecule Detection under Ambient, Aqueous Conditions: A Tribute to Richard Keller

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QM/MM Simulation of Chemical & Biochemical Reaction Pathways: Recent Developments & Applications

Sponsored by COMP, Cosponsored by PHYS

MONDAY EVENING

Section A

Pennsylvania Convention Center
Halls D/E

Sci-Mix

G. S. Engel, Organizer

8:00 - 10:00

347-350, 360, 363, 367-370, 378-379, 381, 386, 391, 394, 396, 398, 400-401, 407-408, 410-411, 414, 416, 420-421, 423, 435-436, 441, 444, 447, 449, 457, 462, 466, 468-470, 477, 479-480, 483-485. See subsequent listings.

TUESDAY MORNING

Section A

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy East

Advanced Potential Energy Surfaces

Ab initio Molecular Dynamics

Cosponsored by COMP

T. L. Head-Gordon, C. Skylaris, Organizers

A. Alexandrova, Presiding

8:00 PHYS **186**. First principles molecular dynamics of heterogeneous materials. G.A. Galli

8:30 PHYS **187**. Molecular simulations on neuronal G-protein coupled receptors. P. Carloni

9:00 PHYS **188**. Optimization of an exchange-correlation density functional for water. M. Fernandez-Serra, M. Fritz, J.M. Soler

9:30 PHYS **189**. Unified theoretical approach to chemical reactions in gas phase and in solution. F. Pietrucci, A. Saitta

9:50 Intermission.

10:00 PHYS **190**. First-principles and force field based simulations of organic/inorganic halide perovskites. U. Rothlisberger

10:30 PHYS **191**. Confinement effects on ab-initio liquid water. L. Pestana, T.L. Head-Gordon

11:00 PHYS **192**. Modeling black titania with first principles and reactive field molecular dynamics simulations. A. Selloni, S. Selcuk

11:30 PHYS **193**. Dipole polarizability of a water molecule in liquid water. R.A. Distasio

Section B

DoubleTree by Hilton Hotel Philadelphia
Center City

Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

A. Nitzan, M. R. Wasielewski, Organizers

J. M. Anna, R. D. Pensack, Presiding

8:00 PHYS **194**. Untangling ultrafast spectroscopy of earth abundant iron light harvesters using theory. L.A. Fredin

8:35 PHYS **195**. Effects of aggregation on the photophysics and dynamics of a high performing conjugated organic polymer. T. Fauvell, L.X. Chen, L. Yu, N. Jackson

8:55 PHYS **196**. Vibrational and electronic evolution of photoexcited porphyrin: Multidimensional pump-degenerate four-wave mixing spectra. B. Abraham, L. Gundlach

9:15 Intermission.

9:30 PHYS **197**. Photophysics and spectroscopy of carotenoid dimers. M.J. Tauber

9:50 PHYS **198**. Multiscale model of light harvesting by photosystem II in plants. D. Bennett, K. Amarnath, A. Schneider, G.R. Fleming

10:10 PHYS **199**. Catalytic cycle of water splitting in photosystem II: QM/MM characterization. K. Yang, V.S. Batista

10:30 Intermission.

10:40 PHYS **200**. Electronic structure and early-time dynamics of higher-lying excited states in light harvesting complex 1 from Rhodospirillum rubrum. P. Ting, P.D. Dahlberg, S.C. Massey, C. Hunter, G.S. Engel

11:00 PHYS **201**. Charge recombination suppressed by destructive quantum interference in heterojunction materials. R. Tempelaar, J. Koster, R. Havenith, J. Knoester, T.C. Jansen

11:35 PHYS **202**. Electronic transitions directed by quantum confinement for increased quantum efficiency in methylammonium lead iodide perovskite quantum dots. D. Vogel, A. Kryjevski, T.M. Inerbaev, D. Kilin

Section C

DoubleTree by Hilton Hotel Philadelphia
Center City

Concerto A/B

Frontiers of Solar System Chemistry: Planets to Comets & Beyond

Chemistry: Surfaces & Sub-Surfaces

S. N. Milam, Organizer

R. L. Hudson, Organizer, Presiding

M. S. Gudipati, Presiding

8:00 PHYS **203**. Water on the Moon and Mercury: To be or not to be? T.M. Orlando

8:35 PHYS **204**. Tholins as coloring agents on solar system bodies: New results from Pluto. D. Cruikshank, C. Materese, S.A. Sandford, H. Imanaka, M. Nuevo, S. Stern, H. Weaver, C. Olkin, L. Young, K. Ennico-Smith, N. COMP Team

9:10 PHYS **205**. Carbonaceous coatings produced via surface-mediated reactions: Are they fluffy? F.T. Ferguson, N. Johnson, J. Nuth

9:30 Intermission.

9:45 PHYS **206**. Surface of the Moon and its interaction with the external environment. J. Keller

10:20 PHYS **207**. Clathrates in the outer Solar System: occurrence and detection. D. Nna-Mvondo

10:55 PHYS **208**. Capture of hyperthermal CO₂ by amorphous water ice via molecular embedding. G. Langlois, W. Li, K.D. Gibson, S.J. Sibener

Section D

DoubleTree by Hilton Hotel Philadelphia
Center City

Assembly E

Intrinsically Disordered Proteins: Structure, Function & Interactions

N. Fawzi, J. Mittal, Organizers

S. M. Vaiana, Presiding

8:00 PHYS **209**. Crowding effects on intrinsically disordered proteins. D. Thirumalai

8:30 PHYS **210**. Macromolecular crowding effects on the intrinsically disordered proteins: A simple model reveals complex behavior. Y. Kim, C. Miller, J. Mittal

9:00 PHYS **211**. Conformations and exchange dynamics of FlgM, an intrinsically disordered protein, in dilute and crowded conditions. P.E. Smith, A. Banks, H. Zhou

9:30 Intermission.

9:50 PHYS **212**. Disordered proteins and tardigrade survival. S. Piszkiwicz, A. Mehta, B. Goldstein, T. Boothby, G.J. Pielak

10:20 PHYS **213**. Intrinsically disordered proteins as physical drivers of membrane traffic. J.C. Stachowiak

10:50 PHYS **214**. Selective diffusion in the nuclear pore. D. Cowburn, S. Sparks

Section E

DoubleTree by Hilton Hotel Philadelphia
Center City

Assembly F

Physical Chemistry Meets AMO

K. Brown, M. C. Heaven, Organizers

B. Heazlewood, Presiding

8:00 PHYS **215**. Vibrational energy relaxation of vibration-cavity polariton modes. A.D. Dunkelberger, K. Fears, B.T. Spann, B. Simpkins, J. Owrutsky

8:30 Intermission.

8:45 PHYS **216**. Probing the internal energy content of cold molecular ions. J.H. Bartlett, R.A. VanGundy, A.B. Dermer, M.L. Theis, K.J. Mascartolo, M.C. Heaven

9:15 PHYS **217**. Supersonic flows meet lasers in the service of astrochemistry. I.R. Sims

Section F

DoubleTree by Hilton Hotel Philadelphia
Center City

Maestro A

Physical Chemistry of Atmospheric Processes

Oxidants & Radicals

E. C. Browne, P. Ziemann, Organizers

J. D. Raff, K. R. Wilson, Presiding

8:00 PHYS **218**. Some known unknowns in atmospheric oxidation chemistry. W. Brune, K.E. Christian, D.O. Miller, B.C. Baier, J. Mao

8:35 PHYS **219**. Radical chemistry and ozone production in central London. D. Heard

9:10 PHYS **220**. Wall loss rates of HO₂ and several organic peroxy radicals onto common sampling materials. E. Wood, S. Kundu, B. Deming, D. Rollings

9:30 PHYS **221**. Identifying the major formation pathways of highly oxidized multifunctional (HOM) compounds from autoxidation of α -pinene. M. Ehn, O. Peräkylä, C. Yan, L. Quéiéver, M. Riva, M.P. Rissanen, D.R. Worsnop

10:05 Intermission.

10:25 PHYS **222**. Withdrawn.

10:45 PHYS **223**. Temperature, NO_x emissions and O₃: Insights from observations in the southeast U.S. R.C. Cohen

11:20 PHYS **224**. New insights into low-NO_x isoprene oxidation chemistry. J. Rivera, E. Praske, R. Zhao, J.D. Crounse, A. Lee, K. Skog, K. Bates, J.P. Abbatt, J. Mao, G.S. Tyndall, P. Wennberg, F. Keutsch

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Section G

DoubleTree by Hilton Hotel Philadelphia
Center City

Maestro B

**Metal & Semiconductor
Nanoclusters with Atomic Precision:
Fundamentals & Applications**

R. Jin, G. Wang, J. Zheng, *Organizers*

M. Steir, *Organizer, Presiding*

8:00 PHYS 225. Ligand effects in the synthesis of metal nanoclusters and their catalysis. N. Zheng

8:35 PHYS 226. Atomically precise alloy nanocluster: synthesis, properties and application. M. Zhu

9:10 PHYS 227. Structure and properties of size-controlled alloy nanoclusters. P. Zhang

9:45 Intermission.

10:00 PHYS 228. Tailoring the properties of thiolate protected bimetallic clusters. A. Tlahuice-Flores

10:35 PHYS 229. Modeling the structure-dependent stability of thiolated metal nanoparticles. M. Taylor, G. Mpourmpakis

10:55 PHYS 230. Heavily doped Au₂₅(Ag_x(SC₆H₁₁)₁₈)₂ nanoclusters: silver goes from core to surface. Q. Li, S. Wang, R. Jin

11:15 PHYS 231. Templated synthesis of Alloy nanocluster with atomically precise: Metal exchange. S. Wang

**Modeling Water & Solvation in
Biochemistry: Developments
& Applications**

Sponsored by COMP, Cosponsored by PHYS

**Impacts of Nanotechnology &
Single Molecule Spectroscopy
in Biology & Medicine**

*Sponsored by ANYL, Cosponsored by
BIOL, COLL, MPPG and PHYS*

Quantum Mechanics

Sponsored by COMP, Cosponsored by PHYS

**QM/MM Simulation of Chemical &
Biochemical Reaction Pathways:
Recent Developments & Applications**

Sponsored by COMP, Cosponsored by PHYS

TUESDAY AFTERNOON**Section A**

DoubleTree by Hilton Hotel Philadelphia
Center City

Ormandy East

PHYS Division Awards Symposium

G. S. Engel, *Organizer, Presiding*

1:00 PHYS 232. Single-molecule imaging reveals nanometer-scale fundamentals of cell biology and plasmonics. J.S. Biteen

**Technical program information
known at press time.**

**The official technical program
for the 252nd ACS National
Meeting is available at:
www.acs.org/Philadelphia2016**

‡ Cooperative Cosponsorship

1:35 PHYS 233. Attosecond pump-probe spectroscopy of electron correlation dynamics. W. Li

2:10 PHYS 234. Progress and applications of first-principles force fields from symmetry-adapted perturbation theory. J.R. Schmidt

2:45 Intermission.

