10:00 ORGN **702.** Artificial zinc enzymes based on molecularly imprinted cross-linked micelles for selective hydrolysis. **M. Arifuzzaman**, Y. Zhao

10:20 ORGN **703.** Probing interactions between hydrocarbons and auxiliary guests inside cucurbit[8]uril. **R. Rabbani**, E. Masson

10:40 ORGN **704.** Sequence control in dynamic metallo-supramolecular oligomers assembled with cucurbit[8]uril. **K. Kotturi**

Synthesis & Chemistry of Agrochemicals

Sponsored by AGRO, Cosponsored by ORGN

THURSDAY AFTERNOON

Synthesis & Chemistry of Agrochemicals

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PHYS

Division of Physical Chemistry

J. Shea, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Advanced Electrocatalysis for Energy Conversion & Storage (see *CATL*, Sun, Mon)

Simulations of Polymeric Materials: Molecular- to Macroscale (see *POLY*, Sun, Mon)

Advances in Computational Catalysis (see *CATL*, Mon, Tue, Wed)

Photoresponsive Nanoparticles: From Fundamentals of Excitation to Applications Systems (see *ENVR*, Mon, Tue, Wed, Thu)

New Directions in Conformational Sampling Methods (see *COMP*, Tue)

SOCIAL EVENTS:

JPC-PHYS Reception, 5:00 PM: Tue

SUNDAY MORNING

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

PAHs & the Organic Inventory of the Gas Phase: Observations, Theory & Experiments

P. Bera, X. Tielens, *Organizers*

J. Bouwman, *Presiding*

8:00 PHYS **1.** Some key questions involving PAHs and astrochemistry. **L.J. Allamandola**

8:35 PHYS **2.** Polycyclic aromatic hydrocarbons and related forms of interstellar carbon. **G. Sloan**

9:05 PHYS **3.** Astronomical modelling of interstellar PAHs. **O. Berné**

9:35 Intermission.

10:05 PHYS **4.** High-resolution IR spectroscopy of the isolated aromatic universe: Bad vibrations at work. **W.J. Buma**, E. Maltseva, A. Petrignani, J. Oomens, C. Mackie, A. Candian, X. Tielens, T.J. Lee, X. Huang

10:35 PHYS **5.** Computation of the infrared spectra of polycyclic aromatic hydrocarbons. **C.W. Bauschlicher**

11:05 PHYS **6.** Signatures and evolution of astronomical aromatic molecules. S.D. Wiersma, A. Candian, W. Roeterdink, J. Bakker, J. Oomens, W.J. Buma, **A. Petrignani**

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Electronic Structure & Reactivity of Organic and Organometallic Compounds

W. Grochala, E. Zurek, *Organizers*

O. G. Eisenstein, *Presiding*

8:00 Introductory Remarks.

8:20 PHYS **7.** Structural chemistry, fuzzy logic and the law. **J. Bernstein**

8:50 PHYS **8.** Rational design of Fe-based catalysts for Fischer-Tropsch synthesis from theoretical prediction to experimental confirmation. **X. Wen**, Y. Yang, Y. Li

9:20 PHYS **9.** Ligand noninnocence in metallocorroles: Insights from optical and X-ray absorption spectroscopies. **A. Ghosh**

9:40 PHYS **10.** π–stacking pancake bonding. **M. Kertesz**

10:00 Intermission.

10:20 PHYS **11.** Planar hypercoordinate carbon atoms. **G. Merino**

10:50 PHYS **12.** Roald Hoffmann's role in the development of the Woodward-Hoffmann Rules. **J. Seeman**

11:20 PHYS **13.** Orbital control of single molecule conductivies and electrical switching properties of organometallic complexes. **H. Berke**, F. Lissel, F. Schwarz, G. Kastlunger, E. Lörtscher, R. Stadler, K. Venkatesan, H. Riel

11:40 PHYS **14.** Organic chemistry at Stony Brook: Learning the basics with a glimpse at the complex yet to come. **J.W. Lauher**

Section C

Walter E. Washington Convention Center
Room 152A

Liquid Theory: Symposium in honor of Ben Widom

K. Koga, R. F. Loring, *Organizers*

D. Ben-Amotz, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PHYS **15.** RNA branching, and the size of long RNA molecules. **W.M. Gelbart**, S. Singaram, A. Ben-Shaul

8:35 PHYS **16.** From complex fluids and interfaces to very complex fluids and even more complex interfaces. **K.A. Dawson**

9:05 PHYS **17.** Topology in biology. **J. Yeomans**

9:35 PHYS **18.** Withdrawn.

10:05 Intermission.

10:20 PHYS **19.** Van der Waals disappointed: First experimental tests of mean-field theory. **J. Levelt Sengers**

10:40 PHYS **20.** Finding simplicity in complexity: Lessons I have learned from Ben Widom. **M.A. Anisimov**

11:00 PHYS **21.** Integral equation theory of coarse-graining. **M. Guenza**

11:20 PHYS **22.** Are there two forms of liquid water? Can the Widom Line settle the dispute? **H.E. Stanley**

Section D

Walter E. Washington Convention Center
Room 151A

Electronic Structure Methods for Complex Chemical Systems

Many-body Perturbation Theory, Random Phase Approximation & Beyond

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, *Organizers*

A. Grüneis, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **23.** Excited-state phenomena in condensed matter: GW, GW-BSE, and beyond. **S.G. Louie**

8:30 PHYS **24.** Electronic excitations at solid-liquid interfaces. **J. Lischner**

8:55 PHYS **25.** Real-space representation of electron-hole interaction kernel in excitonic systems. **A. Chakraborty**

9:10 Intermission.

9:20 PHYS **26.** Effect of crystal packing on the electronic properties of molecular crystals. **N. Marom**

9:45 PHYS **601.** Effect of crystal packing on the excitonic properties of rubrene polymorphs. **X. Wang**, T. Garcia, S. Monaco, B. Schatschneider, N. Marom

10:00 PHYS **27.** The optical properties of stilbene from first-principles. **K. Lewis**, C.B. Rinderspacher, S. Sharifzadeh, J. Andzelm

10:15 PHYS **28.** Beyond RPA: Kernels and renormalization. **A. Ruzsinszky**

10:40 PHYS **29.** Convergence behavior of RPA renormalized many-body perturbation theory and applications to periodic systems. **J.E. Bates**, N. Sengupta, J. Sensenig, A. Ruzsinszky

10:55 Intermission.

11:05 PHYS **30.** Self-consistent temperature dependent Green's function methods applied to solids and molecules. **D. Zgid**, A. Rusakov, S. Iskakov

11:30 PHYS **31.** Combining density functional theory and Green's function theory: Range-separated, non-local, dynamic hybrid functional. **A. Kananenka**, D. Zgid

11:45 PHYS **32.** Towards rigorous *ab initio* quantum embedding for realistic systems in the framework of Green's function theory. **L. Tran**, A. Kananenka, D. Zgid

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion

First Principles Modeling of Liquid/Solid Interfaces

K. L. Jungjohann, J. A. Keith, *Organizers*

A. Heyden, *Presiding*

8:00 PHYS **33.** Modelling metal electrolyte interfaces from density functional theory based molecular dynamics. J. Le, M. Iannuzzi, A. Cuesta, **J. Cheng**

8:20 PHYS **34.** Quantum/continuum simulations of solid/liquid interfaces under applied voltage. **I. Dabo**

8:55 PHYS **35.** Integrating first principles theory and experimental characterization at the solid/liquid interface. **K. Letchworth-Weaver**

9:30 PHYS **36.** Catalysis at the solid-liquid interface: Tools and challenges. **A. Heyden**, M.S. Saleheen

10:05 Intermission.

10:20 PHYS **37.** Cation effects on Pt electrode surface chemistry – insights from DFT. **M.J. Janik**, I.T. McCrum

10:55 PHYS **38.** Modeling solid-liquid interfaces in batteries: Degradation/acid-base reactions, electric double layers, and challenges. **K. Leung**

11:30 PHYS **39.** *Ab initio* studies of ultrathin ionic liquid films on Au (111) surface. M. Liu, **Q. Wu**

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Catalytic Promiscuity & the Emergence of New Proteins

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

Q. Cui, G. J. Poelarends, N. Tokuriki, *Organizers*

S. C. Kamerlin, *Organizer, Presiding*

8:00 Introductory Remarks.

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TECHNICAL PROGRAM

8:10 PHYS **40.** Adaptation of phosphatases as regulators, catalysts, and housekeepers. **K.N. Allen**

8:50 PHYS **41.** Structural and functional innovations in the real-time evolution of new ($\beta\alpha$)8 barrel enzymes. **W. Patrick**

9:30 PHYS **42.** Identical active sites in hydroxynitrile lyases show opposite enantioselectivity and reveal possible ancestral mechanism. B. Jones, S. Bata, **R.J. Kazlauskas**

9:50 Intermission.

10:20 PHYS **43.** Three-dimensional structure and substrate profile for a newly identified phosphotriesterase that catalyzes the hydrolysis of organophosphate flame retardants and plasticizers. **F.M. Raushel**, A.N. Bigley, D.F. Xiang, M.F. Mabanglo

11:00 PHYS **44.** Insight on the role of an active site scaffold in TET2 required for the step-wise oxidation of 5-methylcytosine. H. Torabifard, M.Y. Liu, R.M. Kohli, **G.A. Cisneros**

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS Early-Career Award in Experimental Physical Chemistry: Symposium in honor of Professor Wei Min

J. E. Shea, *Organizer*

X. Xie, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **45.** SRS microscopy: The quest for sensitivity. **X. Xie**

8:45 PHYS **46.** Electric fields and enzyme catalysis. **S.G. Boxer**

9:25 Intermission.

9:40 PHYS **47.** Recent advances in surface-enhanced femtosecond stimulated Raman scattering (SE-FSRS). **R.P. Van** Duyne

10:20 PHYS **48.** Size, dimensionality and strong electron correlation in nanoscience. **L.E. Brus**

11:00 PHYS **49.** Stimulated Raman imaging of vibrational tags for biomedicine. **W. Min**

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

The Exascale Challenge

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Nanotechnology & Single Cell Analysis in Biology & Medicine

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Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding

Sponsored by COMP, Cosponsored by PHYS

ACS COMP Symposium in honor of Peter Pulay

Gradients, Properties & Electron Correlation

Sponsored by COMP, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Spectroscopy: Meeting the Needs of Astronomers with Experiments & Theory

P. Bera, X. Tielens, *Organizers*

J. Pearson, *Presiding*

1:00 PHYS **50.** Dehydrogenation of polycylic aromatic hydrocarbons. **A. Candian**

1:20 Discussion.

1:30 PHYS **51.** Laboratory spectroscopy in astrochemistry. **S.L. Widicus** Weaver

2:05 PHYS **52.** TISA. **J. Cernicharo**

2:35 Intermission.

3:05 PHYS **53.** Complex chemistry of star formation: New insights from the atacama large millimeter/submillimeter array. **J. Jorgensen**

3:35 PHYS **54.** Accurate IR line lists for SO2 isotopologues. **X. Huang**, T.J. Lee, D. Schwenke

4:05 PHYS **55.** New virtual tools for astrochemistry. **V. Barone**, N. Tasinato, C. Puzzarini, D. Licari, L. Spada

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Electronic Structure & Reactivity of Organic and Organometallic Compounds

W. Grochala, E. Zurek, *Organizers*

X. Wen, *Presiding*

1:00 PHYS **56.** Minding the gap: Quantum studies of the singlet-triplet splittings in aromatic diradicals. **C.A. Parish**

1:30 PHYS **57.** On some differences between low-coordinate carbon and silicon compounds. **Y. Apeloig**

2:00 PHYS **58.** Supramolecular chemistry of highly reduced buckybowls. **A.Y. Rogachev**

2:30 PHYS **59.** Molecular orbitals: A powerful tool from structure, reactivity to NMR. **O.G. Eisenstein,** C. Raynaud, C. Coperet

3:00 Intermission.

3:20 PHYS **60.** Sigma-hole supported interactions across the periodic table. **K. Donald**

3:50 PHYS **61.** Activation of small molecules by mono and dinuclear Ni(II) and Cu(II) Schiff base complexes. **M.J. Calhorda**

4:20 PHYS **62.** Dawn rise of new M-M' bonds: An experimental/theoretical 21st-century approach to Alchemize gold en route to sensitizing genuine, ligand-unassisted d10-d10 covalent metal-metal bonds. **M.A. Omary**, B.M. Otten, K. Melancon, M. Ghimire, M. Raweshdeh-Omary

4:40 PHYS **63.** Metalla-[2 + 1] and [2 + 4] cycloadditions of 2-metalla-butadienes and ethylene. **E. Greer**, K. Kwon, C. Cosgriff, E. Votto, A. Badziai, X. Cui

Section C

Walter E. Washington Convention Center
Room 152A

Liquid Theory: Symposium in honor of Ben Widom

D. Ben-Amotz, K. Koga, *Organizers*

R. F. Loring, *Organizer, Presiding*

1:00 PHYS **64.** Crystalline ordering and large fugacity expansions for hard core lattice particles. **J.L. Lebowitz**, I. Jauslin

1:30 PHYS **65.** New thermodynamic model for asymmetric solutions. **A. Karmakar**, E.R. Batista, P. Yang

1:50 PHYS **66.** Chiral symmetry breaking in isotropic liquids. **F. Stillinger**

2:20 PHYS **67.** Improved estimates of the excess chemical potential from particle insertion and removal. **J.C. Rasaiah**, G. Hummer

2:40 PHYS **68.** Surface interactions mediated by a liquid: Shape, orientation and heterogeneity. **A. Luzar**

3:10 Intermission.