3:05 PHYS 235. Single molecule dynamics at soft interfaces: from basic science to a \$100,000,000,000 problem. C.F. Landes

3:40 PHYS 236. Beam and single particle approaches to nanoparticle surface chemistry. S.L. Anderson

4:15 PHYS 237. Many-body molecular dynamics: Towards computer simulations with chemical and spectroscopic accuracy from the gas to the condensed phase. F. Paesani

4:50 PHYS 238. How do metal ions direct ribozyme folding? D. Thirumalai, N. Denesyuk

**Impacts of Nanotechnology &
Single Molecule Spectroscopy
in Biology & Medicine**

*Sponsored by ANYL, Cosponsored by
BIOL, COLL, MPPG and PHYS*

**QM/MM Simulation of Chemical &
Biochemical Reaction Pathways:
Recent Developments & Applications**

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING**Section A**

DoubleTree by Hilton Hotel Philadelphia
Center City

Ormandy East

**Accelerating Discovery: Citizen
Science, Big Data & Machine
Learning for Physical Chemistry**

A. Aspuru-Guzik, J. Hachmann, *Organizers,
Presiding*

8:00 Introductory Remarks.

8:05 PHYS 239. Accelerating scientific discovery through crowdsourced computing. J. Hinde, E. Pyzer-Knapp

8:35 PHYS 240. Open chemistry: Community tools for chemistry and materials science. M.D. Hanwell

9:05 PHYS 241. Bridging the theory-experiment gap: Cognitive calibration for high throughput simulation. E.O. Pyzer-Knapp, A. Aspuru-Guzik

9:35 Intermission.

9:50 PHYS 242. From structural analysis to fingerprints for molecular property predictions. M. Haghighatlar, J. Hachmann

10:10 PHYS 243. Learning data-driven molecular fingerprints with convolutional neural networks on graphs. D. Duvenaud, D. Maclaurin, J. Aguilera-Iparraguirre, R. Gomez-Bombarelli, T. Hirzel, A. Aspuru-Guzik, R.P. Adams

10:40 PHYS 244. Many-body representations for machine learning models of molecular properties. B. Huang, O. von Lilienfeld

11:00 Intermission.

11:10 PHYS 245. Data aggregation, curation and modeling approaches to deliver prediction models to support computational toxicology at the EPA. A.J. Williams, K. Mansouri, T. Martin, C. Grulke, J. Wambaugh, R. Judson, A. Richard, G. Patlewicz, I. Shah

11:40 PHYS 246. Learning from 50 million and counting: Efficient molecular optimization strategies. G. Hutchison

Section B

DoubleTree by Hilton Hotel Philadelphia
Center City

Assembly F

Advanced Potential Energy Surfaces

**Applications of Advanced Potential
Energy Models & Methods**

Cosponsored by COMP

T. L. Head-Gordon, C. Skylaris, *Organizers*

F. Paesani, *Presiding*

8:00 PHYS 247. Projector embedding approach for multiscale coupled-cluster calculations on enzyme-catalyzed reactions. A.J. Mulholland, S. Bennie, M. van der Kamp, R. Penniford, M. Stella, F.R. Manby

8:30 PHYS 248. Rapid dynamic simulations of metalloproteins for predictions of metal-dependent performance of metalloenzymes. A. Alexandrova

9:00 PHYS 249. How important is thermal expansion in modeling molecular crystals? Accurate electronic structure predictions beyond 0 K. G.J. Beran

9:30 PHYS 250. Describing correlation in the ¹(TT) singlet fission intermediate. A. Chien, P.M. Zimmerman

9:50 Intermission.

10:00 PHYS 251. What can we learn about force-fields from the crystal structure prediction of pharmaceuticals? S.L. Price

10:30 PHYS 252. What has polarization ever done for us? R.T. Bradshaw, N.A. Mohamed, J.W. Essex

11:00 PHYS 253. Protein simulations in solution and in crystals using advanced force fields. D.A. Case

11:30 PHYS 254. Parallelization schemes for solving Poisson-Boltzmann equation via finite-difference method: Implementations in DelPhi and applications. E. Alexov

Section C

DoubleTree by Hilton Hotel Philadelphia
Center City

Ormandy West

Advances in Biological Imaging

J. S. Biteen, A. B. Hummon, *Organizers*

L. J. Webb, *Organizer, Presiding*

8:00 PHYS 255. Imaging proteins at the truly single molecule level. J. Longchamp, S. Rauschenbach, S. Abb, C. Escher, T. Latychevskaia, K. Kern, H. Fink

8:40 PHYS 256. Visualizing translation synthesis by Pol IV in Live E. coli cells at single-molecule resolution. E.S. Thrall, J. Kath, J. Loparo

9:00 PHYS 257. Single-molecule fluorescence microscopy reveals the localization and dynamics of starch-digesting proteins in the human gut bacterium *Bacteroides thetaiotaomicron*. H. Tuson, M. Foley, E. Martens, N. Koropatkin, J.S. Biteen

9:40 Intermission.

10:00 PHYS 258. Molecular structure of biomimetic surfaces based on scanning tunneling microscopy. A.F. Raigoza, L.J. Webb

10:40 PHYS 259. Nano-MRI: Achieving nanoscale magnetic resonance imaging of individual biological molecules and assemblies using mechanical detection and dynamic nuclear polarization. C.E. Issac, H. Nguyen, P.T. Nasr, E.A. Curley, M.C. Boucher, J.A. Marohn

11:10 PHYS 260. Two-photon absorption spectra of stilbene and phenanthrene. M. de Wergifosse, A.L. Houk, C.G. Elles, A. Krylov

Section D

DoubleTree by Hilton Hotel Philadelphia
Center City

Aria A/B

**Dynamics of Natural & Artificial
Systems For Energy Conversion:
Insights Gained from Spectroscopic
Methods & Theory**

Financially supported by Coherent

A. Nitzan, M. R. Wasielewski, *Organizers*

J. M. Anna, *Presiding*

8:00 PHYS 261. Unraveling interfacial aggregate properties and surface vibronic interactions via doubly-resonant sum frequency spectroscopy. S. Sengupta, L. Bromley, D. Eisenbeck, S. Das, L.A. Velarde

8:35 PHYS 262. Effect of morphology on single fission: Insight from theory. X. Feng, D. Casanova, A. Krylov

8:55 PHYS 263. Beyond Kasha's exciton model for molecular aggregates: H- to J-aggregate transformation in perylene-based π -stacks. N. Hestand, F.C. Spano

9:15 Intermission.

9:30 PHYS 264. Direct imaging of energy transport in solar energy harvesting systems by ultrafast nanoscopy. L. Huang

10:05 PHYS 265. Experimentally measuring and manipulating coherent energy transport in supramolecular excitonic nanowires through energetic disorder. J.R. Caram, S. Doria, M.G. Bawendi, S. Lloyd

10:25 PHYS 266. Probing the density of states at buried organic interfaces with electronic sum frequency generation spectroscopy. R. Pandey, A.P. Moon, J.A. Bender, S.T. Roberts

10:45 Intermission.

11:00 PHYS 267. Tracking exciton dynamics in diketopyrrolopyrrole-based low bandgap conjugated polymers using femtosecond stimulated Raman spectroscopy. J. Dasgupta

11:20 PHYS 268. Electronic and nuclear contributions to time-resolved optical and X-ray absorption spectra of hematite thin films and their relevance to photocatalysis. D. Hayes, R.G. Hadt, J. Emery, A.B. Martinov, X. Zhang, K.A. Fransted, M.L. Shelby, J. Hong, L.X. Chen

11:40 PHYS 269. Direct observation of two triplet pair intermediates in singlet exciton fission. R.D. Pensack, E. Ostroumov, A. Tilley, S. Mazza, C. Grieco, K. Thorley, J.B. Asbury, D.S. Seferos, J.E. Anthony, G.D. Scholes

Section E

DoubleTree by Hilton Hotel Philadelphia
Center City
Concerto A/B

Frontiers of Solar System Chemistry:
Planets to Comets & Beyond

Laboratory Investigations

R. L. Hudson, *Organizer*
S. N. Milam, *Organizer, Presiding*
A. L. Mattioli, *Presiding*

- 8:00** **PHYS 270.** RNA Oligomerization at high pressure using mineral catalysts and imidazole activated ribonucleotides. L.B. McGown, B. Burcar, K. Rogers, M. Ackerson, E. Garbenis, B. Watson
- 8:35** **PHYS 271.** MM/Submm spectroscopic studies of the gas-phase products of interstellar ice analogues. A. Mesko, S.L. Widicus Weaver, S.N. Milam
- 8:55** **PHYS 272.** Adsorption and processing of complex organic molecules on dust grains. W. Brown
- 9:15** Intermission.
- 9:30** **PHYS 273.** Surface science investigations of physics and chemistry at icy interfaces. A. Rosu-Finsen, D. Marchione, A. Abdulgaliil, J. Thrower, M. Collings, M.R. McCoustra
- 10:05** **PHYS 274.** Insights on Titan's organic aerosol formation from the laboratory. M.G. Trainer, T.J. Gautier, J. Seebree, C.M. Anderson, M.J. Loeffler, J. Stern, S.D. Domagal-Goldman, X. Li, V.T. Pinnick
- 10:40** **PHYS 275.** Kinetics and mechanisms of the acid-base reaction between NH_3 and HCOOH in interstellar ice analogs. J. Bergner, K. Oberg
- 11:00** **PHYS 276.** Non-Norrish type production of HCN in the UV photolysis of asymmetric ketones. L. Digiacobbe, J.M. Smith, M.J. Wilhelm, H. Dai