3:30 PHYS **69.** Structural crossover in binary hard-sphere mixtures: Experiment and theory. **R. Evans**

4:00 PHYS **70.** Changes in the hydration structure of imidazole upon protonation: Neutron scattering and molecular simulations. **P. Jungwirth**

Section D

Walter E. Washington Convention Center
Room 151A

Electronic Structure Methods for Complex Chemical Systems

Extended Systems

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, *Organizers*

J. Lischner, *Presiding*

1:00 PHYS **71.** Single- and multi-exciton phenomena in organic systems from first principles. **J. Neaton**

1:25 PHYS **72.** Singlet-fission from first-principles: Role of crystal symmetry and structure. **S. Refaely-Abramson**, F.H. da Jornada, S.G. Louie, J. Neaton

1:40 PHYS **73.** Unraveling excitation energy transfer mechanisms in plasmonic nanoantennas. **N.V. Ilawe**, M.B. Oviedo, B.M. Wong

1:55 PHYS **74.** Stochastic electronic strcture methods: Improving scaling by introducing a controlled statistical error. **E. Rabani**, R. Baer, D. Neuhauser

2:20 PHYS **75.** Probing the mechanism of tip-molecule charge transfer in the STM setup: A non-adiabatic molecular dynamics study. **J. Jankowska**, O.V. Prezhdo

2:35 Intermission.

2:45 PHYS **76.** High-accuracy trial wave functions on the cheap: Stochastic variational algorithms for quantum chemistry. **B.M. Rubenstein**

3:10 PHYS **77.** Fully quantum simulation of surface enhanced Raman scattering from real-time *ab-initio* methods. **J. Kretchmer**, G. Chan

3:25 PHYS **78.** GPU-enabled real-time electron dynamics of nitrogen-doped graphene nanoflakes. **S. Allec**, M.B. Oviedo, B.M. Wong

3:40 Intermission.

3:50 PHYS **79.** Finite size corrections in coupled cluster theory calculations of solids and surfaces. **A. Grüneis**

4:15 PHYS **80.** Random phase approximation calculations based on patching exchange-correlation potential. **C. Huang**

4:30 PHYS **81.** Condensed-phase spin-unrestricted MP2 forces: A complex case of hydrated electron. **V. Rybkin**, J. Wilhelm

4:45 PHYS **82.** Finite-temperature second-order Green's function approach to electronic correlations in solids. **A. Rusakov**, L. Tran, S. Iskakov, D. Zgid

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion

Insights for Catalysis and Charge Transport

K. L. Jungjohann, J. A. Keith, *Organizers*

M. Sfeir, *Presiding*

1:00 PHYS **83.** Characterizing transport in electrochemical energy conversion devices with X-ray computed tomography. **I. Zenyuk**

1:35 PHYS **84.** In situ transient optical studies of charge transport in nanostructured photocatalytic materials. **M. Sfeir**

2:10 PHYS **85.** Electron transfer in thermally heterogeneous environments: A new paradigm for heat transport between molecules and at molecule-metal interfaces. **G. Craven**, A. Nitzan

2:45 Intermission.

3:05 PHYS **86.** Interplay of mass transfer and local pH effects in CO_2 reduction electrocatalysis. D. Raciti, **C. Wang**

3:40 PHYS **87.** Central role of bicarbonate in the electrochemical reduction of carbon dioxide on gold. M. Dunwell, Q. Lu, J.G. Chen, Y. Yan, F. Jiao, **B. Xu**

4:15 PHYS **88.** Spectroscopic investigation of oxygenate adsorption, diffusion, and reaction at solid catalyst surfaces in the presence of semi-aqueous solvent systems. L. Qi, A. Chamas, W. Elliott, D.W. Hoyt, N.M. Washton, R.M. Rioux, **S.L. Scott**

‡ *Cooperative Cosponsorship*

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Computational Tools for Enzyme Evolution & Functional Annotation

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

Q. Cui, S. C. Kamerlin, G. J. Poelarends, N. Tokuriki, *Organizers*

D. Major, *Presiding*

1:00 PHYS **89.** Evolution of enzyme specificity. **J.M. Thornton**, J.D. Tyzack, A.J. Ribeiro, G.L. Holliday, I. Sillitoe, C.A. Orengo, S. Martinez Cuesta, S. Rahman, N. Furnham

1:40 PHYS **90.** From big data to enzyme chemical function: The nitroreductase superfamily as a model system. **E. Akiva**, J.N. Copp, N. Tokuriki, P.C. Babbitt

2:20 PHYS **91.** QM/MM computations and experimental studies reveals an unexpected intermediate in thymidylate synthase catalysis. S.A. Kholodar, V. Moliner, **A. Kohen**

2:40 Intermission.

3:10 PHYS **92.** Understanding allosteric modulation of beta lactamase function and bacterial drug resistance. **P. Kasson**, G. Cortina, M. Latallo

3:50 PHYS **93.** Don't forget to set the function to low: Predicting modifiable protein residues and effects of their variation. **Y. Bromberg**

4:30 PHYS **94.** Towards engineering radical enzymes: Thermodynamic reaction profiling and mechanistic insights into QueE. **C.M. Jaeger**

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS Early-Career Award in Theoretical Chemistry: Symposium in honor of Professor Lasse Jensen

J. E. Shea, *Organizer*

L. Jensen, *Presiding*

1:00 PHYS **95.** Nanoscale optical interactions in precise assemblies. **P.S. Weiss**

1:30 PHYS **96.** New strategies for surface-enhanced sensing: Carbenes as thiol replacements and hyper-Raman based detection. **J.P. Camden**

2:00 PHYS **97.** Electronic structure theory and plasmonics. **G.C. Schatz**

2:30 Intermission.

2:45 PHYS **98.** Atomistic simulations of surface-enhanced spectroscopies. **L. Jensen**

3:15 PHYS **99.** Tip-enhanced Raman spectroscopy with Angstrom resolution. **R.P. Van Duyne**

3:45 PHYS **100.** Molecular force spectro-microscopy through tip-enhanced Raman scattering. J. Lee, N. Tallarida, L. Rios, **V.A. Apkarian**

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

New Architectures

Sponsored by COMP, Cosponsored by PHYS

Nanotechnology & Single Cell Analysis in Biology & Medicine

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Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding

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ACS COMP Symposium in honor of Peter Pulay

Gradients, Properties & Electron Correlation

Sponsored by COMP, Cosponsored by PHYS

MONDAY MORNING

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Hot Cores & Corinos

P. Bera, X. Tielens, *Organizers*

T. J. Lee, *Presiding*

8:00 PHYS **101.** Recent advances in molecular excitation studies. **L. Wiesenfeld**, A. Faure

8:20 PHYS **102.** Photolysis of astrochemically relevant ammonia ices. **C.R. Arumainayagam**, C. Buffo, H. Schneider

8:40 PHYS **103.** Rotational spectroscopy as a tool to investigate molecules in space: Laboratory measurements and quantum-chemical calculations. **C. Puzzarini**

9:00 PHYS **104.** Synthesis of biomolecules in interstellar medium. **S.K. Chakrabarti**, A. Das, L. Majumdar

9:20 PHYS **105.** Temperature dependent 3.3 µm spectra of PAHs: An anharmonic theoretical approach. **C. Mackie**

9:40 Discussion.

9:50 Intermission.

10:20 PHYS **106.** Molecular complexity in hot cores and hot corinos. **C. Ceccarelli**

10:55 PHYS **107.** ALMA and Herschel observations of hot cores and corinos. **L.C. Darek**

11:25 PHYS **108.** Phosphorus-bearing molecules in massive star-forming clouds. **F. Fontani**, V. Rivilla, P. Caselli, A. Vasyunin, M. Beltran

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Progress in Inorganic Chemistry

W. Grochala, E. Zurek, *Organizers*

R. Dronskowski, *Presiding*

8:00 PHYS **109.** Oriented electric fields as future smart reagents in chemistry. **S.S. Shaik**, D. Mandal, R. Ramanan

8:30 PHYS **110.** Chemical bonds: A lucky bag (eine Wundertüte). **G. Frenking**

9:00 PHYS **111.** Three independent concepts: Oxidation state, effective charge, pair charges - bonding of elements in high oxidation states. **W. Schwarz**

9:20 PHYS **112.** Oxidation states, naturally: A NBO view of counting electrons. **J.S. D'Acchioli**

9:40 PHYS **113.** Exploring the structure, dynamics and reactivity of solvated electrons: From alkali metal-water explosions to non-explosive ways. **P. Jungwirth**

10:00 Intermission.

10:20 PHYS **114.** Ab initio theory of electronic Berry phase effect and topological materials: The role of symmetry and chemical bonding. **J. Feng**

10:50 PHYS **115.** Could we make shorter Zn-Zn bonds? **S. Alvarez**, J. Echeverria, A. Falceto

11:20 PHYS **116.** Chemistry of boron and physics of frustration in boron and boron compounds. **T. Ogitsu**

11:40 PHYS **117.** Silicon borides at 1atm and under pressure. **G. Gao**, X. Liang, L. Wang, C. Shao

Section C

Walter E. Washington Convention Center
Room 152A

Liquid Theory: Symposium in honor of Ben Widom

D. Ben-Amotz, R. F. Loring, *Organizers*

K. Koga, *Organizer, Presiding*

8:00 PHYS **118.** Solvation, structure, and scaling in models for simple and complex mixtures. **J.D. Weeks**, A. Gao

8:30 PHYS **119.** Widom's formula and the utility of chemical modeling in the theory of solutions. **L.R. Pratt**

9:00 PHYS **120.** Thermodynamics of hydrophobic hydration: Experimental facts. **C. Cerdeirina**

9:30 PHYS **121.** How are hydrophobic and pH-responsive polymers functioning in nanochannels? **I. Szleifer**, K. Huang

10:00 Intermission.

10:20 PHYS **122.** Lattice-based adsorption isotherms for solute activities and surface tensions of complex aqueous solutions. **C. Dutcher**, L. Nandy, H. Boyer

10:40 PHYS **123.** Cosolvent effects on hydrophobic polymer collapse. **N. van der Vegt**

11:00 PHYS **124.** Curious case of non-equilibrium finance. **M. Lipkin**

11:20 PHYS **125.** Onset of turbulence. **B.J. Alder**

Section D

Walter E. Washington Convention Center
Room 151A

Electronic Structure Methods for Complex Chemical Systems

Noncolvalent Interactions, Nanosystems & Solvation

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, *Organizers*

C. Isborn, *Presiding*

8:00 PHYS **126.** First-principles exciton models, with application to singlet fission. **J. Herbert**, A. Morrison, J. Liu

8:25 PHYS **127.** Unravelling singlet fission mechanism in quinoidal systems. **M. Momeni**

8:40 PHYS **128.** Photochemical dynamics for intramolecular singlet fission in covalently-bound pentacene dimers. **Z. Lin**, H. Iwasaki, T.A. Van Voorhis

8:55 PHYS **129.** Equilibrium geometries and binding energy scaling relationships for aromatic excimers and exciplexes: A TDDFT and NEVPT2 study. **R. Krueger**, G. Blanquart

9:10 Intermission.

9:20 PHYS **130.** Fully converged GW quasiparticle calculations for large systems. **P. Zhang**

9:45 PHYS **131.** Excited-state forces in TDDFT and the Bethe-Salpeter equation. **D.A. Strubbe**

10:10 PHYS **132.** Evolution from the plasmon to exciton state in atomically precise gold nanoparticles. **M. Zhou**, M. Sfeir, C. Zeng, Y. Chen, S. Zhao, T. Higaki, R. Jin

10:25 PHYS **133.** Dressed atom design of charge-transfer force fields. **S.R. Atlas**, G. Amo-Kwao

10:40 Intermission.

10:50 PHYS **134.** Computational design of asymmetric organocatalysts. **S.E. Wheeler**

11:15 PHYS **135.** Simplified methods for the computation of electronic absorption and circular dichroism spectra. **C. Bannwarth**, S. Grimme

11:30 PHYS **136.** Quantum yields made easy: Towards an evaluation of non-radiative rates. **A.W. Kohn**, Z. Lin, T.A. Van Voorhis

11:45 PHYS **137.** Unique electronic structure of iron carbene photosensitizers. **L.A. Fredin**, P. Persson

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TECHNICAL PROGRAM

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion

Liquid/Carbon Interfaces & Excited States

K. L. Jungjohann, J. A. Keith, *Organizers*

A. J. Morris, *Presiding*

8:00 PHYS **138.** Understanding the intrinsic water wettability of graphitic surfaces. **L. Li**

8:35 PHYS **139.** Electrochemical properties of clean graphite electrodes. **H. Liu**, L. Li

9:10 PHYS **140.** Sulfur composite for high capacity lithium sulfur battery. U. Gulzar, R. Proietti, **C. Capiglia**

9:45 Intermission.