Section F

DoubleTree by Hilton Hotel Philadelphia
Center City
Assembly E

Intrinsically Disordered Proteins:
Structure, Function & Interactions

N. Fawzi, J. Mittal, *Organizers*
T. Mittag, *Presiding*

- 8:00** **PHYS 277.** Sequence effects on hydrodynamic size for intrinsically disordered proteins described from experimental polyproline II propensities. S. Whitten
- 8:30** **PHYS 278.** Determination of statistical ensembles of intrinsically disordered proteins using NMR measurements. M. Vendruscolo
- 9:00** **PHYS 279.** Internal dynamics and chain expansion: the role of electrostatics in amyloid versus non-amyloid IDPs of the Ct family. S.M. Vaiana
- 9:30** Intermission.
- 9:50** **PHYS 280.** Phase transitions and multiphase liquid coexistence in living cells. C. Brangwynne
- 10:20** **PHYS 281.** Biophysics of protein disorder: Single molecules to droplets. A.A. Deniz
- 10:50** **PHYS 282.** Liquid-liquid phase separation of the low complexity domain of hnRNP2A. V. Ryan, C. Chabata, N. Fawzi

- 11:10** **PHYS 283.** On the edge of disorder: Effects of oxidative damage on proteins and chaperone networks. A. de Graff, K. Dill

Section G

DoubleTree by Hilton Hotel Philadelphia
Center City
Maestro A

Physical Chemistry of
Atmospheric Processes
Chemistry at Interfaces

- E. C. Browne, P. Ziemann, *Organizers*
M. Ehn, F. Keutsch, *Presiding*
- 8:00** **PHYS 284.** Interfacial oxidation of catechol. M.I. Guzman, E.A. Pillar-Little, R. Zhou
- 8:20** **PHYS 285.** Free radical reaction pathways and the evolution of organic aerosol. K.R. Wilson
- 8:55** **PHYS 286.** Heterogeneous reactivity of biogenic volatile organic compounds on mineral aerosol surfaces. R.Z. Hinrichs
- 9:15** **PHYS 287.** Effect of reaction environments on the atmospheric photochemistry of pyruvic acid and related oxoacids. V. Vaida, A. Reed Harris, R. Rapf
- 9:50** Intermission.
- 10:10** **PHYS 288.** Nonlinear optical spectroscopy of aerosol surfaces. Y. Rao, Y. Wu, W. Li, B. Xu, X. Li, Y. Wu, Y. Qian, Y. Zeng, H. Wang, V.F. McNeill, H. Dai
- 10:30** **PHYS 289.** Chiral-Selective atmospheric reaction of limonene and α -pinene probed by sub-wavenumber sum frequency generation vibrational spectroscopy at interfaces. L. Fu, H. Wang
- 10:50** **PHYS 290.** Probing fluxional dynamics of α -pinene adsorption to solid surfaces. H. Chase, M. Upshur, J. Ho, B. Psciuk, B. Rudshteyn, H. Wang, R.J. Thomson, V.S. Batista, F. Geiger
- 11:10** **PHYS 291.** Molecular-level insights into reactive nitrogen oxide chemistry on soil surfaces. J.D. Raff, M.A. Donaldson, N. Scharko

Section H

DoubleTree by Hilton Hotel Philadelphia
Center City
Maestro B

Metal & Semiconductor
Nanoclusters with Atomic Precision:
Fundamentals & Applications

- R. Jin, M. Sfeir, J. Zheng, *Organizers*
G. Wang, *Organizer, Presiding*
- 8:00** **PHYS 292.** Computational insights into catalysis by ligand-protected nanoclusters. D. Jiang
- 8:35** **PHYS 293.** Modeling TiO_2 aerogels from nanoparticles to networks. N.Q. Le, I. Schweigert
- 8:55** **PHYS 294.** Ultrasmall palladium nanoclusters as effective catalyst for oxygen reduction reaction. S. Zhao, H. Zhang, S. House, R. Jin, J. Yang, R. Jin
- 9:15** Intermission.
- 9:30** **PHYS 295.** Ultrasmall luminescent gold nanoparticles for ratio-metric pH sensing. J. Zheng

- 10:05** **PHYS 296.** Metal oxide based heterostructure nanowire arrays for multi-mode chemical sensors at elevated temperature. P. Gao

- 10:40** **PHYS 297.** Structural changes in $\text{Au}_{25}(\text{SR})_{16}$ nanoparticles after photoexcitation. K.M. Weerawardene, C.M. Aikens

Impacts of Nanotechnology &
Single Molecule Spectroscopy
in Biology & Medicine

Sponsored by ANYL, Cosponsored by
BIOL, COLL, MPPG and PHYS

QM/MM Simulation of Chemical &
Biochemical Reaction Pathways:
Recent Developments & Applications

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy East

Accelerating Discovery: Citizen
Science, Big Data & Machine
Learning for Physical Chemistry

A. Aspuru-Guzik, J. Hachmann, *Organizers*,
Presiding

- 1:00** **PHYS 298.** Deductive and inductive modelling of electronic properties in the organic molecular design space. R. Ramakrishnan
- 1:30** **PHYS 299.** First principles evolution of emitters for organic light emitting diodes. B.G. Levine, Y. Shu
- 2:00** **PHYS 300.** Computational generation and screening of metal-organic frameworks for gas storage and separations. D.A. Gomez-Gualdrón, Y.J. Colón, Y.G. Chung, R. Snurr
- 2:30** Intermission.
- 2:45** **PHYS 301.** Accelerating materials research through the effective use of data. T. Mueller
- 3:15** **PHYS 302.** Using machine-learning to create predictive material property models. C. Wolverton
- 3:45** Intermission.
- 4:00** **PHYS 303.** Predicting the electronic structure and properties of inorganic materials with machine learning. O. Isayev
- 4:30** **PHYS 304.** Not-so-short chat on entropy in materials science. S. Curtarolo

Section B

DoubleTree by Hilton Hotel Philadelphia
Center City
Assembly F

Advanced Potential Energy Surfaces
MM from QM

Cosponsored by COMP

T. L. Head-Gordon, C. Skylaris, *Organizers*
L. V. Slipchenko, *Presiding*

- 1:00** **PHYS 305.** Developing model Hamiltonians for electron-molecule interactions. K.D. Jordan, T. Odbadrakh
- 1:30** **PHYS 306.** Charge transfer models for molecular simulation. S.W. Rick

- 2:00** **PHYS 307.** Multiple contributions to the exchange potential for semi-classical electrons. J. Herzfeld, S. Ekesan

2:30 Intermission.

- 2:45** **PHYS 308.** Estimation of QM/MM polarization energy for small molecules using force-field approaches. Y. Shao

- 3:15** **PHYS 309.** Advancements in adaptive multiscale QM/MM approaches. R. Walker, A.W. Goetz

- 3:45** **PHYS 310.** MP2 hydration free energies of simple salts predicted through adaptive force matching. F. Wang, J. Li

- 4:15** **PHYS 311.** Self-adaptive Reactive Force Fields (SERFF): force matching for molecular dynamics simulation of reactive materials. N. Goldman

Section C

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy West

Advances in Biological Imaging

A. B. Hummon, L. J. Webb, *Organizers*
J. S. Biteen, *Organizer, Presiding*

- 1:00** **PHYS 312.** Biological imaging with vibrationally resonant sum-frequency generation microscopy. Y. Han, J. Hsu, V. Raghunathan, E. Polma, N. Ge
- 1:40** **PHYS 313.** Super-resolution molecular imaging with photostable nanoprobes. M.B. Prigozhin, P.C. Maurer, A.M. Courtis, X. Zheng, N. Liu, J. Collins, S. Aloni, F. Ogletree, R. Macfarlane, Y. Cui, J. Rao, P. Alivisatos, S. Chu
- 2:00** **PHYS 314.** Spatiotemporal Organization of the E. coli Cytoplasm. J.C. Weisshaar
- 2:40** **PHYS 315.** Electro-spray-ion beam deposition for high-resolution imaging of biomolecules by STM. S. Abb, G. Rinke, L. Harnau, R. Gutzler, S. Rauschenbach, K. Kern
- 3:00** Intermission.
- 3:20** **PHYS 316.** Polymer mechanics in the initiation and robustness of bacterial biofilms. V. Gordon
- 4:00** **PHYS 317.** Single-molecule imaging neuronal receptor ion channel dynamics in living cells by a new combined single-molecule patch-clamp electric recording and FRET spectroscopic microscopy. H. Lu
- 4:30** **PHYS 318.** Organelle specific single molecule imaging of oligomeric protein structures. A.M. Loe, F. Moonschi, C.I. Richards

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.

Section D

DoubleTree by Hilton Hotel Philadelphia
Center City
Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

J. M. Anna, A. Nitzan, M. R. Wasielewski,
Organizers

G. S. Engel, *Presiding*

1:00 PHYS 319. Enhancement of Resonance Energy transfer via evanescent field. X. Chen, A. Poudel, M.A. Ratner

1:20 PHYS 320. Spectroscopy and excited-state dynamics of a series of BODIPY-based A-D-A small-molecule organic solar cells acceptors. E.R. Young, S.J. Hendel, A. Krishnamurthy

1:40 PHYS 321. Fluorescent carbon nanotube defects feature substantial vibronic reorganization. M. Kim, L. Adamska, N.F. Hartmann, H. Kwon, J. Liu, K. Velizhanin, Y. Piao, L.R. Powell, B. Meany, S.K. Doorn, S. Tretiak, Y. Wang

2:00 Intermission.

2:20 PHYS 322. Nanoscopic imaging of energy transfer from single plasmonic particles to semiconductor substrates via STEM/EELS. G. Li, C. Cherqui, N. Bigelow, G. Duscher, P. Straney, J. Millstone, D.J. Masiello, J.P. Camden

2:40 PHYS 323. Enhancing photocarrier generation through interlayer coupling in graphene-WS₂ heterostructures. L. Yuan, T. Chung, Y. Chen, L. Huang

3:00 PHYS 324. Ultrafast charge transfer in PbSe binary nanocrystal superlattices with well-controlled energy landscapes. S. Li, Y. Wu, N. Gogotsi, C.B. Murray, J.B. Baxter

3:20 PHYS 325. Multi-chromophore exciton down-conversion in acene and perylene aggregates through space-separated singlet fission. C.T. Chapman, G.C. Schatz

Section E

DoubleTree by Hilton Hotel Philadelphia
Center City
Concerto A/B

Frontiers of Solar System Chemistry: Planets to Comets & Beyond

Atmospheres & Gas-Phase Chemistry

R. L. Hudson, *Organizer*

S. N. Milam, *Organizer, Presiding*

S. L. Widicus Weaver, *Presiding*

1:00 PHYS 326. Unveiling the chemical complexity of planetary atmospheres through ground and space-based observations. A. Moullet

1:35 PHYS 327. Spectroscopy and photochemistry of nitriles relevant to Titan's atmosphere. T.S. Zwier, K. Jawad, D. Mehta-Hurt, B.M. Hays

2:10 PHYS 328. Dimerization of methanimine and its charged species in the atmosphere of Titan and interstellar/cometary ice analogs. D. Skouteris, N. Balucani, V. Barone, S. Falcinelli, N. Fagnas Lago, M. Rosi

2:30 PHYS 329. Ammonium hydrosulfide and its role in coloring Jupiter's clouds. M.J. Loeffler, R.L. Hudson

2:50 Intermission.

3:05 PHYS 330. Laboratory investigations into the complex organic chemistry of Titan. M.A. Smith

3:40 PHYS 331. Neutral gas-phase chemistry in upper planetary atmospheres. N. Balucani

4:15 PHYS 332. Photon induced aerosol formation in planetary atmospheres: Photochemical hydration of sulfur dioxide. J.A. Kroll, D.J. Donaldson, V. Vaida

Section F

DoubleTree by Hilton Hotel Philadelphia
Center City

Assembly E

Intrinsically Disordered Proteins: Structure, Function & Interactions

N. Fawzi, J. Mittal, *Organizers*

C. Brangwynne, *Presiding*

1:00 PHYS 333. Artificial cytoplasm based on liquid-liquid phase coexistence: Towards responsive compartmentalization of biomolecules and reactions. C.D. Keating

1:30 PHYS 334. NPM1 facilitates nucleolar assembly through phase separation with ribosomal components. D.M. Mitrea, J.C. Hunter, C.S. Guy, D. Ban, P.R. Banerjee, C.B. Stanley, A.A. Deniz, R. Kriwacki

2:00 PHYS 335. Aberrant phase transition of stress granules triggered by misfolded proteins and prevented by chaperone function. S. Alberti

2:30 Intermission.

2:50 PHYS 336. ALS mutations disrupt phase separation mediated by an α -helical region of the TDP-43 low complexity C-terminal domain. A. Conicella, G. Zerze, J. Mittal, N. Fawzi

3:10 PHYS 337. Karyopherin beta2 rapidly disaggregates disease-linked RNA-binding proteins with intrinsically disordered, prion-like domains. J. Shorter

3:40 PHYS 338. Role of disordered regions in mediating liquid-liquid phase separation and compartmentalizing cells. T. Mittag

4:10 PHYS 339. Phosphorylation of the low complexity domain of FUS regulates assembly and inhibits aggregation. Z. Monahan, V. Ryan, K.A. Burke, N. Fawzi, F. Shewmaker

Section G

DoubleTree by Hilton Hotel Philadelphia
Center City
Maestro B

Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications

R. Jin, M. Sfeir, G. Wang, *Organizers*

J. Zheng, *Organizer, Presiding*

1:00 PHYS 340. Probing the catalytic activities of the core and shell of Au₂₅ nanoclusters. Z. Wu

1:35 PHYS 341. Atomically precise assemblies of fluorescent silver clusters on DNA scaffolds. E. Gwinn

2:10 PHYS 342. Clusters with a twist: DNA-stabilized fluorescent silver clusters. S. Swasey, N. Karimova, C.M. Aikens, O. Lopez-Acevedo, L. Espinosa Leal, E. Gwinn

2:30 Intermission.

2:50 PHYS 343. Photoelectronic properties of nanostructures at hetero-interface regions. K. Nobusada

3:25 PHYS 344. Observing isomerism at the nanoscale and its implications: the case of Au₂₈(SR)₂₄ nanoclusters. Y. Chen, R. Jin

3:45 PHYS 345. Controlling the atomic structure of Au₃₀ nanocluster by bulky ligand: 1-adamantanethiolate vs. tert-butylthiolate. T. Higaki, C. Liu, C. Zeng, R. Jin, Y. Chen, N.L. Rosi, R. Jin

4:05 PHYS 346. Closo-Si₁₂C₁₂ molecule from cluster to crystal: Optical property predictions. X.F. Duan, L.W. Burggraf

Impacts of Nanotechnology & Single Molecule Spectroscopy in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL, MPPG and PHYS

QM/MM Simulation of Chemical & Biochemical Reaction Pathways: Recent Developments & Applications

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WEDNESDAY EVENING

Section A

Pennsylvania Convention Center
Hall D

PHYS Poster Session

G. S. Engel, *Organizer*

6:00 - 8:00

PHYS 347. National Science Foundation initiatives for 2017. A. Wilson, C.A. Bessel, J. Lighty, K. Covert, T. Patten, S. Tam-Chang, L. He, T.D. Mitchell, D.A. Rockcliffe, E. Goldfield

PHYS 348. National Science Foundation (NSF) Division of Chemistry: Programmatic structure and funding opportunities. A. Wilson, M. Bushey, K. Cook, C. Foss, T. Li, M. Langell, S. Rychnovsky, C.A. Murillo, E. Goldfield

PHYS 349. National Science Foundation (NSF) Division of Chemistry: Broader impacts, broadening participation, education, outreach. A. Wilson, T. Higgins, G. Yancey, M. Hawkins, M. Jenkins, M. Wampamba, M. Stewart, E. Pfeiffer, I. Johnson, K. Noble

PHYS 350. NSF Graduate Research Fellowship Program for chemistry and chemical engineering students. T.B. Higgins, M. Bushey, T. Patten

PHYS 351. Synthesis and characterizations of MoS₂Se_{2-x} and WS₂Se_{2-x} solid solutions. M.T. Nguyen, A. Sen Gupta, J. Shervin, H. Akamatsu, A. Elias, M. Terrones, J. Zhu, V. Gopalan, T.E. Mallouk

PHYS 352. Effect of repeated hydration and dehydration cycles on water uptake into brown carbon thin films. A. Muentner Edwards

PHYS 353. Determination of rate constants for acetonylperoxy/hydroperoxy self reactions and cross reaction via Infrared kinetic spectroscopy. F.J. Grieman, A. Hui, M. Okumura, S.P. Sander

PHYS 354. Peculiarities of the glycerol-water eutectic mixture. M. Debraine, P. Siemienski, R.A. Huttemann, B.H. Milosavljevic

PHYS 355. Ultrafast photoinduced dynamics in CdSe and CdSe/ZnS quantum dots using femtosecond time-resolved fluorescence upconversion spectroscopy. R.D. Rajapaksha

PHYS 356. Investigation of singlet fission structural dynamics with femtosecond stimulated Raman spectroscopy for organic photovoltaic applications. S.M. Hart, R.R. Frontier

PHYS 357. CN vibrational relaxation dynamics of cyano-phenylalanine. J. Rodgers, W. Zhang, C. Bazewicz, J. Chen, S.H. Brewer, F. Gai

PHYS 358. Spatial coherence of holes in conjugated polymer films. R. Ghosh, C.M. Pochas, F.C. Spano

PHYS 359. Charge redistribution in excited state lumichrome. S.E. Meckel, V.A. Spata, D.T. Barnard, R.F. Pauszek, S. Matsika, R.J. Stanley

PHYS 360. Excited-state investigation of the ultrafast electrocyclic reaction for a molecular photochromic switch. C. Jones, V.A. Spata, S. Matsika

PHYS 361. Time-resolved surface-enhanced Raman spectroscopy. J.D. Schultz, N.C. Brandt, R.R. Frontier

PHYS 362. Probing DNA-carbon nanotube complex formation by fluorescence spectroscopy. K. Wagner, C. Williams, L.M. Nebel

PHYS 363. Advancing the sensitivity and selectivity of 2D-IR spectroscopy. W. Zhang, B. Markiewicz, J. Chen, F. Gai

PHYS 364. Quantum control of nuclei. Q. Wang

PHYS 365. Integrated panchromatic light-harvesting antenna and charge-separation array: Excited-state photodynamics. H. Kang, G. Hu, D. Niedzwiedzki, C.R. Kirmaier, D.F. Bocian, J.S. Lindsey, D. Holten

PHYS 366. Direct measurement of solvent-induced perturbations to the molecular geometry of N₃ on TiO₂ using heterodyne-detected vibrational SFG. C. Rich, A.T. Krummel

PHYS 367. Near-field scanning optical microscopy investigations of individual supramolecular light-harvesting nanotubes. K. Ng, S. Belh, A. Chowdhury, N. Yehya, M. Patel, G. Huffman, D.M. Eisele

Technical program information known at press time.

The official technical program for the 252nd ACS National Meeting is available at:

www.acs.org/Philadelphia2016

- PHYS 368.** Spin resolved relaxation dynamics applied to aqueous cobalt doped anatase nanowire. S.J. Jensen, T.M. Inerbaev, D. Kilin
- PHYS 369.** Unraveling spectral fluctuations in surface-enhanced Raman spectroscopy. S. Lambeth, M.D. Sonntag
- PHYS 370.** Characterizing glassy materials with Raman spectroscopy. A. Lipshaw, T. Moseley, M.D. Sonntag
- PHYS 371.** Molecular diffusion and photothermal kinetics studied by second harmonic generation. R. Kumal, H. Nguyen, M. Abu-Laban, B.P. Kruger, D. Hayes, R.L. McCarley, L.H. Haber
- PHYS 372.** Nuclear magnetic resonance studies of polycarbonate films for high power thin film capacitors. S. Lai, D.A. Boyles, J. Fontanella, S. Greenbaum
- PHYS 373.** Measuring ultrafast dynamics of single ZnO nanostructures by ultraviolet femtosecond Kerr-gated wide-field fluorescence microscopy. J. Blake, J. Nieto-Pescador, Z. Li, L. Gundlach
- PHYS 374.** Saturated structured illumination microscopy of silk. B. Jones, S. Stranich
- PHYS 375.** Effects of fluctuating electronic environments on the OH vibrational frequency of water. K. Jeon, M. Yang
- PHYS 376.** EPR spectra of alkyl-bridged copper(II) porphyrin dimers in fluid solution: evaluation of exchange interaction modulated by conformational change. R. Wang, A. Brugh, M.J. Therien, M.D. Forbes
- PHYS 377.** Ultrafast charge transfer dynamics at interfaces. J. Nieto-Pescador, B. Abraham, L. Gundlach
- PHYS 378.** Time resolved infrared emission of highly excited acetylene derivatives with an indirect signature of elusive vinylidene species. V. Trunnikova, S. Rachmil-Etter, J.M. Smith, M.J. Wilhelm, H. Dai
- PHYS 379.** Ultrafast dynamics of drug-protein complex. S. Yamazaki, A.M. Scott
- PHYS 380.** Infrared matrix isolation studies of the reaction of trimethylaluminum with ozone. D.M. Sriyathne, B.S. Ault
- PHYS 381.** Spin-labeling electron paramagnetic resonance and Overhauser dynamic nuclear polarization characterizations of the folding of IA₃, an intrinsically disordered protein. K. Dunleavy, Z. Sorrentino, E. Milshteyn, G.E. Fanucci
- PHYS 382.** Experimental investigations of the decomposition of ionic liquids. S.D. Chambreau, G.L. Vaghjani, D. Popolan-Vaida, S.R. Leone, T. Brown, J. Lee, R.N. Zare
- PHYS 383.** Characterization of hydrogen bonding in sulfonic acid-ionic liquid solutions. J. Tomlin, O.C. Fiebig, A. Miller, D.J. Walczyk, L. Yu, T.D. Vaden
- PHYS 384.** Fingerprinting n-propyl cyanide for the Cologne Database for Molecular Spectroscopy. O. Wilkins, N. Wheres, H. Mueller, F. Lewen, S. Schlemmer, A. Walters, R. Vicente, D. Liu, R. Garrod, A. Bellocche, K. Menten
- PHYS 385.** Investigation of thermochromic behavior of triphenylmethane dye Acid Blue 90 in low molecular weight polyethylene glycol and its mixtures with 1-dodecanol. N. Barashkov, I. Irgibaeva, A. Mantel, A. Aldongarov, T. Sakhno
- PHYS 386.** Progress towards directly detecting ultracold chemical reactions between trapped KRb molecules. M. Hu, Y. Liu, Y. Chen, K. Ni
- PHYS 387.** Aggregation of N-methylacetamide at aqueous surfaces. Y. Wu, Y. Wu, B. Xu, H. Dai, J. Liu, Y. Rao
- PHYS 388.** Method for performing in-trap photoionization in a miniature ion trap mass spectrometer. C.N. Stedwell, J.D. DeBord, M. Spencer, D. Rafferty
- PHYS 389.** Laboratory measurements of carbon dioxide self-quenching rates. K.J. Castle, C. Flynn
- PHYS 390.** Measuring the electron scattering cross-section of water vapor using lab-based ambient pressure XPS. Y. Khalifa, A. Broderick, J.T. Newberg
- PHYS 391.** Scattering-type scanning near-field optical microscopy with reconstruction of vertical interaction. L. Wang, X. Xu
- PHYS 392.** Molecular road map to tuning ground state absorption and excited state dynamics of near-infrared chromophores. Y. Bai, O. Jean-Hubert, H. Yoo, M.J. Therien
- PHYS 393.** Investigation of FTIR spectra of gamma-irradiated polytetrafluoroethylene. T. Sakhno, S. Sychkova, Y. Sakhno, N. Barashkov
- PHYS 394.** Novel fluorophore-quencher pair for short distance measurements. M. Hilaire, T. Troxler, F. Gai
- PHYS 395.** Molecular level understanding of photo-bleaching and oxidative-redding via electron transfer in fluorescent proteins. A. Acharya, A. Kolomeisky, A. Krylov
- PHYS 396.** Simple method to introduce an ester vibrational probe into proteins. I. Ahmed, F. Gai
- PHYS 397.** Study on the compatibility of Azo-Tetrazolate based high energy materials using DSC. M. Yousef, K. Hudson, B.C. Berry
- PHYS 398.** Photo-induced excited state dynamics: water-splitting in titanium-doped microporous silica. W. Sapp, R.T. Koodali, D. Kilin
- PHYS 399.** Novel structure for a gas-phase bimolecular heterodimer formed between a protic acid and a haloethylene: The microwave spectrum and molecular structure of hydrogen chloride-(Z)-1-Chloro-2-fluoroethylene. M.D. Marshall, H.O. Leung, H.K. Tandon
- PHYS 400.** Quantum confinement controlled photo-induced charge-transfer excitons in carbon nanotube and semiconducting nanostructure interfaces. A.R. Erck, D. Kilin
- PHYS 401.** Electronic structure properties of graphene binding with low-concentration fluorine. Y. Duan, C.C. Stinespring, B. Chorpene
- PHYS 402.** Ideal and real gas heat capacity of cesium atoms at high temperatures. L. Biolsi
- PHYS 403.** Molecular dynamics of laser assisted decomposition of unstable molecules at the surface of carbon nanotubes. B. Disrud, D. Kilin
- PHYS 404.** Thermodynamics of mixed electrolyte solutions: A new look at an old topic. R. Wigent, M. Siddiq, D. Henriques
- PHYS 405.** Computing couplings with QM/MMpol models using Q-Chem/CHARMM interface. Q. Zeng, W. Liang
- PHYS 406.** Total and differential cross sections of open-shell and excited-state species from equation-of-motion coupled-cluster Dyson orbitals. S. Gozem, A. Krylov
- PHYS 407.** Application of a many-body decomposition scheme to the local mode vibrations of (H₂O)_n water clusters (n=6, 21). J. Heindel, D.P. Schofield
- PHYS 408.** Cis-Trans isomerization mechanisms of muconic acid. A. Zaczek, T.M. Korter
- PHYS 409.** Enzyme design: Identifying mutations to alter important dynamics in complex systems. I. Zoi, S.D. Schwartz
- PHYS 410.** Proton transfer mechanisms in aminonaphthols. H.E. Rudel, M.S. Groves, K. Takematsu
- PHYS 411.** Theoretical investigation of the effect of substitution on the fluorescence properties of anthracene. S. Abou-Hatab, S. Matsika
- PHYS 412.** Trend-based feature selection in molecular descriptor space. M. Haghighatari, J. Hachmann
- PHYS 413.** GW versus wavefunction approaches. Q. Ou, J.E. Subotnik
- PHYS 414.** IR-UV double resonance spectroscopy of a cold protonated fibril-forming peptide: NNQQNY+H⁺. A.F. DeBlase, C.P. Harrilal, P.S. Walsh, S.A. Mcluckey, T.S. Zwier
- PHYS 415.** Potential energy surfaces and dynamics of N₂ + O → NO + N reaction. W. Lin, D.G. Truhlar
- PHYS 416.** Nuclear quantum effects and classical potential energy surfaces: Two classical quasiparticles per quantum particle. A. Sinitskiy, G.A. Voth
- PHYS 417.** MD simulations of coumarin 153 solvation in [Im₄⁺][BF₄⁻] / dipolar cosolvent mixtures. B. Conway, M. Liang, X. Zhang, M. Maroncelli
- PHYS 418.** Tool for screening possible MOF/TiO₂ interface linker species. J. Domenico, M.E. Foster, K.W. Sohlberg
- PHYS 419.** Integration of the probability density of the hydrogen 2p orbital within isosurfaces. I. Rhile
- PHYS 420.** Bridging the gap between continuous and atomistic models in heat transfer. J.M. Espinosa Duran, Y. Sereda, A. Abi Mansour, P. Ortoleva
- PHYS 421.** Theoretical evaluation of center-substituted zwitterionic polymethines for all-optical switching applications. S.B. Shiring, R. Gieseeking, A.K. Jen, S.H. Jang, J.E. Bredas
- PHYS 422.** Computation of the force generated by a single surface-mounted switchable rotaxane. G. Bazargan, K.W. Sohlberg
- PHYS 423.** Experimental and theoretical investigation of 1-butanol pyrolysis. N. Balucani, D. Stranges, D. Skouteris, L. Pacifici, S. Falcinelli, M. Rosi
- PHYS 424.** Estimating the entropy and quantifying the impurity of a swarm of surface-hopping trajectories: A new perspective on decoherence. W. Ouyang, J.E. Subotnik
- PHYS 425.** Rate constants and surface hopping. A. Jain, J.E. Subotnik
- PHYS 426.** Crystal simulations of small ligand molecules: Challenges for current force fields. M. Huang, D.M. York
- PHYS 427.** Mixed semi-classical approaches to nonadiabatic dynamics: Capturing detailed balance. N. Bellonzi, A. Jain, J.E. Subotnik
- PHYS 428.** Mathematical modeling of gas desorption from a metal organic super container cavity. W. Sapp, Z. Wang, D. Kilin
- PHYS 429.** Effect of high refractive index nanoparticles on charge-transfer state lifetime. J.C. Mohammed, M. Ziffer, D.S. Ginger
- PHYS 430.** Structural and electronic properties of CuO_n (n = 1 - 6) clusters and their water reaction effect using ab initio Monte Carlo simulations. G. Bae
- PHYS 431.** Photophysical characterization of an enzymatically-synthesized dually fluorescent FAD cofactor. K. Jacoby, R.J. Stanley, D.M. Yearseley
- PHYS 432.** Photoluminescence of gold nanorods. E. Sung, S. Link
- PHYS 433.** Interfacial charge transfer dynamics of organic/inorganic heterojunction probed by ultrafast transient electronic sum frequency generation. B. Xu, Y. Wu, D. Sun, C. He, H. Dai, Y. Rao
- PHYS 434.** Role of inorganic acidity on templated vanadate composition and dimensionality. A. Nourmahnad, M.B. Wenny, J. Schrier, A.J. Norquist
- PHYS 435.** Electrochemical and photophysical characterization of BODIPY-based A-D-A and D-A small molecule acceptors for use in organic solar cells. S.J. Hendel, A. Krishnamurthy, E.R. Young
- PHYS 436.** Replicating prebiotic astrochemistry through the use of a silicate grain surface analog. A.N. Carey, M.C. Foster
- PHYS 437.** Charge accommodation in n-doped ethynyl-bridged π-conjugated porphyrin arrays. I. Goodenough, J. Rawson, P. Angiolillo, M.J. Therien
- PHYS 438.** Modeling protocols for ORR and OER catalysts in solar water splitting. Y. Pal, G. Wu, J. Hachmann
- PHYS 439.** Pinpointing recombination pathways in copper zinc tin sulfide quantum dots. G.S. Doucette, J.B. Asbury, R.J. Stewart
- PHYS 440.** Characterization of the chemical interaction between singlewalled carbon nanotubes and titanium dioxide nanoparticles. K.C. Silva, P. Corio, J.J. Santos
- PHYS 441.** Charge recombination of organic-inorganic halide perovskite single crystals. C. He, H. Yin, L. Jin, A.J. Lewis, X. Li, B. Xu, H. Dai, B.B. Wayland, Y. Rao