10:05 PHYS **141.** Bridging the divide: Metal organic frameworks as molecular solids and their solution reactivity. **A.J. Morris**

10:40 PHYS **142.** Development of electron-hole multicomponent coupled-cluster theory (eh-mcCC): An excite-first correlate-later approach to electronic excitation. **A. Chakraborty**

11:15 PHYS **143.** Multi-electron transfer via photo-excited quinoidal bithiophene to anthraquinone. **H. Kim**, N. Abeyasinghe, R. Ho Wu, R. Vázquez, B. Keller, T.G. Goodson, P.M. Zimmerman

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Computational Approaches to Enzyme Design

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

S. C. Kamerlin, G. J. Poelarends, N. Tokuriki, *Organizers*

Q. Cui, *Organizer, Presiding*

8:00 PHYS **144.** Computational design and screening of mutant enzyme libraries. **D. Janssen**, H. Arabnejad, X. Niu, E. Lanfranchi, H.J. Wijma

8:40 PHYS **145.** Design and evolution of gated protein tunnels. **J. Damborsky**, D. Bendar, S. Marques, P. Kokkonen, M. Musil, J. Stourac, L. Sumbalova, O. Vavra, R. Nemeth, Z. Prokop

9:20 PHYS **146.** Redefining enzyme catalysis: Chemical control in the biosynthesis of terpenes. **D.T. Major**

9:40 Intermission.

10:10 PHYS **147.** Application of computational modeling in biocatalysis and enzyme design. **A. Rodriguez-Granillo**

10:50 PHYS **148.** Enzyme catalysis: Insights from valence bond. A. Sharir-Ivry, V. Rajapandian, **A. Shurki**

11:30 PHYS **149.** Hamiltonian replica exchange molecular dynamics: A fast and reliable method in the computational enzymology toolbox. **D. Petrovic**, B. Strodel

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS Award in Theoretical Chemistry Symposium in honor of Professor David Reichman

J. E. Shea, *Organizer*

E. Rabani, *Presiding*

8:00 PHYS **150.** Theoretical studies of neutral and charged quasiparticle dynamics in novel materials. **D.R. Reichman**

8:35 PHYS **151.** Molecules on metal surfaces: Exciting but highly non-intuitive nonadiabatic dynamics. **J.E. Subotnik**, W. Dou

9:10 PHYS **152.** Condensed phase quantum chemistry. **G. Chan**

9:45 Intermission.

10:00 PHYS **153.** Towards accurate first-principles spectroscopy in condensed phases. **T.C. Berkelbach**

10:35 PHYS **154.** Gardner transition: A new lens for glasses. **P. Charbonneau**

11:10 PHYS **155.** Ultra-high transient photocurrent peak in PbSe nanocrystals arrays. J. Gao, L. Kidon, P. Alivisatos, **E. Rabani**

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Large Scale Electronic Structure

Sponsored by COMP, Cosponsored by PHYS

Nanotechnology & Single Cell Analysis in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL and PHYS

Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding

Sponsored by COMP, Cosponsored by PHYS

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Sponsored by COMP, Cosponsored by MEDI and PHYS

ACS COMP Symposium in honor of Peter Pulay

Gradients, Properties & Electron Correlation

Sponsored by COMP, Cosponsored by PHYS

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

‡ *Cooperative Cosponsorship*

MONDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Solar Eclipse Viewing & Discussion

X. Tielens, *Organizer*

P. Bera, *Organizer, Presiding*

1:00 PHYS **156.** Solar eclipse. **P. Bera**, X. Tielens

2:00 PHYS **157.** Solar eclipse: Vieiwing and discussion. **A. Tielens**, P. Bera

3:00 PHYS **158.** Solar eclipse: Discussions. **P. Bera**, A. Tielens

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Concepts & Methodology

W. Grochala, E. Zurek, *Organizers*

S. S. Shaik, *Presiding*

1:00 PHYS **159.** What we can learn from the DOE (and LOBSTER providing it). **R.V. Dronskowski**

1:30 PHYS **160.** Intrinsic resolution of molecular electronic wave functions and energies in terms of quasi-atoms and their interactions. **K. Ruedenberg**

1:50 PHYS **161.** First-principles derived descriptors for rational design of functional molecular materials. E. Berquist, **D. Lambrecht**

2:10 Intermission.

2:30 PHYS **162.** Self-adaptive force matching for molecular dynamics simulation of reactive materials under extreme conditions. **N. Goldman**

2:50 PHYS **163.** Label algorithm for oriented quasi-atomic orbitals. **A.C. West**, M.W. Schmidt, M. Gordon, K. Ruedenberg

3:10 PHYS **164.** Chemistry with semi-classical electrons: Reaction trajectories auto-generated by sub-atomistic force fields. C. Bai, S. Kale, **J. Herzfeld**

3:30 PHYS **165.** Understanding hydrogen bonds from a Kohn-Sham molecular orbital perspective: Pauli matters. **S.C. van der Lubbe**, C. Fonseca Guerra

Section C

Walter E. Washington Convention Center
Room 152A

Liquid Theory: Symposium in honor of Ben Widom

D. Ben-Amotz, K. Koga, *Organizers*

R. F. Loring, *Organizer, Presiding*

1:00 PHYS **166.** Current-generating double layer shoe with a porous sole. **A. Kolomeisky**, A. Kornyshev

1:30 PHYS **167.** Mapping electronic structure Hamiltonian to an Ising type Hamiltonian. **S. Kais**

1:50 PHYS **168.** How high is the entropy of a high entropy alloy? **M. Widom**

2:20 PHYS **169.** Statistical mechanical modeling of quasiparticles in condensed phases. **R. Remsing**

2:40 PHYS **170.** Classical engine with ideal efficiency and nonzero power: Is it possible? J. Koning, **J.O. Indekeu**

3:10 Intermission.

3:30 PHYS **171.** Thermodynamics and kinetics of nano-scale drying transitions. Y. Altabet, **P.G. Debenedetti**

4:00 PHYS **172.** Understanding and characterizing the context-depending hydrophobicity of nanostructured solutes. E. Xi, V. Venkateshwaran, **A. Patel, S. Garde**

4:20 PHYS **173.** Confinement-induced compression and high pressure phases in nanopores. **K.E. Gubbins**

Section D

Walter E. Washington Convention Center
Room 151A

Electronic Structure Methods for Complex Chemical Systems

Emerging Directions in Electronic Structure

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, *Organizers*

F. A. Evangelista, *Presiding*

1:00 PHYS **174.** Potential energy surfaces and Berry phases beyond the Born-Oppenheimer approximation. **E. Gross**

1:25 PHYS **175.** Quasiparticle spectra from stochastic many-body methods. **V. Vlcek**, R. Baer, E. Rabani, D. Neuhauser

1:40 PHYS **176.** Exchange-correlation functionals for chemical applications from the strong-coupling limit of DFT. **S. Vuckovic**

1:55 PHYS **177.** Beyond Koopmans: Modelling ionization energies in solution. **P. Slavicek**

2:10 Intermission.

2:20 PHYS **178.** Progress in excited state variational principles for molecules and solids. **E. Neuscamman**

2:45 PHYS **179.** Correlated electronic structure methods based on spin-projection for open-shell systems. **T. Tsuchimochi**

3:10 PHYS **180.** Symmetry breaking and restoration by similarity transformation. **M. Degroote**, G.E. Scuseria

3:25 Intermission.

3:35 PHYS **181.** Quantum embedding for complex systems. **G. Chan**

4:00 PHYS **182.** Projection-based quantum embedding for molecular and periodic systems. **D. Chulhai**, J. Goodpaster

4:15 PHYS **183.** Simulation of atomic force microscopy with density embedding theory and its implementation to realspace DFT code PARSEC. **Y. Sakai**

4:30 PHYS **184.** Colle-Salvetti based functional for the inclusion of electron-proton correlation in multicomponent density functional theory. **K. Brorsen**, Y. Yang, M. Pak, S. Hammes-Schiffer

4:45 PHYS **185.** Machine learning acceleration of non-local density functionl theory. **N. Geva**, T.A. Van Voorhis, T. Thonhauser

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion

Insights for Batteries

K. L. Jungjohann, J. A. Keith, *Organizers*

B. L. Lucht, *Presiding*

1:00 PHYS **186.** Generation and evolution of materials in the anode solid electrolyte interphase (SEI) of lithium ion batteries. **B.L. Lucht**

1:35 PHYS **187.** Grand challenge in battery designs through better understanding of the interfaces. **B. Liaw**

2:10 PHYS **188.** Heterogeneity in the SEI and failure statistics in Li ion battery pouch cells. **S.J. Harris**, P. Lu

2:45 Intermission.

3:05 PHYS **189.** In-situ spectro-imaging of lithium transport and reactions at electrolyte/electrode interface in batteries. W. Zhang, B. Swartzentruber, W.M. Mook, K.L. Jungjohann, **F. Wang**

3:40 PHYS **190.** Revealing mechanisms for electrolyte decomposition from first-principles consistent with operando X-ray photoemission spectra. **D. Prendergast**, A.I. Baskin, Y. Yu, C. Valero-Vidal, N. Hahn, Q. Liu, K.R. Zavadil, B.W. Eichhorn, E. Crumlin

4:15 PHYS **191.** Withdrawn.

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Discovery & Engineering of Industrially Relevant Enzymes

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

Q. Cui, S. C. Kamerlin, N. Tokuriki, *Organizers*

G. J. Poelarends, *Organizer, Presiding*

1:00 PHYS **192.** Discovery of a reductive aminase for chiral amine synthesis. **N. Turner**

1:40 PHYS **193.** Engineering nature's protein repertoire for food, pharma and the bio-based economy. **R. de Jong**

2:20 PHYS **194.** Using experimental and computational data to expand the utility of a suite of flavin-dependent monooxygenases. **A.R. Narayan**

2:40 Intermission.

3:20 PHYS **195.** Re-engineering esterases for amide bond synthesis. **J.J. Lalonde**, D. Entwistle, C. Micklistch, R. Voladri

4:00 PHYS **196.** Atom- and step efficient modular synthetic enzyme cascades to chiral building blocks and active pharmaceutical ingredients. R. Oeggl, J. Wachtmeister, V. Erdmann, J. Kulig, T. Sehl, A. Jakoblinnert, **D. Rother**

4:40 PHYS **197.** Characterization of site- and stereoselective Rieske oxygenases from the saxitoxin biosynthetic pathway. **A.L. Lukowski**, M. Hinze, A.R. Narayan

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS/Journal of Physical Chemistry Lectureship Award: Symposium in honor of Professor Zahra Fakhraai

J. E. Shea, *Organizer*

Z. Fakhraai, *Presiding*

1:00 PHYS **198.** Electron-plasmon and plasmon-exciton interactions in molecular junctions. **A. Nitzan**, M. Galperin, M. Sukharev

1:35 PHYS **199.** Assembly of anisotropic nanoparticles in polymer nanocomposite films. **R.J. Composto**

2:10 PHYS **200.** Rationalizing simulations with experiments on the dynamics of confined glasses. **R. Riggleman**, Z. Fakhraai

2:45 Intermission.

3:15 PHYS **201.** Theories of activated diffusion and structural relaxation in multi-component polymer liquids and glasses. **K.S. Schweizer**

3:50 PHYS **202.** Using surface structure and mobility to build more organized glasses with physical vapor deposition. **M.D. Ediger**

4:25 PHYS **203.** Long-range correlated dynamics in organic and inorganic glasses. **Z. Fakhraai**, Y. Zhang, T. Liu, R. Stephens, E. Glor, K. Wahid, G. Angrand, R. Riggleman

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Electronic Structure

Sponsored by COMP, Cosponsored by PHYS

Nanotechnology & Single Cell Analysis in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL and PHYS

Transformative Research & Excellence in Education Award

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Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding

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Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Sponsored by COMP, Cosponsored by MEDI and PHYS

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

S. O. Kelley, J. E. Shea, *Organizers*

8:00 - 10:00

127, 129, 135, 143, 176, 197, 231, 277, 289, 313, 316-317, 329, 335, 346, 361, 394-395, 398, 403, 416-418, 425, 427, 437, 439, 457, 460, 461-462, 465, 469-470, 474-477, 480, 483, 485, 487-489, 492, 495, 497, 504, 509-510, 518-519, 522, 527, 532, 538, 540-541. See previous listings.

TUESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Hot Cores & Corinos

P. Bera, X. Tielens, *Organizers*

E. Herbst, *Presiding*

8:00 PHYS **204.** Astronomical model studies related to the composition of hot cores and hot corinos. **S. Charnley**

8:30 PHYS **205.** SOFIA/EXES high spectral resolution observations of Orion IRc2. **N. Rangwala**, X. Huang, K. Acharyya, R. Le Gal, S. Colgan, T.J. Lee, E. Herbst

9:00 Intermission.

9:30 PHYS **206.** Ion-induced reactions in hot cores and corinos. **W.D. Geppert**, M. Larsson

10:00 PHYS **207.** Complex organic molecules in star-forming regions: hot cores and hot corinos. **V. Rivilla**

10:20 Discussion.