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- PHYS 442.** Deposition of coiled silver nanowire ring by spraying method. B. Seong, H. Park, I. Chae, X. Wang, H. Lee, H. Jang, L. Lin, D. Byun
- PHYS 443.** Solvent-mediated surface binding and population of molecules onto TiO₂ particles. H. Fang, B. Xu, B.G. DeLacy, H. Dai, Y. Rao
- PHYS 444.** Interactions between positrons and chiral quartz crystals. F. Wu, Y. Jean, D. Vanhorn
- PHYS 445.** Direct observation of diffusional dynamics of nanoparticles on solid substrates by using liquid phase TEM. J. Park, S. Choi, D. Weitz
- PHYS 446.** AuBr₃ for microscopic-photochemical-laser-traced-electrodeposition (μPLATE) aqueous electrochemical and photochemical studies. C.N. Lafratta, P. Lawrence, E. Will, C. Sirko
- PHYS 447.** Tunable luminescence and exciton dynamics from 2D organic-inorganic hybrid perovskite single crystals [(C₁₀H₂₁NH₃)₂PbX₂ (X=I, Br, Cl)] for optoelectronic applications. H. Yin, L. Jin, C. He, X. Li, D. Kaan, B. Xu, D. Wozniak, Y. Wu, Y. Wu, A.J. Lewis, G. Dobreiner, H. Dai, B.B. Wayland, Y. Rao
- PHYS 448.** Bio-inspired super thin and high conductive silver thin film patterning by EHD jet printing method. H. Jang, B. Seong, J. Bae, D. Byun, L. Lin
- PHYS 449.** Influence of surface chemistry on electronic structure in organo-halide perovskites investigated by surface passivation. K.T. Munson, J.B. Asbury
- PHYS 450.** Friction near metal surfaces. W. Dou, A. Nitzan, J.E. Subotnik
- PHYS 451.** Can surface-enhanced Raman scattering identify the drug mechanism of platinum-based anticancer drugs? S. Khan, N. Mirsaleh-Kohan
- PHYS 452.** Pyrene luminescence quenching by iodide anion in poly(vinyl alcohol) solutions. R.L. Cohn, B.H. Milosavljevic
- PHYS 453.** Real time observation of unimolecular decay of Criegee intermediates to OH radical products. Y. Fang, F. Liu, V.P. Barber, M.I. Lester
- PHYS 454.** Unimolecular decay dynamics of vibrationally activated Criegee intermediates to OH products. H. Li, N.M. Kidwell, M.I. Lester
- PHYS 455.** UV + VUV double-resonance studies of autoionizing Rydberg states of the hydroxyl radical. A.M. Green, F. Liu, M.I. Lester
- PHYS 456.** Extremophile photolyases: a comparative study of temperature-dependent DNA repair. D.T. Barnard, R.A. McBride, K. Jacoby, R.J. Stanley
- PHYS 457.** Role of APOBEC3B and APOBEC3A in oncogenesis. N. Agarwal, E. Schutsky, R.M. Kohli
- PHYS 458.** Effects of evolution on reaction dynamics in apicomplexa lactate dehydrogenases. M. Varga, M.W. Dzierlenga, S.D. Schwartz
- PHYS 459.** Conformational transition of histone-complexed DNA molecules in a dense array of nanoposts: a computational study. H. Joo, Y. Kang, J. Kim
- PHYS 460.** Conformation and cohesion factors stabilizing crystalline GABA polymorphs. S.J. Dampf, T.M. Korter
- PHYS 461.** Evaluation and comparison of sorbitol cocrystal stabilities. T. Dierks, T.M. Korter
- PHYS 462.** Suppressing Aβ42 toxicity with potentiated Hsp104 variants in a yeast model of Alzheimer's disease. S. Sudesh, J. Stillman, K. Mack, J. Shorter
- PHYS 463.** Effects of aqueous ionic liquids on the structures and unfolding kinetics of myoglobin and BSA proteins. K.G. DeFrates, S. Hanna, O.C. Fiebig, T.D. Vaden
- PHYS 464.** Influence of water on protein folding and unfolding. N. Steinke, R.J. Gillams, C.D. Lorenz, S.E. McLain
- PHYS 465.** Structural studies of cis and trans peptide conformers of caprylactam and perlargolactam: subjects for predictions of ¹³C NMR deuterium isotope shifts. E. Kleist, B.S. Hudson
- PHYS 466.** All-atom models for unfolded state structure and dynamics. W. Zheng, R.B. Best
- PHYS 467.** Specific and nonspecific interactions between tetrapropylammonium ions and aromatic side chains. B. Ding, D. Mukherjee, J. Chen, F. Gai
- PHYS 468.** Assembly mechanism of nanostructured whey protein filaments. A. Kamada, N. Mittal, D. Söderberg, C. Lendel, F. Lundell
- PHYS 469.** Kinetics and mechanism of light-induced disulfide cleavage in a protein environment. R.M. Abaskharon, F. Gai
- PHYS 470.** 5-Cyanotryptophan as a novel site-specific CD probe of protein structures. D. Mukherjee, F. Gai
- PHYS 471.** Rational design, synthesis, and NMR characterization of beta-cyclodextrin derivatives with high affinities for fentanyl. D. Kennedy, C.A. Valdez, E.Y. Lau, B.P. Mayer
- PHYS 472.** Effects of nucleotide changes in single strands of RNA, and their applications to engineering microRNA biosensors. B. Lydon, S. Ranganathan, A.A. Chen
- PHYS 473.** Computational study of the combustion and atmospheric decomposition of 1,3-pentadiene and 1,4-pentadiene. S.D. Mondal, A.C. Davis
- PHYS 474.** Coexistence of different electron transfer mechanisms in the DNA repair process by photolyase. W. Lee, G. Kodali, R.J. Stanley, S. Matsika
- PHYS 475.** Cardiolipin membranes as photoreduction inhibitors in ferricytochrome C: A resonance Raman study. D. Malyska, R. Schweitzer-Stenner
- PHYS 476.** Estimating biological productivity with triple oxygen isotopes in the Arctic Ocean. A. Zhou, R.H. Stanley, B. Ji, Z.O. Sandwith, W.J. Williams
- PHYS 477.** Pseudo-phosphorylation of the tau protein and its implication for aggregation. D. Prokopovich, L. Larini
- PHYS 478.** Biofilm hydrology: label-free characterization of the hydration behavior of native biofilms. R.T. McDonough, H. Zheng, M. Ailla, J. Goodisman, J. Chaiken
- PHYS 479.** Examination of the potential posttranslational modification of Hsp104. J. Lin, J. Shorter
- PHYS 480.** Designing novel peptides to regulate enzyme activity. A. Cooper, L. Larini
- PHYS 481.** Lipid-bound conformations of alpha-synuclein revealed by site-specific SCN groups. K. Fiore, D. Konstantinovskiy, C.H. Londergan
- PHYS 482.** Exploring oxidation state dependent conformational changes of cytochrome C on cardiolipin containing liposomes. B. Milorey, L. Serpas, L. Pandiscia, R. Schweitzer-Stenner
- PHYS 483.** Cationic conjugated polymers for discrimination of microbial pathogens. H. Yuan
- PHYS 484.** Catalytic nitrogen-containing heterocycles studied by gas phase fluorescence spectroscopy in a purpose-built ion trap mass spectrometer. A.L. Ferzoco, V. Rajagopal
- PHYS 485.** In-Situ observations of surface properties of aerosols. Y. Wu, W. Li, B. Xu, X. Li, Y. Wu, Y. Qian, Y. Zeng, H. Wang, V.F. McNeill, H. Dai, Y. Rao
- PHYS 486.** Understanding the physical changes in atmospheric aerosols due to humidification: application of an ambient pressure, variable humidity transmission electron microscope. M. Giordano, W. Harlow, M. Taheri, P.F. DeCarlo
- PHYS 487.** Thermochemistry and kinetic analysis on the oxiranyl radical unimolecular dissociation and association with O₂: A theoretical study. J.W. Bozzelli, H. Wang
- PHYS 488.** Minimum energy conical intersection characterization using active space configuration interaction methods. B. Fales, B. Levine
- PHYS 489.** Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept and a pilot implementation. Y. Mao, P. Horn, M.P. Head-Gordon

Section B

DoubleTree by Hilton Hotel Philadelphia Center City
Ormandy West

Advances in Biological Imaging

A. B. Hummon, L. J. Webb, *Organizers*
J. S. Biteen, *Organizer, Presiding*

8:00 **PHYS 497.** Gigapixel super-resolution cellular imaging by optimized photoblinking and epi-illumination. S. Manley, K. Douglass, C. Steben, A. Archetti, A. Lambert

8:40 **PHYS 498.** Expansion microscopy with conventional antibodies and fluorescent proteins. J.C. Vaughan, A.R. Halpern, T. Chozinski, H. Okawa, H. Kim, G.J. Tremel, R.O. Wong

9:20 Intermission.

9:40 **PHYS 499.** Brillouin imaging to measure elastic properties of marine biomaterials. K.J. Koski

10:00 **PHYS 500.** Single-Particle tracking multiplex Raman imaging of targeting-peptide attached Au-nanobridged nanopag particles moving inside a single live cell. Y. Suh

10:30 **PHYS 501.** Towards a 'universal' fluorescent tag: unravelling the ultrafast photodynamics of maleimides. M. Staniforth, W. Quan, T. Karsili, R.K. O'Reilly, V. Stavros

Section C

DoubleTree by Hilton Hotel Philadelphia Center City
Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

J. M. Anna, A. Nitzan, M. R. Wasielewski, *Organizers*

S. C. Massey, *Presiding*

8:00 **PHYS 502.** Random-phase approximation model for excited-state spectroscopy. M.A. Mosquera, M.A. Ratner, G. Schatz

8:25 **PHYS 503.** Coupled wavepackets for non-adiabatic molecular dynamics: A generalization of Gaussian wavepacket dynamics to multiple potential energy surfaces. A. White, S. Tretiak, D. Mozyrsky

8:50 **PHYS 504.** Semi-classical Path-Integral Dynamics for understanding energy transfer and charge separation processes in light harvesting systems. P. Huo

9:15 Intermission.

9:40 **PHYS 505.** Ultrafast spectroscopy of photosynthetic light harvesting systems. G.S. Engel

10:15 **PHYS 506.** Nature of dynamic disorder in lead-halide perovskite photovoltaics: a combined molecular dynamics and density functional theory study. L. Tan, D.A. Egger, F. Zheng, L. Kronik, A.M. Rappe

10:40 **PHYS 507.** Recent advances and application of efficient nonadiabatic excited-state MD for modeling interchromophoric energy transfer in extended π-conjugated molecules. T. Nelson, L. Alfonso Hernandez, S. Fernandez-Alberti, S. Tretiak

THURSDAY MORNING

Section A

DoubleTree by Hilton Hotel Philadelphia Center City
Ormandy East

Accelerating Discovery: Citizen Science, Big Data & Machine Learning for Physical Chemistry

A. Aspuru-Guzik, J. Hachmann, *Organizers, Presiding*

8:00 **PHYS 490.** Data mining and machine learning in colloidal self assembly. S.C. Glotzer

8:30 **PHYS 491.** Sorting out a process-structure-property relationship in polymer organic electronics. N. Persson, M. McBride, J. Lu, E. Reichmanis, M. Grover

9:00 **PHYS 492.** Accelerating discovery of new processing paths of heterogeneous materials for desired properties. O. Wodo

9:30 Intermission.

9:45 **PHYS 493.** Statistical learning for discovering chemical pathways. K. Rajan

10:15 **PHYS 494.** Applying Bayesian optimization to catalyst discovery. S.F. Carr, R.M. Garnett, C. Lo

10:45 Intermission.

11:00 **PHYS 495.** Dark Reactions Project: Machine learning-assisted materials discovery using failed experiments. J. Schrier

11:30 **PHYS 496.** Accelerating the discovery of reaction mechanisms with an ab initio nanoreactor. L. Wang

Section D

DoubleTree by Hilton Hotel Philadelphia
Center City
Concerto A/B

**Frontiers of Solar System Chemistry:
Planets to Comets & Beyond**
Chemistry: Theory, Models & Methods

S. N. Milam, *Organizer*

R. L. Hudson, *Organizer, Presiding*

R. C. Fortenberry, *Presiding*

8:00 PHYS 508. Theoretical studies of venus atmospheric chemistry involving compounds of sulfur and chlorine. D.E. Woon

8:35 PHYS 509. Computing highly accurate spectroscopic line lists for characterization of planetary atmospheres: CO₂ and SO₂ line lists needed for modeling Venus. T.J. Lee, X. Huang, D. Schwenke

9:10 PHYS 510. Spectra of novel trace gasses in planetary atmospheres. R.C. Fortenberry

9:30 Intermission.

9:45 PHYS 511. Sulfur photochemistry in planetary atmospheres. M. Kumar, J.S. Francisco

10:20 PHYS 512. Mechanisms for the abiotic synthesis of adenine, guanine, uracil and thymine via UV-induced oxidation of purine and pyrimidine in astrophysical ices. P.P. Bera, M. Nuevo, C.K. Materese, S.A. Sandford, T.J. Lee

10:40 PHYS 513. Calculating photoionization and photodetachment spectra from correlated wave functions. S. Gozem, A. Krylov

Section E

DoubleTree by Hilton Hotel Philadelphia
Center City
Assembly E

**Intrinsically Disordered Proteins:
Structure, Function & Interactions**

N. Fawzi, *Organizer*

J. Mittal, *Organizer, Presiding*

8:00 PHYS 1. IDPs as critical regulators of the cell cycle. W. Peti

8:30 PHYS 2. Dueling activation and repression in intrinsic disorder-mediated allostery. J. Li, J.T. White, H.N. Motlagh, E.B. Thompson, V.J. Hilser

9:00 PHYS 3. Exploring protein-protein interactions involving intrinsically disordered regions by using carbon-detected NMR techniques. H. Roder, R. Fazlieva, E.A. Golemis, K.S. Campbell, H. Cheng

9:30 Intermission.

9:50 PHYS 4. Role of intrinsically disordered coat protein loops in phage P22 capsid assembly. A.T. Alexandrescu, A. Rizzo, L. Fraser, T. Tripler, N. D'Lima, M. Suhanovsky, K. Parent, C. Teschke

10:20 PHYS 5. Small molecule binding to the intrinsically disordered protein c-Myc: Specificity and inhibition. S.J. Metallo

10:50 PHYS 6. Investigating the role of N-terminal acetylation on alpha-synuclein structure and function. E. Rhoades

11:20 PHYS 7. Intrinsically disordered regions of proteins in signaling and disease. S. Gnanakaran

Section F

DoubleTree by Hilton Hotel Philadelphia
Center City
Maestro A

**Physical Chemistry of
Atmospheric Processes**
Acids & Bases in the Atmosphere

E. C. Browne, P. Ziemann, *Organizers*

M. Freedman, G. D. Smith, *Presiding*

8:00 PHYS 514. Studying aerosol formation and growth with the world's cleanest can. J. Smith, M. Lawler, D. Draper

8:35 PHYS 515. Unexpected behavior of fine particle acidity. R. Weber, H. Guo, T. Russell, A. Nenes

9:10 PHYS 516. Nanoparticle organic chemistry relevant to new particle formation. M.V. Johnston

9:45 Intermission.

10:05 PHYS 517. Thermodynamics of small clusters of H₂SO₄, H₂O, and dimethylamine. D. Hanson, P.H. McMurry, C.N. Jen

10:40 PHYS 518. How acidic is carbonic acid? D. Pines, P. Kiefer, S. Daschakraborty, Y. Motro, Y. Miller, J.T. Hynes, E. Pines

11:00 PHYS 519. Absorption of near uv light by HNO₂/NO₂ on sapphire surfaces. L. Zhu

Section G

DoubleTree by Hilton Hotel Philadelphia
Center City
Maestro B

**Metal & Semiconductor
Nanoclusters with Atomic Precision:
Fundamentals & Applications**

M. Steir, G. Wang, J. Zheng, *Organizers*

R. Jin, *Organizer, Presiding*

8:00 PHYS 520. Mapping of defects in individual silicon nanocrystals using real-space spectroscopy. D.A. Kisilitsyn, V. Kocovski, J.M. Mills, S. Chiu, C. Gervasi, B. Taber, A.E. Rosenfield, O. Eriksson, J. Ruz, A. Goforth, G. Nazin

8:20 PHYS 521. Direct observation of individual colloidal nanocrystals by using graphene liquid cell TEM. J. Park, S. Choi, D. Weitz, P. Alivisatos

8:40 PHYS 522. Withdrawn.

9:00 Intermission.

9:20 PHYS 523. New chemistry that directly tailors excitons in semiconducting carbon nanotubes. H. Kwon, A. Furmanchuk, M. Kim, B. Meany, Y. Guo, G. Schatz, Y. Wang

9:40 PHYS 524. Energy transfer between nanoplasmons mediated by a molecular system. M.A. Ochoa, A. Nitzan

10:00 PHYS 525. Multi-photon lithography of 3D micro-structures in Ge-doped AsSe chalcogenide glasses. C.M. Schwarz, C. Grabill, B. Gleason, R. Sapia, J. Barker, C. Rivero-Baleine, K. Richardson, A. Pogrebnyakov, T.S. Mayer, S.M. Kuebler

10:20 PHYS 526. Photophysics of composite metal/dielectric nanostructures and implications for energetic electron transfer. J.J. Foley

**Vibrational Nanospectroscopy for
Chemical & Biochemical Analysis**

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THURSDAY AFTERNOON

Section A

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy East

**Accelerating Discovery: Citizen
Science, Big Data & Machine
Learning for Physical Chemistry**

A. Aspuru-Guzik, J. Hachmann, *Organizers, Presiding*

1:00 PHYS 527. Exploration of data driven force field development for industrial application. W.C. Swope, M. Johnston, E.O. Pyzer-Knapp, R. Anderson, D. Bray, L. Wang

1:30 PHYS 528. Folding@home dares schizophrenia, or molecular dynamics simulations of not-molecular-dynamics-accessible (NMDA) receptors. A. Sinititskiy, N. Stanley, V.S. Pande

2:00 Intermission.

2:15 PHYS 529. Nonlinear reconstruction of macromolecular folding funnels from univariate time series. A. Ferguson

2:45 PHYS 530. Computer assisted identification of metabolite mass spectra: How can machine learning and quantum mechanics help? E. Cauet, I. Laponogov, J. McKenzie, K.A. Veselkov, Z. Takats

Section B

DoubleTree by Hilton Hotel Philadelphia
Center City
Ormandy West

Advances in Biological Imaging

A. B. Hummon, L. J. Webb, *Organizers*

J. S. Biteen, *Organizer, Presiding*

1:00 PHYS 531. Ultra-high resolution three dimensional imaging throughout whole cells. F. Huang

1:40 PHYS 532. Towards 3-D snapshot volumetric imaging: Novel methods of microscopy and image reconstruction to achieve 3-D volumes with single snapshot exposures. M.K. Daddysman, A. Selewa, X. Huang, T. Huynh, J. Jureller, N.J. Ferrier, M. Hereld, N.F. Scherer

2:00 PHYS 533. Molecular binding mechanisms for probing amyloid peptide structures revealed by using scanning tunneling microscopy. C. Wang

2:40 Intermission.

3:00 PHYS 534. Using sub-diffraction Raman imaging to investigate the functional role of the transmembrane bacteriorhodopsin lattice. C.T. Graefe, W.R. Silva, R.R. Frontiera

3:20 PHYS 535. Measuring single-cell respiration rates using a phosphorescence-based imaging approach. K. Ojha, J. Ertle, M. Konopka

3:40 PHYS 536. Removal of single-molecule localization bias using a metasurface polarization filter. M.P. Backlund, A. Arbabi, P. Petrov, E. Arbabi, S. Saurabh, A. Faraon, W.E. Moerner

4:20 PHYS 537. Visualizing microbial population dynamics in the larval zebrafish gut. R. Parthasarathy

5:00 PHYS 538. 3D Multi-resolution Microscopy: Advances in contextualized and target-locked microscopy in live cells. S. Hou, K. Welsher

Section C

DoubleTree by Hilton Hotel Philadelphia
Center City
Concerto A/B

**Frontiers of Solar System Chemistry:
Planets to Comets & Beyond**
Chemistry & Planetary Astrobiology

S. N. Milam, *Organizer*

R. L. Hudson, *Organizer, Presiding*

M. J. Mumma, *Presiding*

1:00 PHYS 539. From interplanetary chemistry to planetary biology. S.A. Benner, H. Kim, E. Biondi

1:35 PHYS 540. DNA Photolysis runs hot and cold: How nature adapts to extreme conditions. R.J. Stanley, S. Munshi, D.T. Barnard, R.A. McBride

2:10 PHYS 541. Life's first handshake-Interstellar detection of the chiral molecule propylene oxide. B. McGuire, P.B. Carroll, R. Loomis, I. Finneran, P. Jewell, A. Remijan, G.A. Blake

2:30 PHYS 542. Analytical methods for the study of soluble organic compounds in meteorites. J.C. Aponte, H.L. McLain, H.V. Graham, J.E. Elsila, D.P. Glavin, J.P. Dworkin

2:50 Intermission.