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Recent Advances in High Pressure Chemistry

W. Grochala, *Organizer*

E. Zurek, *Organizer, Presiding*

8:00 PHYS **208.** Borophenes, borospherenes and boron. **E.D. Jemmis**

8:30 PHYS **209.** Bonds vs bands, or how it is easier to understand electronic structure and phase diagram of ice: Canondrums and smoking guns. **A.L. Tchougreeff**

9:00 PHYS **210.** Thermodynamic stabilization of nitrogen pentafluoride. **D. Kurzydlowski**, P. Zaleski-Ejgierd

9:20 PHYS **211.** Withdrawn.

9:40 PHYS **212.** Novel superconductivity in hydrides at high pressures. **H. Liu**, I. Naumov, R. Hoffmann, N. Ashcroft, R. Hemley

10:00 Intermission.

10:20 PHYS **213.** Topological study of chemical bonds under pressure: The case of solid hydrogen. **V. Labet**, V. Riffet, J. Contreras-Garcia

10:50 PHYS **214.** Cobalt-hydrogen system under high pressure: A theoretical perspective. **T. Jaron**, W. Grochala

11:10 PHYS **215.** Superconducting phases of phosphorus hydride under pressure: Stabilization via mobile molecular hydrogen. **T. Bi**, D.P. Miller, A. Shamp, E. Zurek

11:30 PHYS **216.** Superconductivity in scandium hydrides under pressure. **X. Ye**, N. Zarifi, E. Zurek, R. Hoffmann, N. Ashcroft

11:50 Discussion.

Section C

Walter E. Washington Convention Center
Room 152A

Gaseous Ion Chemistry & Surface Reactions

The Chemistry of Cold Ions

A. K. Badu-Tawiah, H. Chen, *Organizers*

C. Bleiholder, *Presiding*

8:00 PHYS **217.** Unraveling the spectral signatures of divatlent metal binding to surfactancts at the air-water interface with crygenic ion vibrational (CIVP) spectroscopy. **M.A. Johnson**

8:40 PHYS **218.** Observation of excited quadrupole-bound states in cryogenically-cooled deprotonated 4-cyanophenol anions. **G. Zhu**, Y. Liu, L. Wang

9:00 PHYS **219.** Cryogenic linear ion trap with expanded electrode spacing designed for fluorescence spectroscopy of excited state charge transfer complexes. **A.L. Ferzoco**, V. Rajagopal, C. Stokes

9:40 Intermission.

10:00 PHYS **220.** Single-Conformation spectroscopy and isomerization of cryocooled peptide ions. A.F. Deblase, C.P. Harrilal, J.T. Lawler, S.A. Mcluckey, **T.S. Zwier**

10:40 PHYS **221.** From multiply-charged anions to ultracold anions: High-Resolution resonant photoelectron imaging via dipole-bound excited states. **L. Wang**

Section D

Walter E. Washington Convention Center
Room 151A

Electronic Structure Methods for Complex Chemical Systems

Correlated Electronic Structure Methods for Complex Systems

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, *Organizers*

E. Neuscamman, *Presiding*

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TECHNICAL PROGRAM

8:00 PHYS **222.** Single-reference coupled-cluster and equation-of-motion coupled-cluster methods for multi-reference problems: CC(*P;Q*) formalism. **P. Piecuch**, J. Shen, N.P. Bauman, I. Magoulas

8:25 PHYS **223.** Electron correlation methods for near-degenerate states based on the driven similarity renormalization group. **F.A. Evangelista**, C. Li

8:50 PHYS **224.** Attenuated coupled cluster: A novel single-reference approach for strongly correlated systems. **J.A. Gomez**, G.E. Scuseria

9:05 PHYS **225.** Extending the reach of the CCSD(T) method by massive parallelism and reduced scaling. **C. Peng**, F. Pavosevic, E.F. Valeev

9:20 Intermission.

9:30 PHYS **226.** Correlation energies through incremental full configuration interaction. **P.M. Zimmerman**

9:45 PHYS **227.** Truncating the configuration interaction (CI) expansion through modified orthogonalization of molecular orbitals. **A.C. West**, M.W. Schmidt, M. Gordon, K. Ruedenberg

10:00 PHYS **228.** Multiconfiguration quantum embedding methods. **S. Bernales Candia**, H. Pham, G.E. Scuseria, L. Gagliardi

10:15 PHYS **229.** Multi-reference calculations of NMR shifts in open-shell actinide complexes. **F. Gendron**, J. Autschbach

10:30 Intermission.

10:40 PHYS **230.** One-particle many-body Green's function theory: Algebraic recursions, linked-diagram and irreducible-diagram theorems, and general-order algorithms. **S. Hirata**

11:05 PHYS **231.** Orbital-free density functional theory with atom-centered density matrices. **W.C. Witt**, J. Dieterich, F. Libisch, E.A. Carter

11:20 PHYS **232.** Charge transfer excited states: A balanced and efficient wave function ansatz in variational Monte Carlo. **N.S. Blunt**, E. Neuscamman

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion

Insights for Batteries & Liquid/Oxide Interfaces

K. L. Jungjohann, J. A. Keith, *Organizers*

M. F. Fernandez-Serra, *Presiding*

8:00 PHYS **233.** Coupling in-situ TEM and ex-situ analysis to understand heterogeneous sodiation of antimony. **D. Mitlin**

8:35 PHYS **234.** Towards tunable electrochemistry of two-dimensional materials. **M. Velicky**, R.A. Dryfe

9:10 PHYS **235.** Mechanistic insights into oxygen reduction reactions in non-aqueous metal-air batteries. Y. Zhang, X. Zhang, J. Wang, S. Ma, L. Guo, S. Rawal, W.C. McKee, **Y. Xu**, Z. Peng

9:30 Intermission.

9:45 PHYS **236.** Molecular dynamics simulations of alkali halide adsorption to water-alumina interfaces. **R. Wang**, K. Millan, R. Remsing, S. Piontek, A. Tuladhar, L. Magidson, V. Carnevale, M. Klein, E. Borguet

10:05 PHYS **237.** Simulations of the liquid/solid interface. **H. Metiu**, H. Kristoffersen, R. Liu, J.E. Shea

10:40 PHYS **238.** Withdrawn.

11:15 PHYS **239.** Interplay between surface termination and polarization in photocatalysis on perovskite oxide surfaces. **M.F. Fernandez-Serra**, M. Dawber, B. Pamuk, M. Kaltak

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Membrane Proteins: Structure, Activity & Drug Development

Structure & Dynamics of Membrane Proteins

F. Marassi, *Organizer*

M. J. Cocco, *Organizer, Presiding*

O. Beckstein, *Presiding*

8:00 PHYS **240.** Signaling-related mobility changes in functional chemotaxis receptor arrays by solid-state NMR. M. Kashefi, **L.K. Thompson**

8:30 PHYS **241.** Cellular structural biology probing prokaryotic and eukaryotic membrane protein complexes *in-situ* at atomic resolution. **M. Kaplan**

9:00 PHYS **242.** Blocking the neurite outgrowth inhibitor (Nogo) to promote neuroregeneration. **M.J. Cocco**

9:20 Intermission.

9:40 PHYS **243.** Probing the conformational rearrangements in Bcl-2 proteins, Bax and Bid at the initiation of apoptosis. **N. Tjandra**

10:10 PHYS **244.** Intrinsically disordered membrane enzymes selenoprotein S and selenoprotein K. Z. Zhang, J. Liu, R. Cheng, **S. Rozovsky**

10:40 Intermission.

11:00 PHYS **245.** Structure and function of electrogenic sodium/proton antiporter membrane proteins. **O. Beckstein**, D.L. Dotson, M. Coincon, P. Uzdavinys, E. Nji, C. Lee, S. Yashiro, Y. Huang, W. Chen, J. Shen, A.D. Cameron, D. Drew

11:30 PHYS **246.** Reverse q-titration of integral membrane proteins in nanodiscs. A. Laguerre, F. Loehr, E. Henrich, B. Hoffmann, F. Bernhard, **V. Doetsch**

Section G

Walter E. Washington Convention Center
Room 151B

Physical Chemistry Research at Undergraduate Institutions

Materials

T. Hopkins, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PHYS **247.** Shedding light on colloidal surfaces: Exposing molecular behavior and chemical reactivity at the solid-liquid interface. **M. Subir**

8:45 PHYS **248.** Finding Goldlilocks in nanoscience research at PUI institutions. **J.J. Peterson**

9:05 PHYS **249.** Microwave spectra and molecular structures of 2-(trifluoromethyl)-oxirane and 2-vinyloxirane, two candidates for chiral analysis via noncovalent chiral tagging. **M.D. Marshall**, H.O. Leung, M. Acha, K. Wang

9:25 PHYS **250.** Unlocking the electronic genome of halogenated polycyclic aromatic hydrocarbons with undergraduate students. **S. Jezowski**, B. Schatschneider

9:45 Intermission.

10:05 PHYS **251.** Cation exchange in colloidal nanocrystals: New advances and new possibilities. **P.G. Van Patten**

10:45 PHYS **252.** Computational molecular dynamics study of heteroepitaxial growth patterns comparing Cu/Ni and Pt/Ni on Ni(111) and Ni(100). **K. Haug**, B. Nguyen, P. Ly

11:05 PHYS **253.** Guided-wave plasmon polariton modes. **J. Leger**, H. Nguyen, R. Owen, S. Clark, B. Johnson

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Molecular Dynamics

Sponsored by COMP, Cosponsored by PHYS

Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding

Sponsored by COMP, Cosponsored by PHYS

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Sponsored by COMP, Cosponsored by MEDI and PHYS

TUESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Organic Inventory of Protoplanetary Disks

P. Bera, X. Tielens, *Organizers*

P. Caselli, *Presiding*

1:00 PHYS **254.** Organic inventory of protoplanetary disks: Recent insights and future prospects with ALMA and JWST. **C. Walsh**

1:35 PHYS **255.** ALMA observation of molecules in protoplanetary disks. **S. Guilloteau**

2:05 PHYS **256.** Molecular clues from inner planet-forming disks. **J. Najita**

2:35 Intermission.

3:00 PHYS **257.** Planet formation in protostellar disks. **G. Laughlin**

3:30 PHYS **258.** Properties and origins of cometary and asteroidal organic matter delivered to the early Earth. **S. Messenger**, A.N. Nguyen

4:00 PHYS **259.** Possibility to locate the position of the H_2O snowline in protoplanetary disks through spectroscopic observations. **S. Notsu**, H. Nomura, C. Walsh, T. Hirota, M. Honda, E. Akiyama, T. Millar

4:20 PHYS **260.** Measurements of the thermo-chemical evolution of the planet-forming region in disks. **A. Banzatti**, K.M. Pontoppidan, C. Salyk, G. Herczeg, E. van Dishoeck, G.A. Blake, I. Pascucci

4:40 Discussion.

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Bonding in Bioorganic Systems

W. Grochala, E. Zurek, *Organizers*

J. Feng, *Presiding*

1:00 PHYS **261.** Understanding the emergence of contractility in acto-myosin networks. J. Komianos, **G. Papoian**

1:20 PHYS **262.** Chemistry of the nitrogenase P-cluster: Structural and electronic flexibility. **K. Tatsumi**, G. Moula

1:40 PHYS **263.** Role of dynamics in enzymatic electrophilic aromatic substitution. **K.M. Merz**

2:00 PHYS **264.** From metal-based chirality to second coordination sphere chirality... and back: Artificial metalloenzymes. **T.R. Ward**

2:20 PHYS **265.** Speciation at solid/liquid interfaces in the thermal or electrochemical hydrogenation of organic compounds. D. Cantu, **R.S. Weber**, Y. Wang, M. Lee, M.T. Nguyen, S. Akhade, A. Padmaperuma, M. Lilga, V. Glezakou, R. Rousseau

2:40 Intermission.

3:00 Discussion.

3:40 PHYS **266.** Bonding with Roald. **B.Z. Shakhashiri**

Section C

Walter E. Washington Convention Center
Room 152A

Gaseous Ion Chemistry & Surface Reactions

Ion/Surface Interactions

H. Chen, *Organizer*

A. K. Badu-Tawiah, *Organizer, Presiding*

1:00 PHYS **267.** Ion-based synthesis of functional materials. **T. Pradeep**

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

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1:40 PHYS **268.** Synthesis, stability, and immobilization on surfaces of phosphine-ligated gold clusters. **G.E. Johnson**, M. Ligare, U. Reveles, J. Laskin

2:20 Intermission.

2:40 PHYS **269.** Understanding and exploiting surface chemistry to direct the *in situ* synthesis and placement of nanostructures. **A.V. Walker**

3:20 PHYS **270.** Electron induced surface reactions of $C_3H_5Fe(CO)_2Mn(CO)_5$: Metal center impact on the behavior of organic ligands. **I. Unlu**

Section D

Walter E. Washington Convention Center
Room 151A

Electronic Structure Methods for Complex Chemical Systems

Ultra-efficient Electronic Structure Methods & Molecular Dynamics

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, *Organizers*

S. Refaely-Abramson, *Presiding*

1:00 PHYS **271.** Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. **S. Tretiak**

1:25 PHYS **272.** Exciton coupled-cluster theory for large-scale electronic structure calculations: Test application on Ben clusters. Y. Liu, **A.D. Dutoi**

1:40 PHYS **273.** Modeling excited states in the condensed phase. **C. Isborn**

2:05 PHYS **274.** First-principles derived descriptors for linear response properties. E. Berquist, **D. Lambrecht**

2:20 Intermission.

2:30 PHYS **275.** Computational synthesis and characterization by large quantum and reactive molecular dynamics simulations. **A. Nakano**

2:55 PHYS **276.** Non-adabatic dynamics of the 1,2-dioxetane chemiluminescence. M. Vacher, I.F. Galvan, A. Brakestad, H.O. Karlsson, **R. Lindh**

3:10 PHYS **277.** Accelerating the simulation of nonadiabatic dynamics through an efficient augmented surface hopping algorithm in Q-Chem. **G.R. Medders**, J.E. Subotnik

3:25 Intermission.

3:35 PHYS **278.** Scalable algorithms for real-space and real-time first-principle calculations. **E. Polizzi**

4:00 PHYS **279.** Interpolative separable density fitting decomposition for accelerating large-scale hybrid functional calculations. **W. Hu**, L. Lin, C. Yang

4:15 PHYS **280.** Density-to-potential inversions in density functional theory with atom-centered bases and multiwavelet bases. **X. Zhang**, E.A. Carter

4:30 PHYS **281.** Projector augmented wave based Kohn-Sham density functional theory simulations with reduced order scaling. **G.J. Martyna**

4:45 Concluding Remarks.

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Structure-Function Relationships in Enzyme Evolution

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

Q. Cui, S. C. Kamerlin, G. J. Poelarends, *Organizers*

N. Tokuriki, *Organizer, Presiding*

1:00 PHYS **282.** Capturing and designing for electrostatic preorganization in enzymes. **A. Alexandrova**

1:40 PHYS **283.** Computation of enzyme cold adaptation. **J. Åqvist**

2:20 PHYS **284.** What makes enzymes work? Using pressure and temperature to probe properties needed for enzyme activity. **J.M. Rodgers**, R. Hemley, T. Ichiye

2:40 Intermission.

3:10 PHYS **285.** Resurrected ancestral proteins as scaffolds for protein engineering. **J. Sanchez-Ruiz**

3:50 PHYS **286.** Role of conformational dynamics in the evolution of novel retro-aldolase activity. **S. Osuna**, A. Romero-Rivera, M. Garcia-Borràs

4:30 PHYS **287.** Mechanism-informed refinement reveals altered substrate binding mode for catalytically competent nitroreductase. **A.F. Miller**, W. Pitsawong, R.L. Koder, C. Haynes, D. Rodgers

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Membrane Proteins: Structure, Activity & Drug Development

Structure & Dynamics of Membrane Proteins

M. J. Cocco, F. Marassi, *Organizers*

C. D. Schwieters, W. D. Van Horn, *Presiding*

1:00 PHYS **288.** NMR study of the pre-fusion to post-fusion transition of the gp41 ecto domain. C.S. Chiliveri, J. Roche, J.L. Baber, R. Ghirlando, J. Ying, J. Louis, **A. Bax**

1:30 PHYS **289.** Dissecting the polymodal gating and modulation of TRP channels. **W.D. Van Horn**

2:00 PHYS **290.** Hidden dynamics in the unfolding of individual bacteriorhodopsin proteins. **M. Siewny**, H. Yu, D. Edwards, A. Sanders, T. Perkins

2:20 PHYS **291.** Revealing the structural basis for GPCR signaling through atomic-level simulation. **R.O. Dror**

2:50 Intermission.

3:10 PHYS **292.** Solid-state NMR of membrane proteins. **S. Opella**

3:40 PHYS **293.** Software tools to assist membrane structure determination. **C.D. Schwieters**

4:10 PHYS **294.** Enabling proton transfer in classical simulations. **T. Lazaridis**

4:40 PHYS **295.** Structure base analysis of production and purification of human leukemia interferon. **Y.S. Ting**

Section G

Walter E. Washington Convention Center
Room 151B

Physical Chemistry Research at Undergraduate Institutions

Photophysics & Reactivity

T. Hopkins, *Organizer*

J. Leger, *Presiding*

1:00 PHYS **296.** Organic chemistry catalyzed by undergraduate theorists. **R.J. Cave**

1:40 PHYS **297.** Elucidating the excited-state proton and electron transfer processes in substituted anthraquinone dyes using single-molecule spectroscopy. **K.L. Wustholz**

2:20 Intermission.

2:40 PHYS **298.** Utilizing ionic liquids as solvents to control chirality. **T. Hopkins**

3:00 PHYS **299.** Onset of oscillations in the Beluosov-Zhabotinsky reaction: Undergraduate research experience. **H.M. Hastings**, D.R. Myers, P. Dooley, S.G. Sobel, R.J. Field, D. Guralnick, S. Rafikova, M. Zahed

3:20 PHYS **300.** Characterization of excited electronic states by cavity ringdown spectroscopy. **S. Drucker**

4:00 PHYS **301.** Photophysics of cyano-substituted hydroquinones: Promising candidates as super photoacids with tunable acidity. **M. Zahid**, A. Mansha, G. Grampp, I.A. Bhatti, P. Jacques, S. Asim

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Data & Automation

Sponsored by COMP, Cosponsored by PHYS

Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding

Sponsored by COMP, Cosponsored by PHYS

Computational Studies of Membranes & Membrane-Bound Systems

Membrane Bilayers

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Chemistry of Dark Clouds: Chemical Networks Connecting Gas & Dust

P. Bera, X. Tielens, *Organizers*

T. Millar, *Presiding*

8:00 PHYS **302.** Gas-grain chemistry in dark clouds: Successes and remaining puzzles. **E. Herbst**

8:35 PHYS **303.** Molecular inventory of dark clouds: Observations and theory. **P. Caselli**

9:05 PHYS **304.** Formation of complex organics and nitrogen-containing organics by ion-molecule and intracluster reactions. **M.S. El-Shall**

9:35 PHYS **305.** Time-resolved reactive scattering to study atom-addition reactions on ices: A case study of $H+O_3>OH+O_2$. **G. Vidali**, J. He, S. Emtiaz

9:55 Intermission.

10:00 PHYS **306.** Chemical kinetics and tunneling on dust grains. **G. Nyman**

10:30 PHYS **307.** Exotic organosilicon chemistry in molecular clouds: From crossed molecular beams to computational chemistry. **R. Kaiser**

11:00 PHYS **308.** Complex organic molecule formation under dark cloud conditions: The laboratory view. **H. Linnartz**

11:30 PHYS **309.** Production and infrared spectra of hydrogenated free radicals and protonated species important in interstellar media. **Y. Lee**, M. Tsuge, K.A. Haupa

11:50 Discussion.

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Structure & Properties of Materials

W. Grochala, E. Zurek, *Organizers*

P. Edwards, *Presiding*

8:00 PHYS **310.** Towards rational design of chemical reactions. **F. Bickelhaupt**

8:30 PHYS **311.** Li insertion in SiCO anode materials: On the way to understand capacity and mechanisms. **P. Kroll**, S. Haseen

9:00 PHYS **312.** Tuning the band-edge orbitals of perovskite photovoltaic materials via strain, layering, and doping. **R. Berger**, C. Grote, N. Onishi, K. Tsui

9:20 PHYS **313.** Theory predition of a novel Si-He compound: Structure, property and synthesis. **E. Xu**, T. Li

9:40 PHYS **314.** Orbital approach to superconductivity and superfluidity. **P. Love**

10:00 Intermission.

10:20 PHYS **315.** New bridges with the isolobal analogy: Electron counting in intermetallic phases and strategies for materials discovery. **D. Fredrickson**

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10:50 PHYS **316.** Electron delocalization in σ-bonded one-dimensional chains. **M. Jovanovic**, J. Michl

11:10 PHYS **317.** Layered chalcogenides and the density-of-energy (DOE) function. **P. Konze**, M. Küpers, R. Dronskowski

11:30 PHYS **318.** Computational discovery of high-pressure materials. **M. Amsler**, C. Wolverton, V. Hegde

11:50 Discussion.

Section C

Walter E. Washington Convention Center
Room 152A

Gaseous Ion Chemistry & Surface Reactions

Solution Chemistry in the Gas-Phase

A. K. Badu-Tawiah, H. Chen, *Organizers*

G. E. Johnson, *Presiding*

8:00 PHYS **319.** Structural biology in the gas phase: New techniques for the rapid analysis of protein sequence, structure and stability. J.D. Eschweiler, Y. Tian, D. Polasky, **B.T. Ruotolo**

8:40 PHYS **320.** Protein structure prediction guided by covalent labeling mass spectrometry data. M.L. Aprahamian, S.H. Hinckley, V.H. Wysocki, **S. Lindert**

9:20 Intermission.

9:40 PHYS **321.** Two-dimensional, time-resolved trapped ion mobility spectrometry-mass spectrometry (TIMS/TIMS-MS) to study conformations of peptides and proteins. F. Liu, M. Ridgeway, M. Park, **C. Bleiholder**

10:20 PHYS **322.** Effects of charge state on the structures of protein ions: Results from cation-to-anion proton-transfer reactions (CAPTR). **M.F. Bush**

Section D

Walter E. Washington Convention Center
Room 151A

Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion

New Methods for Measuring & Modeling Liquid/Solid Interfaces

K. L. Jungjohann, J. A. Keith, *Organizers*

B. Peters, *Presiding*

8:00 PHYS **323.** Nanoscale electrochemistry probed by tip-enhanced Raman spectroscopy. **M. Mattei**, G. Goubert, G. Kang, G.C. Schatz, R.P. Van Duyne

8:20 PHYS **324.** Modeling atomically dispersed catalysts on amorphous supports at multiple scales. A. Fong, Y. Wang, S.L. Scott, **B. Peters**

8:55 PHYS **325.** *In situ* molecular imaging of the solid-liquid interface using microfluidics. **X. Yu**

9:30 PHYS **326.** Computational insights to charge transfer reactions at the complex electrode/SEI/electrolyte interface. Y. Li, **Y. Qi**

10:05 Intermission.

10:20 PHYS **327.** Probing liquid-solid interfaces. **G. Veith**, R. Sacci, J. Browning, M. Doucet, J. Kim

10:55 PHYS **328.** *In-operando* neutron reflectometry: Depth profiles of solid liquid interfaces. **J. Dura**

11:30 PHYS **329.** Towards high-resolution ultra-low-field NMR and MRI of heterogeneous systems endowed by nuclear spin hyperpolarization. **D. Barskiy**, C. Slack, T. Sjolander, J. King, A. Pines

Section E

Walter E. Washington Convention Center
Rooms 159A/B

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

New Strategies to Expand the Scope of Enzyme Engineering

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

Q. Cui, G. J. Poelarends, N. Tokuriki, *Organizers*

S. C. Kamerlin, *Organizer, Presiding*

8:00 PHYS **330.** Antibody-enzyme conjugates for targeted glycocalyx editing. **C.R. Bertozzi**

8:40 PHYS **331.** Evolution and applications of split RNA polymerase biosensors. **B.C. Dickinson**

9:20 PHYS **332.** Peptide affinity reagents for Rivax vs. Abrax: A combined computational/experimental approach to untangle selectivity in structurally similar proteins. **M. Hurley**, D.A. Sarkes, D.N. Stratis-Cullum

9:40 Intermission.

10:10 PHYS **333.** Promiscuity, serendipity and metabolic innovation. **S.D. Copley**, J. Kim, J. Flood, J. Kershner, M. Kristofich

10:50 PHYS **334.** Designing highly specific protein-based small molecule biosensors. **V. Raman**

11:30 PHYS **335.** Computational studies of laboratory-evolved tryptophan synthase variants for stand-alone function. **M. Maria Solano**, J. Iglesias, S. Osuna

11:50 Concluding Remarks.

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Membrane Proteins: Structure, Activity & Drug Development

Structure & Dynamics of Membrane Proteins

M. J. Cocco, *Organizer*

F. Marassi, *Organizer, Presiding*

W. Im, *Presiding*

8:00 PHYS **336.** (Passive to active) chaser: NMR and MD of membrane proteins. **W. Im**

8:30 PHYS **337.** Loop dynamics of outer membrane protein OprG contribute to amino acid transport in Pseudomonas aeruginosa. **L.K. Tamm**

9:00 PHYS **338.** NMR structure and function of membrane proteins in membranes. **F. Marassi**

9:20 Intermission.

9:40 PHYS **339.** Receptor mediated uptake: Structure and function of Neisseria Opa proteins. **L.M. Columbus**

10:10 PHYS **340.** Solid-state NMR of protein/lipid contacts of viral fusion peptides. **D.P. Weliky**

10:40 Intermission.