3:05 PHYS 543. RNA and Protein: A Match made in the Hadean. L.D. Williams

3:40 PHYS 544. Self-assembly of prebiotic materials from impact events of amino acid mixtures. N. Goldman

Section D

DoubleTree by Hilton Hotel Philadelphia
Center City
Assembly E

**Intrinsically Disordered Proteins:
Structure, Function & Interactions**

J. Mittal, *Organizer*

N. Fawzi, *Organizer, Presiding*

1:00 PHYS 545. Using site-specific vibrational probe groups to document changes in the dynamic conformational distribution of disordered proteins when binding to lipids or to other proteins. C.H. Londergan, K. Fiore, D. Konstantinovskiy

1:30 PHYS 546. Site-specific vibrational probe pairs for 2D IR studies of biomolecular conformational dynamics. M.J. Tucker

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1:50 PHYS 547. Structural trends in intrinsically disordered proteins due to increased protein length: A course-grained free energy approach. F.X. Vazquez, R. Zhou

2:10 PHYS 548. Phosphorylation and oligomerization of the microtubule associated protein tau. L. Larini

2:30 Intermission.

2:50 PHYS 549. Investigating HIV Vif interactions with host proteins. K. Ball, M.P. Jacobson, J.D. Gross

3:10 PHYS 550. Understanding MDM2-p53 binding through Markov state model approaches. G. Zhou, G.A. Pantelopulos, S. Mukherjee, V.A. Voelz

3:30 PHYS 551. Formation of amyloid fibril on two-dimensional surface. Y. Lin, E.J. Pettersson, Z. Fakhraai

Section E

DoubleTree by Hilton Hotel Philadelphia Center City
Maestro A

Physical Chemistry of Atmospheric Processes

Aerosols: Water, Phase & Optics

E. C. Browne, P. Ziemann, *Organizers*

D. Hanson, J. Smith, *Presiding*

1:00 PHYS 552. Impact of relative humidity on the optical properties of clay aerosols. J. Morang, T. Galpin, M.E. Greenslade

1:20 PHYS 553. Listening to what ambient aerosols have to say: Measuring UV-visible absorption spectra using photoacoustic spectroscopy. D.A. Fischer, S. Phillips, G.D. Smith

1:55 PHYS 554. Probing the morphology, diffusivity, and volatility of secondary organic matter using aerosol optical tweezers. K. Gorkowski, H. Beydoun, M.J. Polen, N.M. Donahue, R.C. Sullivan

2:15 PHYS 555. Measurements of particle phase transitions using synthesized nanoparticles. M. Petters, N. Rothfuss, S. Petters, D. Pagonis, M.S. Claflin, L.B. Algrim, Z. Finewax, P. Ziemann, E. Levin, S. Kreidenweis

2:50 Intermission.

3:05 PHYS 556. Role of nucleation mechanism on the size dependent morphology of organic aerosol. M.B. Altaf, A. Zuend, M. Freedman

3:25 PHYS 557. pH Dependence of liquid-liquid phase separation in mixed organic-inorganic particles. D.J. Losey, M. Freedman

3:45 PHYS 558. Liquid-liquid phase separation in organic aerosol. M. Freedman

4:20 PHYS 559. How will particle mixing states modify CCN activity? D. Vu, S. Gao, A. Asa-Awuku

4:40 PHYS 560. Characterizing ice nucleation activity of carbon nanotubes. V. Alstadt, J.N. Dawson, M. Freedman

Section F

DoubleTree by Hilton Hotel Philadelphia Center City
Maestro B

Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications

R. Jin, M. Sfeir, J. Zheng, *Organizers*

G. Wang, *Organizer, Presiding*

1:00 PHYS 561. Towards accurate description of transition-metal clusters and bioinorganic systems: A time-dependent formulation of perturbation theory for strong electron correlation. A. Sokolov, G. Chan

1:30 PHYS 562. Doping of sub-nano oxide-deposited Pt cluster catalysts for selective dehydrogenation. A. Alexandrova

2:00 PHYS 563. Controlling gold nanoclusters with atomic precision. R. Jin

Section H

DoubleTree by Hilton Hotel Philadelphia Center City
Aria A/B

Dynamics of Natural & Artificial Systems For Energy Conversion: Insights Gained from Spectroscopic Methods & Theory

Financially supported by Coherent

J. M. Anna, A. Nitzan, M. R. Wasielewski, *Organizers*

G. S. Engel, *Presiding*

1:00 PHYS 564. Chirality-selective functionalization of semiconducting carbon nanotubes with a conformation switchable molecule. L.R. Powell, Y. Wang

1:20 PHYS 565. Regulating long-wavelength absorptivity and photophysics of oligo(porphinato)metal(II) chromophores through variation of electronically excited state protonic character. Y. Bai, J. Rawson, O. Jean-Hubert, P. Zhang, M.J. Therien

1:40 PHYS 566. Cation-dependent interfacial electron transfer kinetics at dye-sensitized TiO₂ interfaces. T.J. Barr, R. Sampaio, B.N. DiMarco, G.J. Meyer

2:00 Intermission.

2:20 PHYS 567. Tracking photoinitiated and equilibrium dynamics of Photosystem I and model systems. J.M. Anna

2:55 PHYS 568. Employing J-aggregates as efficient FRET acceptor to extract excitons in PbS quantum dots. C. Wang

3:15 PHYS 569. Short-range dispersion interactions stabilize non-cavity solvation of the hydrated electron. W.J. Glover, B.J. Schwartz

Vibrational Nanospectroscopy for Chemical & Biochemical Analysis

Sponsored by ANYL, Cosponsored by PHYS

POLY

Division of Polymer Chemistry

M. Jeffries-El, T. White and C. Lipscomb, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Bioderived & Bioinspired Polymers
(see PMSE, Sun, Mon, Tue, Wed)

Materials, Devices & Switches
(see ORGN, Sun, Wed)

SOCIAL EVENTS:

Reception, 6:00 PM: Tue

Reception, 5:30 PM: Wed

Breakfast, 7:30 AM: Tue

Luncheon, 12:00 PM: Sun, Mon, Tue

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A

Sheraton Philadelphia Downtown Hotel
Salon 10

Advanced Functional Copolymers & Biomaterials

Cosponsored by PMSE

E. B. Berda, *Organizer*

L. F. Deravi, J. Foster, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 POLY 1. Heparin-mimicking polymers with anticoagulant and enzyme stabilization properties. N. Ayres, Y. Huang, Q. Chai

8:35 POLY 2. Toward fibrous biomaterial scaffolds: Manufacturing and functionalization strategies. L. Korley, A.M. Jordan, N. Wanasekara

9:05 POLY 3. Biomaterials for tissue engineering: Mimicking nature from the macroscopic to the molecular scale. S. Camarero-Espinosa, J. Cooper-White, B. Rothen-Rutishauser, C. Weder, J. Foster

9:35 POLY 4. Peptide functionalized poly(ester urea)s for regenerative medicine. M. Becker

10:05 Intermission.

10:20 POLY 5. Dynamic bio-inspired materials by buckling of polymer films and multilayers. R.C. Hayward

10:50 POLY 6. Pro-angiogenic biodegradable elastomer for the in situ tissue regeneration. S. Lee, J. Gao, K. Lee, Y. Wang

11:20 POLY 7. Supramolecular biomaterials: Making use of dynamic interactions. E.W. Meijer

11:50 POLY 8. Isocyanate-free polyurethanes from cyclic carbonate functionalized fatty esters. K. Zhang, S.J. Talley, A.M. Nelson, M. Chen, A. Hudson, E. Margareta, R.B. Moore, T.E. Long

Section C

Sheraton Philadelphia Downtown Hotel
Parlor B

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

A. Chen, M. Petr, *Presiding*

8:00 POLY 9. Synthesis of donor-acceptor type polymers by click chemistry of cycloaddition/retro-electrocyclization. W. Huang

8:20 POLY 10. Synthesis and characterization of novel pyrimidine donor-acceptor polymers. V. Karmegam, S.S. Gunathilake, M.C. Biewer, M.C. Stefan

8:40 POLY 11. Alignment of conjugated polymer nanowires for electronic and optoelectronic applications. E. Egap, M. Chang

9:00 POLY 12. Withdrawn.

9:20 POLY 13. Structure-property relationships for polyelectrolytes: thermal stability, film morphology and supramolecular assembly with conjugated polyelectrolytes. X. Yang, M. Bedford, W. Wan, C. Conrad, E. Colter, E. Freeman, L. Hu, G. Chumanov, R. Smith

9:40 POLY 14. Preparation of resonance stabilized phosphonium polyelectrolytes by RAFT polymerization. T. Womble, K.J. Noonan

10:00 POLY 15. pH on the Photophysical Studies of Metallopolymer Phosphorus Sensors containing trimesa-PPETE/Cu²⁺. A. Chen, W. Wu, Z. Qing, A. Niyogango, W.E. Bernier, W.E. Jones

10:20 POLY 16. Chromonic liquid crystal hydrogels. R. Kularatne, V.S. Godakhindi, T.H. Ware

10:40 POLY 17. Another step to zero band gap plastics: a soluble, low band gap bishthiadiazole based electrophoretic polymer. M. Icli Ozkut

11:00 POLY 18. Oligothioetheramides: A novel strategy for the assembly of sequence-defined macromolecules. M. Porel, C.A. Alabi

11:20 POLY 19. Synthesis of a siloxane thermoplastic elastomer with a functionalizable backbone and its use as a rapid photoactuator. M. Petr, B. Katzman, W. DiNatale, P.T. Hammond

Section D

Sheraton Philadelphia Downtown Hotel
Independence Ballroom B

3rd Symposium on Poly(2-Oxazoline)s & Polypeptides

Financially supported by Serina Therapeutics, GATT Technologies, Polymer Chemistry Innovations, Sigma Aldrich, CEM

H. Schlaad, *Organizer*

R. Hoogenboom, R. N. Zuckermann, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 POLY 20. Design of polypeptide and poly(2-oxazoline) based copolymer biomaterials. S. Lecommandoux, D. Taton, E. Garanger, C. Drappier, C. Legros

9:00 POLY 21. Polypeptoid polymers: Development of new chemistry and functional materials. D. Zhang