11:00 PHYS **341.** Role of membrane on the function of cytchrome-P450. **A. Ramamoorthy**

11:30 PHYS **342.** Magic angle NMR studies of bacterioshodopsin (bR) and the volage depndent anion channel (VDAC). Q. Ni, T. Can, M. Eddy, Y. Su, R. Silvers, L. Andreas, L. Clark, G. Pintacuda, L. Emsley, G. Wagner, J. Herzfeld, **R.G. Griffin**

Section G

Walter E. Washington Convention Center
Room 151B

Physical Chemistry Research at Undergraduate Institutions

Biophysical

T. Hopkins, *Organizer*

J. G. Navea, *Presiding*

8:00 PHYS **343.** Expanding the vocabulary of vibrational probe functional groups. **C.H. Londergan**

8:40 PHYS **344.** Condensed-phase effects on the structural and energetic properties of molecular complexes: Computations and low-temperature IR spectroscopy. **J.A. Phillips**

9:00 PHYS **345.** Simulations reveal new insights into the mechanism of Ubc13-catalyzed ubiquitination. W. Jones, A. Davis, R.H. Wilson, S.G. Zamfir, **I. Sumner**

9:40 Intermission.

10:00 PHYS **346.** Application of chirped-pulse Fourier transform microwave spectroscopy to study the structure and dynamics of biomolecules in the gas phase. **R.G. Bird**

10:20 PHYS **347.** Research with undergraduates: A fabulous career. **G.C. Shields**

10:40 PHYS **348.** Binding modes and pathway of RHPS4 to human telomeric G-quadruplex and duplex DNA probed by all-atom molecular dynamics simulations with explicit solvent. K. Mulholland, F. Siddiquei, **C. Wu**

11:00 PHYS **349.** Getting over the curve: Early experiences in computational chemistry. **J. Kua**

Molecular Mechanics

Force Fields

Sponsored by COMP, Cosponsored by PHYS

Computational Studies of Membranes & Membrane-Bound Systems

Biology in the Membrane

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

The DIBs: Solving a Century Old Problem

P. Bera, X. Tielens, *Organizers*

N. Cox, *Presiding*

1:00 PHYS **350.** Diffuse interstellar bands: Solving a century old problem. **F. Salama**

1:35 PHYS **351.** ESO diffuse interstellar bands large exploration survey (EDIBLES). N. Cox, M. Cordiner, F. Salama, H. Linnartz, **R. Lallement**, M. Yajouri, E. Consortium

2:05 PHYS **352.** Electronic spectroscopy of C60+ and its identification in interstellar space. **J. Maier**

2:35 Intermission.

3:05 PHYS **353.** Diffuse interstellar bands: 100-years-old mystery beginning to be solved. **T. Oka**

3:35 PHYS **354.** Interstellar C_{60}^+: Pro et contra. **G. Galazutdinov**

3:55 PHYS **355.** Constant intensities of diffuse interstellar bands in the spectrum of AE Aur. **J. Krelowski**

4:15 PHYS **356.** Search for infrared DIBs in Barnard 68. **M. Yajouri**, N. Cox, R. Lallement

4:35 Discussion.

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Structure & Properties of Materials

E. Zurek, *Organizer*

W. Grochala, *Organizer, Presiding*

1:00 PHYS **357.** Decarbonisation of fossil fuels: Microwave-promoted deep catalytic dehydrogenation of liquid alkanes. **P. Edwards**, X. Jie, S. Gonzalez-Cortes, T. Xiao, J. Wang, B. Yao, D. Slocombe, H. Al-Megren, J. Dilworth, J.M. Thomas

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

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‡ *Cooperative Cosponsorship*

1:30 PHYS **358.** Engineering chemical bonds at the inorganic-organic interface: A strategy to design high-performance hybrid phosphor materials for energy-efficient lighting technologies. **J. Li**

2:00 PHYS **359.** Journey with Roald: Coherence in molecular junctions – control, structure, insights and measurements. **M.A. Ratner**

2:20 PHYS **360.** Exploring structural space searching for carbon allotropes. **D.M. Proserpio**, V.L. Deringer, G. Csányi, A.A. Golov, A.A. Kabanov

2:40 PHYS **361.** Corannulene η^5-coordination with transition metals: A theoretical study. **X. Lu**, A.Y. Rogachev

3:00 Intermission.

3:20 PHYS **362.** Phosphorene meets metal fragments. **A. Ienco**, G. Manca, C. Mealli, M. Peruzzini

3:50 PHYS **363.** Effect of temperature on the symmetry of molecules and solids: A continuous symmetry measures study. **P. Alemany**

4:20 PHYS **364.** On the Curie-Weiss temperature of a magnetic system composed of nonquivalent magnetic ions. **K.H. Lee**, C. Lee, H.J. Koo, M. Whangbo

4:40 PHYS **365.** Bonding and dynamics in the synthesis of K_2MSbS_4H (M = Zn, Cd). **C. Zheng**, X. Zhang, R. Hoffmann, F. Huang

Section C

Walter E. Washington Convention Center
Room 152A

Gaseous Ion Chemistry & Surface Reactions

Ion Energetics: Gas-Phase versus Micro-Solvated Systems

A. K. Badu-Tawiah, H. Chen, *Organizers*

M. F. Bush, *Presiding*

1:00 PHYS **366.** Anion photoelectron/photodissociation spectroscopy: Radical thermochemistry and solvation dynamics. **W. Lineberger**

1:40 PHYS **367.** Exploring the thermochemistry of neutral acetonitrile and methanol solvation onto ionized halogenated benzenes. **A.C. Pearcy**, K. Mason, S. Platt, M.S. El-Shall

2:00 PHYS **368.** Chemistry on a slide: Hydration gradient effects on rates and mechanisms at the air-water interface. **A.J. Colussi**

2:40 Intermission.

3:00 PHYS **369.** Field-induced droplet ionization illuminates stepwise oxidation of cell membrane lipids by hydroxyl radicals at the air-water interface. X. Zhang, K. Barraza, **J.L. Beauchamp**

3:40 PHYS **370.** Amine substitution studies of atmospherically relevant anionic clusters. **E. Castracane**, E. Racow, Y. Yang, S.E. Waller, J. Kreinbihl, C.J. Johnson

4:00 PHYS **371.** Thermochemistry and mechanisms of the deamidation of asparagine containing peptides. **P.B. Armentrout**, G.C. Boles

Section D

Walter E. Washington Convention Center
Room 151A

Physical Chemistry Research at Undergraduate Institutions

Atmospheric & Gas Phase

T. Hopkins, *Organizer*

M. Subir, *Presiding*

1:00 PHYS **372.** Collaborative experimental and computational investigations of unimolecular reactions of halocarbon species in the gas-phase. **B.E. Holmes**, G.L. Heard

1:40 PHYS **373.** Quantum chemical and statistical rate theory investigations of atmospheric oxidation reactive intermediates. **K.T. Kuwata**

2:00 PHYS **374.** Microwave spectroscopy at Coker College. **G.G. Brown**, S. Gaster, C. Funderburk, T. Taylor

2:40 PHYS **375.** Withdrawn.

3:00 Intermission.

3:20 PHYS **376.** Vector correlations in the photodissociation of NO-containing molecules. **J.A. Bartz**

4:00 PHYS **377.** Towards and understanding of CO_2 microsolvation: Microwave spectroscopy of CO_2 complexes with fluoroethylenes. **R.A. Peebles**, S.A. Peebles, A.M. Anderton, C.L. Christenholz, R.E. Dorris, W.C. Trendell

4:20 PHYS **378.** Automating the analysis of high-resolution rotational spectra. **S.T. Shipman**, J.H. Westerfield, K. Ervin, E. Riffe, E. Johnson

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Membrane Proteins: Structure, Activity & Drug Development

Structure & Dynamics of Membrane Proteins

M. J. Cocco, F. Marassi, *Organizers*

R. Martin, A. Nevzorov, *Presiding*

1:00 PHYS **379.** Functional consequences of membrane protein oligomerization illustrated with proteorhodopsin. **S. Han**, C. Han, M. Idso, S. Hussain

1:30 PHYS **380.** SAS NMR methods development for investigation of biological membranes and membrane proteins. J. Kelly, M.H. Uhelkar, J. Kelz, **R.W. Martin**

2:00 PHYS **381.** Identification of receptor binding to the biomolecular corona of nanoparticles. **Y. Yan**, S. Lara, F. Alnasser, K. Dawson

2:20 Intermission.

2:40 PHYS **382.** Structural studies of the drug transporter EmrE using NMR spectroscopy. **N. Traaseth**

3:10 PHYS **383.** Sensitivity enhancement in solid-state NMR of oriented membrane proteins. S. Koroloff, D. Tesch, S. Milikisiyants, A.I. Smirnov, **A. Nevzorov**

3:40 Intermission.

4:00 PHYS **384.** Insights into structure and dynamics of membrane proteins. S. Wang, D. Good, C. Ing, S. Emami, R. Pomes, L. Brown, **V. Ladizhansky**

4:30 PHYS **385.** M2 proton channel: Structure, dynamics and proton exchange data for understanding drug binding and functional rates. **T.A. Cross**, R. Fu, Y. Miao, A. Wright, J. Paulino

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS/Journal of Physical Chemistry Lectureship Award: Symposium in honor of Professor Randall Goldsmith

J. E. Shea, *Organizer*

J. Vura-Weis, *Presiding*

1:00 PHYS **386.** New variables to dissect in vitro biochemistry with single-molecule resolution. **Q. Wang**

1:40 PHYS **387.** Multidimensional super-resolution imaging. **S.F. Lee**

2:20 Intermission.

2:35 PHYS **388.** Carrier-specific femtosecond extreme ultraviolet spectroscopy of semiconductors. **J. Vura-Weis**

3:15 PHYS **389.** Probing complex interfacial (bio)chemical interactions using silicon photonic microring resonator arrays. **R.C. Bailey**

3:55 PHYS **390.** Optical microresonators as platforms for single-molecule spectroscopy. **R.H. Goldsmith**

Molecular Mechanics

Nucleic Acids

Sponsored by COMP, Cosponsored by PHYS

Computational Studies of Membranes & Membrane-Bound Systems

Transport Across Membranes

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY EVENING

Section A

Walter E. Washington Convention Center
Hall D

PHYS Poster Session

J. E. Shea, *Organizer*

6:00 - 8:00

PHYS **391.** Benchmarking of electrostatic interactions in QM/MM molecular dynamics simulations. **X. Pan**, Y. Shao

PHYS **392.** Cation effects on the first electronic transitions of hydrating water studied by far-UV spectroscopy and quantum chemical calculations. **T. Goto**, A. Ikehata, Y. Morisawa, K. Bec, Y. Ozaki

PHYS **393.** Characterization of the 1,2-propanediol + benzene and 1,2-propanediol + benzene-d_6 liquid-liquid phase equilibria. **K.C. Riley**, C.A. Tibbetts, M. McKibben, C.C. Williamson

PHYS **394.** Solid-state theoretical investigation of elasticity in insensitive explosives. **R. Prendergast**, T.M. Korter

PHYS **395.** Chemical reaction in Pluto's atmosphere: Nitrile formation from C_2H_2 and N_2. **Y. Yarnall**, P.D. Cooper

PHYS **396.** Extreme biophysics: Enzymes under pressure. **Q. Huang**, J.M. Rodgers, R.J. Hemley, T. Ichiye

PHYS **397.** Effect of internal hydrogen bond formation on the predicted thermochemistry of hydroxylated Criegee intermediates. **M.K. Sprague**, K.K. Irikura, T. Bui

PHYS **398.** Impact of material dimensionality on charge transfer dynamics: Case study of dye-sensitized lead halide perovskite solar cells. **A. Forde**, D. Kilin

PHYS **399.** Tip-enhanced Raman spectroscopic study on Pt-Au bimetallic surfaces. **H. Su**, J. Zhong, B. Ren

PHYS **400.** Theory investigation on structure and optical properties of TMTZ single crystal. **M. Yue**, G. Lu

PHYS **401.** Withdrawn.

PHYS **402.** GW method using the Cholesky decomposition technique with applications to QM/QM embedding approaches. **A. Shee**, L. Tran, D. Zgid

PHYS **403.** Withdrawn.

PHYS **404.** Palladium nanoparticles supported on Ce-metal organic framework for efficient CO oxidation and low-temperature CO_2 capture. A. Awad, A. Lin, **M.S. El-Shall**

PHYS **405.** Computationally investigating the mechanism of the histone acetyltransferase, Gcn5. **R.H. Wilson**, I. Sumner

PHYS **406.** Calculation of vibrational structure of astrochemically relevant ions using reparametrized semi-empirical methods. **J.P. Layfield**, J. Arend, W. Fuerste

PHYS **407.** Quantum control of particles moving at surface. **Q. Wang**

PHYS **408.** First-principles studies on the electronic structural, optical and phonon lattice dynamical properties of pure- and La-doped $SrTiO_3$. **Y. Duan**

PHYS **409.** Withdrawn.

PHYS **410.** Molecular docking of selective binding affinity of sulfonamide derivatives as potential antimalarial agents targeting the glycolytic enzymes: GAPDH, aldolase and TPI. N.Y. Forlemu, **P. Watkins**, J. Sloop

PHYS **411.** Electromagnetic property of a plastic-aluminum bi-layer material and its potential application in data decoding for compact disks. **J. Zhang**

PHYS **412.** Understanding the effect of substituents on the rigidity and conjugation length of poly(phenylene ethynylene) using DFT - Tight Binding. **C.J. Zeman**, K.S. Schanze

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TECHNICAL PROGRAM

PHYS **413.** Plasmon-enhanced single-molecule analysis with shell-isolated Ag nanoparticle platform. **C. Li**, J. Li, Z. Tian

PHYS **414.** Plasmon-enhanced quantum dot spontaneous emission and sensitized photoelectrochemical hydrogen evolution using shell-isolated nanoparticles. **Y. Hao**

PHYS **415.** Investigation of deep eutectic solvents containing chloride-free cholinium salts: Synthesis and solvent properties. **N. Barashkov**, T. Sakhno, I. Irgibaeva, A. Mantel

PHYS **416.** Insights into the mechanism of a green/blue phytochrome via absorption and circular dichroism spectroscopies. **J.A. Clinger**, E. Chen, D.S. Kliger, G.N. Phillips

PHYS **417.** Membrane binding and fluidity sensing by α-, β-, and γ-synuclein. **E. O'Leary**, Z. Jiang, J.C. Lee

PHYS **418.** Photoinduced anion exchange in cesium lead halide perovskite nanocrystals. **D.G. Parobek**

PHYS **419.** Withdrawn.

PHYS **420.** Fabrication of light-emitting electrochemical cells (LECs) having screen-printed electrodes. **L. Hyeonseok**

PHYS **421.** High-resolution photoelectron imaging of boron clusters (B_{11}^- and B_{12}^-) and transition-metal doped boron cluster (IrB_3^-). **J.G. Czekner**, L. Cheung, L. Wang

PHYS **422.** Sliding of positively charged nanoparticles along long DNA molecules with flexibility gradient: A Brownian dynamics simulation study. **S. Park**, J. Kim

PHYS **423.** Sequence-dependent binding of a dendrimer with a DNA molecule: A molecular dynamics simulation study. **J. Chae**, J. Kim

PHYS **424.** Probing the stability of the C-terminal domain of type IV pilins under external force. **R.B. Goncalves**, J.L. Baker

PHYS **425.** Enforcing size-consistency in an excited state variational principle. **J. Shea**, E. Neuscamman

PHYS **426.** Crystal structures and electronic properties of Xe-Cl compounds at high pressure. **N. Zarifi**, E. Zurek, J. Tse

PHYS **427.** Efficient construction of real space stenciling factors. **B. Van Der Goetz**, E. Neuscamman

PHYS **428.** Cyanylated cysteine as an infrared reporter of protein-peptide interactions: Experimental measurements, molecular dynamics simulations and semi-quantitative calculations of IR lineshape. **R.J. Xu**, C.H. Londergan

PHYS **429.** Designing boron-based thermally activated delayed fluorescence emitters with improved OLED device properties. **S. Mukhopadhyay**

PHYS **430.** Intramolecular singlet fission in antiaromatic polycyclic hydrocarbon. **Y. Wu**, Y. Wang, D. Zhang, H. Fu

PHYS **431.** New environment sensitive bifunctional ligand-induced aggregation of serum proteins: Possible consequences in biology and electronics. **S. Panja**, S. Datta, P. Mitra, M. Halder

PHYS **432.** Simulating protein-mediated hydrolysis of ATP and other nucleoside triphosphates by combining QM/MM molecular dynamics with advances in metadynamics. **R. Sun**, O. Sode, J.F. Dama, G.A. Voth

PHYS **433.** AFQMC in the infinite basis set limit: The accuracy of combining AFQMC with F12 methods. **H. Hao**, B. Rubenstein

PHYS **434.** In-situ monitoring the electrodeposition ofsilver nanoplates and its catalytic applications. **S. Juanjuan**

PHYS **435.** Chitosan-assisted synthesis of silver hexahedrons on pencil graphite electrodes: Nucleation-growth mechanism and sensing of hydrogen peroxide and hydrazine. **P. Sankaranarayanan**, S. M V

PHYS **436.** Electromagnetic response-mediated intervention of microwave heating on different stages of Maillard reaction. **N. Zhang**, Y. Zhao, D. Fan, B. Yan, J. Huang, J. Zhao, M. Wang, H. Zhang

PHYS **437.** Withdrawn.

PHYS **438.** Plasmonic electricity: Fluorophore induced plasmonic current. **J. Moskowitz**, C.D. Geddes

PHYS **439.** Investigating the influence of low concentration ionic liquids on Trp-cage structural stability. **M. De Souza**, A. Heyert, G.E. Lindberg, J.L. Baker

PHYS **440.** Cyclooxygenase-2 dimerization activity may be influenced by its monomers' glycosylation at Asn^{580}. **J.M. Cunanan**, R. Chan, M. Chen, M. Sevigny, R.W. Hall

PHYS **441.** OC-HOCO complex: Identification and implications for ISM chemistry. **Y. Yarnall**, K. Stelmach, O. Gadzhiev, A. Masunov , P.D. Cooper

PHYS **442.** Influence of protein crowder size on hydration structure and dynamics in macromolecular crowding. **P. Wang**, I. Yu, M. Feig, Y. Sugita

PHYS **443.** Blocked linear method for optimizing large parameter sets in variational Monte Carlo. **L. Zhao**, E. Neuscamman

PHYS **444.** Computational insights into epoxide hydrolase asymmetric hydrations of epoxides. **E. Serrano-Hervás**, F. Feixas, M. Garcia-Borràs, S. Osuna

PHYS **445.** Manipulation and characterization of nanoscale plasmon-induced chemical reaction by electrochemical tip-enhanced Raman spectroscopy. **S. Huang**, X. Wang, Z. Zeng, B. Ren

PHYS **446.** Probing solvent effects on an iodine clock reaction using millifluidic devices. **S. Morley**, B.J. Knurr

PHYS **447.** Redesign of MACiE: A database of enzyme mechanisms. **A.J. Ribeiro**, G.L. Holliday, N. Furnham, J.M. Thornton

PHYS **448.** Withdrawn.

PHYS **449.** Sparse energy sampling in Fock-space variational Monte Carlo. **H. Wei**, E. Neuscamman

PHYS **450.** Cost-effective multi-determinant expansion in quantum Monte Carlo for excited states. **S. Pineda Flores**, E. Neuscamman

PHYS **451.** Super-resolution imaging of fluorophores bound to silica-coated gold nanorods. **A. McLeod**, K.A. Willets, T. Anthony

PHYS **452.** Stepwise hydration of halogen-containing benzene cations in the gas phase: Is it hydrogen of halogen bonding? K. Mason, A.C. Pearcy, I.K. Attah, S. Platt, **M.S. El-Shall**

PHYS **453.** Laser synthesis of palladium nanoparticles incorporated within NH_2-MIL-125(Ti) for the selective hydrodeoxygenation of vanillin, a model for bio-oil upgrade reactions. J. Bobb, A. Awad, **M.S. El-Shall**

PHYS **454.** Spectroscopic and computational investigation of pyran-4-one in its $S_1(n,\pi^*)$ excited state. **M.P. McDonnell**, K.M. Jawad, S.M. Fritz, T.S. Zwier, S. Drucker

PHYS **455.** All-atom simulation and coarse-grained analysis of the type IV pilus filament from Neisseria meningitidis. **J.L. Baker**, R.B. Goncalves

PHYS **456.** STM study on the polymerization of 3,4-ethylenedioxythiophene on Au(111) surface by using different electrochemical treatment. **S. Fu**, I. Liu, Y. Lee

PHYS **457.** Brominated and iodinated < 10 nm carbon nanodots. **R. Knoblauch**, C.D. Geddes

PHYS **458.** Investigating the effect of choline chloride and trivalent cations on late embryogenesis abundant protein consensus sequences. **S. Schmidt**, K. Barrie, M.R. Bunagan

PHYS **459.** Effect of adding lithium chloride or potassium chloride on the tetra-n-butylammonium chloride/water semi-clathrte system using differential scanning calorimetry. **D.C. Henriques**, R.J. Wigent

PHYS **460.** Chiral discrimination by amino acid based deep eutectic solvents. **C. Wright**, T. Hopkins

PHYS **461.** Narrowing limitless: A method for selecting ionic liquids to control protein structure. **A. Heyert**, J.L. Baker, G.E. Lindberg

PHYS **462.** Evaluation of anisotropic, isotropic, and no thermal expansion in the (quasi-)harmonic approximation to accurately calculate thermodynamic properties of organic crystals. **N.S. Abraham**, E. Dybeck, N.P. Schieber, M.R. Shirts

PHYS **463.** Platinum electrode fabrication for in situ spectroelectrochemistry. **E. Gobrogge**, X. Ren, C. Lundgren

PHYS **464.** Circular dichroism study of late embryogenesis abundant proteins in reverse micelles. K. Barrie, **M.R. Bunagan**

PHYS **465.** Photophysical study of ruthenium (II) Tris-(2,2'-bipyridine) encapsulated within Uio-66 metal organic frameworks containing functionalized linkers. **J. Mayers**, R.W. Larsen

PHYS **466.** Comparative analysis of recombinant polyhydroxybutyrate depolymerases from bacterial strains. **D.I. Martinez-Tobon**, A. Elias, D. Sauvageau

PHYS **467.** Withdrawn.

PHYS **468.** Rovibrational spectra of potential interstellar noble gas molecules and small hydrocarbons. **C.M. Novak**, R.C. Fortenberry

PHYS **469.** UV-visible spectroscopy of PAHs and PANHs in supersonic jet: Astrochemical implications. **S. Bejaoui**, F. Salama

PHYS **470.** Salt bridges gate alpha-catenin activation at intercellular junctions. **S. Barrick**, J. Li, X. Kong, A. Ray, E. Tajkhorshid, D.E. Leckband

PHYS **471.** Rainbow of colors in butterfly wings: A photophysical investigation. **F. Chalyavi**, A. Espeset, N.R. Fetto, M. Forister, M.J. Tucker

PHYS **472.** Ab initio self-energy embedding theory for realistic systems. **L. Tran**, A. Kananenka, D. Zgid

PHYS **473.** Molecular properties from range-separated LDA-GF2 hybrid functional. **A. Kananenka**, D. Zgid

PHYS **474.** Distal residues of ornithine transcarbamoylase contribute to electrostatic and dynamics properties of the enzyme. **J. Winters**, L. Ngu, K. Nguyen, L. Makowski, P. Beuning, M. Ondrechen

PHYS **475.** High-resolution spectroscopy of gas phase aromatic molecules. **W. Roeterdink**, W.J. Buma, A. Petrignani

PHYS **476.** Withdrawn.

PHYS **477.** Modeling and simulation approaches for studying competition and cooperativity of actin binding proteins. **G.M. Hocky**, D.R. Kovar, G.A. Voth

PHYS **478.** Development of a stochastic implementation of the second-order Green's function. **B. Winograd**

PHYS **479.** Accurate temperature dependent methods for QM/QM embedding. **A.R. Welden**, D. Zgid

PHYS **480.** Effect of adding sodium chloride on tetra-n- butylammonium chloride/ water semi-clathrate system. **M.A. Siddiq**

PHYS **481.** Green's functions in solid-state electronic structure modeling: Self-consistency, finite temperature, and electronic correlations. **A. Rusakov**, L. Tran, S. Iskakov, D. Zgid

PHYS **482.** Combining the photoreduction of Au(III) and the electrodeposition of Au(I) in a new method to create microscopic gold patterns. **C.N. Lafratta**, C. Sirkoch, P. Lawrence, E. Will

PHYS **483.** Withdrawn.

PHYS **484.** Insights into the molecular structure of hydrogen chloride-cis-1,2-difluoroethylene from ab initio calculation of an intermolecular potential energy surface. **L.H. Yoon**, H.O. Leung, M.D. Marshall

PHYS **485.** Alkyne combustion: Experimental and theoretical studies of formyl radical formation. **M. Drummer**

PHYS **486.** Computational study of quaternary ammonium salts as liquid-liquid phase-transfer catalysts. **T. Schaefer**, J.P. Layfield

PHYS **487.** Growth mechanism of 'sea urchin' shaped ZnO nanostructures and their photocatalytic activity in the degradation of organic dyes. H.D. Kiriarachchi, K.M. AbouZeid, **M.S. El-Shall**

PHYS **488.** Redox potentials and reactivity of redox shuttles from the first principles calculations. **M. Burrows**, R. Tazhigulov, K.B. Bravaya

PHYS **489.** Infrared photodissociation cluster studies on CO_2 interaction with titanium oxide catalyst models. **L.G. Dodson**, M.C. Thompson, J.M. Weber

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

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PHYS **490.** Synthesis of carbonaceous TiO2 nanostructures by laser vaporization controlled-condensation of MIL-125(Ti) and NH2-MIL-125(Ti) and their applications as catalyst support for Pd nanoparticles for Suzuki cross coupling reactions. J. Bobb, A. Awad, **M.S. El-Shall**

PHYS **491.** Acid site correlation to the selectivity for 2-methoxy-4-methylphenol in the hydrodeoxygenation of vanillin by Pd nanoparticles encapsulated within the zirconium-based metal-organic framework UiO-66-NH2. A. Lin, A. Awad, **M.S. El-Shall**

PHYS **492.** Withdrawn.

PHYS **493.** Photophysical properties of 1-pyrenemethylamine hydrochloride. **G.S. DiBattista**, A. Brooks, S. Temple, B.H. Milosavljevic

PHYS **494.** Fabrication of highly nanostructured electrodes. **P. Kharel**, A. Talsania, D. Cahill, F. Dawood

PHYS **495.** Effective removal of heavy metal ions from aqueous solutions by chemically modiefied graphene oxide nanosheets. F.S. Awad, K.M. AbouZeid, **M.S. El-Shall**

PHYS **496.** Ab initio study of triplet states of XeF2 and XeCl2. **G.J. Hoffman**

PHYS **497.** Investigations of prebiotic phosphorus chemistry on the meteoritic mineral schreibersite. **H.L. Abbott-Lyon**

PHYS **498.** Laboratory astrochemistry: Catalytic conversions of methanol to organic molecules over olivine-type silicates. **Q. Li**, W. Dai, B. Liu, P.J. Sarre, A. Cheung

PHYS **499.** Simultaneous photophysical and TA study of liquid-liquid phase yransition in water-rich ideal solution. A. Anmangandla, **P. Martin**, B.H. Milosavljevic

PHYS **500.** Pre-transition droplet formation in liquid-liquid binary systems. **M. McKibben**, S. Rogers, A.R. Wert, K.C. Riley, C.C. Williamson

PHYS **501.** Accelerated electrospray-based reaction discovery: Toward rational design of visible-light-mediated aerobic oxidation of N-heterocycles in ambient air. **A.K. Badu-Tawiah**, S. Jayaraj, Q. Wan, K.M. Davis

PHYS **502.** Solvent polarity driven varied interaction of long chain aliphatic thiol or amines with fluorescent assembly. **J. Jana**, T. Pal

PHYS **503.** Combined experimental and computational investigation on the Sm2O3-BaO system. **W. Gong**

PHYS **504.** Mapping structure-property relations in molecularly tunable fluorescent quantum defects. **M. Kim**, G. Ao, X. He, H. Kwon, X. Wu, M. Zheng, S.K. Doorn, Y. Wang

PHYS **505.** Is carbon monoxide in the pure solid form in the ice mantle? **J. He**, G. Vidali

PHYS **506.** Controlling the magnetic anisotropy of single molecule with STM tip: The crucial roles of structural deformation and electronic states. **X. Wang**, X. Zheng

PHYS **507.** Chirality associated Marcus inverted region observed in pristine single-walled carbon nanotubes via asymmetric-doping-induced electrical potential. **A.T. Liu**, Y. Kunai, A. Cottrill, M. Strano

PHYS **508.** Inhibitory effects of Acanthus montanus leaves extract on microbial influenced corrosion of oil pipe line steel (caused by sulphur reducing bacteria) in anaerobic environment. **I. Nkechi**

PHYS **509.** Evolving new proteins by non-homologous recombination. **G. Rawcliffe**, W. Patrick

PHYS **510.** Direct spectroscopic measurement of inherent and applied interfacial electric fields near an electrode. **J. Patrow**, S.A. Sorenson, J. Dawlaty

PHYS **511.** Decomposition of hydroxylammonium nitrate ionic liquid aerosols on catalytically active metal surfaces. **G.L. Vaghjiani**, S. Chambreau, D.M. Popolan-Vaida, S.R. Leone

PHYS **512.** Chemical signatures in magnetized cloud cores. **S. Hocuk**, P. Caselli

PHYS **513.** Role of anharmonic effects in analysis of astrochemical observations: IR signatures and thermodynamics. **J. Bloino**, M. Biczysko, C. Puzzarini

PHYS **514.** Light-activated synthesis of aryl fluorescent quantum defects in single-walled carbon nanotubes. **X. Wu**, H. Kwon, M. Kim, Y. Wang

PHYS **515.** Withdrawn.

PHYS **516.** Hydrophobic water at a hydrophilic interface. **J.D. Cyran**, M.A. Donovan, E. Tyrode, M. Bonn, E. Backus

PHYS **517.** Intervention of TGase in surimi gel under microwave irradiation. **H. Cao**, D. Fan, J. Huang, X. Jiao, W. Zhou, W. Zhang, J. Zhao, H. Zhang

PHYS **518.** Withdrawn.

PHYS **519.** DNA damage through microwave irradiation generated reactive oxygen species. **T.M. Santaus**, C.D. Geddes

PHYS **520.** Computational challenges in astrochemistry. **M. Biczysko**, J. Bloino, C. Puzzarini

PHYS **521.** Anharmonic temperature effects on the infrared spectrum. **T. Chen**

PHYS **522.** Study of highly excited states of chlorine substituted cumuleneone series with coupled cluster method. **Q.L. Nguyen**, M.M. Murnane, H.C. Kapteyn, W.K. Peters, R.C. Fortenberry

PHYS **523.** Second harmonic generation of water at silica/aqueous interface determined by molecular dynamics. **S. Chen**, S.J. Singer

PHYS **524.** Withdrawn.

PHYS **525.** Molecular dynamics simulations and Markov models of natural and evolved stand-alone LovD enzyme variants. **J. Iglesias**, S. Olsson, F. Noé, S. Osuna

PHYS **526.** Non-adiabatic molecular dynamics with delta self-consistent field excited states (ΔSCF-NA-MD). **E. Pradhan**

PHYS **527.** DFT calculations of Arg and Lys on Au(111) to probe the effects of amino acid conformation and dispersion on binding. **M.C. Small**, J. Terrell, D.A. Sarkes, J. Jahnke, D.N. Stratis-Cullum, M. Hurley

PHYS **528.** Field-controlled nanopore permeation by electrolyte solution. **D. Bratko**, F. Moucka, D. Vanzo, A. Luzar

PHYS **529.** Exploration of reduced scaling approaches to EOM-CCSD. **C. Peng**, E.F. Valeev, J. Zhang

PHYS **530.** Non-reactive dynamics at water-mineral interfaces. **R. Remsing**

PHYS **531.** Organic macromolecules in comet 67P and diffuse interstellar band carriers. **R. Lallement**, J. Bertaux

PHYS **532.** Monovalent and divalent cations at the α-Al_2O_3 (0001)/water interface: How cation identity affects interfacial ordering and vibrational dynamics. **S. Piontek**, K. Millan, R. Wang, A. Tuladhar, R. Remsing, V. Carnevale, M. Klein, E. Borguet

PHYS **533.** Analyzing the role of the product metal ion in DNA polymerase β catalysis. **L. Perera**

PHYS **534.** Reduced scaling many-body methods in non-LCAO representations. **E.F. Valeev**

PHYS **535.** Withdrawn.

PHYS **536.** Study hyddrated electrons with range-separated functionals. **C. Zhou**, V. Vlcek, D. Neuhauser, B.J. Schwartz

PHYS **537.** Insights into sulfide-enhanced oxygen reduction reaction activity by in-situ electrochemical infrared spectroscopy and theoretical simulations. **D. Chen**, Y. Wang, T. Allison, Y. Tong

PHYS **538.** Effect of solvent and substrate on dye molecule orientation for DSSC applications. **J. Domenico**, M.E. Foster, M. Allendorf, K.W. Sohlberg

PHYS **539.** Pentavalent lanthanide nitride-oxides: NPrO and $NPrO^-$ complexes with N≡Pr triple bonds. **S. Hu**

PHYS **540.** Photophysical studies of Ru(II)tris(2,2'-bipyridine) encapsulated within a Zinc(II) – benzene-1,3,5-tricarboxylic acid metal-organic framework. **C. McKeithan**, R.W. Larsen

PHYS **541.** Influence of galactic arm scale dynamic on the molecular composition of dense clouds. **M. Ruaud**, V. Wakelam, P. Gratier, I.A. Bonnel

PHYS **542.** Contributions of an astrochemical European network[1] to the qualitative understanding of physical astrochemistry: Energy transfers and reaction rates. **L. Wiesenfeld**

PHYS **543.** Evidence for the presence of H_n-PAHs in post AGB stars. **C.K. Materese**, J.D. Bregman, S.A. Sandford

PHYS **544.** Magnesium pre-organizes SAM-II riboswitch triplex. **S. Roy**, H. Lammert, R.L. Hayes, B. Chen, R. LeBlanc, T. Dayie, J. Onuchic, K.Y. Sanbonmatsu

THURSDAY MORNING

Section A

Walter E. Washington Convention Center
Room 156

Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets

Chemistry of Atmospheres of Stars & Planets

P. Bera, X. Tielens, *Organizers*

R. L. Hudson, *Presiding*

8:00 PHYS **545.** Molecular spectroscopy of exoplanet atmospheres. **A. Burrows**

8:35 PHYS **546.** Atmospheric chemistry in (currently observable) exoplanets: Review of a suite of techniques. **K. Heng**

9:05 PHYS **547.** Spectroscopic data for characterizing (exo)-planetary atmospheres. **T.J. Lee**

9:35 Intermission.

10:00 PHYS **548.** Astrochemistry of titan. **C. Nixon**

10:30 PHYS **549.** James Webb Space Telescope capabilities for characterizing exoplanet atmospheres. T. Greene

11:00 PHYS **550.** Expanding our knowledge of the ranges of environmental conditions that may have been able to support peptide synthesis on the primitive Earth and elsewhere. **E.T. Parker**

11:30 PHYS **551.** Climatological variations in Titan's atmospheric chemistry mapped using ALMA. **M. Cordiner**, C. Nixon, S. Charnley, N. Teanby, Z. Kisiel, P. Irwin, M. Palmer, J. Lai, X. Thelen, V. Vuitton

11:50 Discussion.

Section B

Walter E. Washington Convention Center
Room 152B

Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann

Insights into Physical Chemistry

W. Grochala, E. Zurek, *Organizers*

A. Hermann, *Presiding*

8:00 PHYS **552.** Ionic ammonia-water mixtures stable at icy planet conditions. V. Naden Robinson, Y. Wang, Y. Ma, **A. Hermann**

8:30 PHYS **553.** Theoretical investigation of singlet fission: Uncovering mechanisms and designing molecules. **N. Ananth**

9:00 PHYS **554.** Quantum chemistry and quantum dynamics studies of intramolecular singlet fission: How bonding affects number doubling of excitons. **T. Zeng**

9:20 PHYS **555.** Jahn-Teller models, symmetric spaces, and quantum phase transitions. **R. Florentino Ribeiro**, J. Yuen-Zhou

9:40 PHYS **556.** Study of proton and electron transfer using quantum master equation methods. **T. Ture**

10:00 Intermission.

10:20 PHYS **557.** Orbital interactions between C_2H_2, BBr_3, and HBr influencing stereospecificity of acetylene bromoboration. H. Semrád, J. Stošek, P. Kubáček, **M. Munzarova**

10:40 PHYS **558.** Density functional perturbational orbital approach in understanding of covalent magnetism through chemical bonds. **D. Seo**

11:00 PHYS **559.** Double Rydberg anions and their Dyson orbitals. **J.V. Ortiz**

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11:20 PHYS **560.** From hydrogen storage materials to metallic and superconducting hydrides. **W. Grochala**

11:40 PHYS **561.** Predicting crystal structures at high pressures. **E. Zurek**

Section C

Walter E. Washington Convention Center
Room 152A

Gaseous Ion Chemistry & Surface Reactions

Ion Spectroscopy

A. K. Badu-Tawiah, H. Chen, *Organizers*

A. L. Ferzoco, *Presiding*

8:00 PHYS **562.** Cryogenic spectroscopy for structural and analytical studies of biomolecular ions. V. Scutelnic, C. Masellis, **T.R. Rizzo**

8:40 PHYS **563.** Coordination chemistry in titanium-carbon dioxide anionic clusters studied by infrared photodissociation spectroscopy. **L.G. Dodson**, M.C. Thompson, J.M. Weber

9:00 PHYS **564.** Probing glycosidic bond stability via energy-resolved single and multiple collision-induced dissociation tandem mass spectrometry approaches: Application to protonated and sodium cationized nucleosides and glycosyl phosphates. **M.T. Rodgers**, R. Wu, Y. Zhu, Z. Yang

9:40 Intermission.

10:00 PHYS **565.** Homochiral serine octamer anions: Infrared spectrum and structure of the chloride adduct. **G. von Helden**

10:40 PHYS **566.** Specific peptide-bond dissociation of some peptide model ions. **C. Liu**

11:00 PHYS **567.** Exploring the dissociation dynamics of radical cations with femtosecond pump-probe spectroscopy: Application to model systems for organophosphorus nerve agents and nitro-based energetic molecules. D. Ampadu Boateng, G. Gutsev, P. Jena, **K.M. Tibbetts**

Section D

Walter E. Washington Convention Center
Room 151A

Physical Chemistry Research at Undergraduate Institutions

Interfaces

T. Hopkins, *Organizer, Presiding*

8:00 PHYS **568.** Atmospheric fate of fly ash: From heterogeneous photochemistry of nitric acid to particle weathering. **J.G. Navea**

8:40 PHYS **569.** Insights into liquid-liquid equilibrium behavior gained from laser light scattering measurements. **C.C. Williamson**

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

9:00 PHYS **570.** Dark reactions project: Undergraduate-driven discovery of new materials with cheminformatics, machine learning, and experiments (and robots) at a small liberal arts college. **J. Schrier**

9:40 Intermission.

10:00 PHYS **571.** Investigating the interfacial structure and partitioning of nitrate ions in reverse micelle structures. **J.D. Patterson**, K.J. Blackshaw

10:20 PHYS **572.** Quantum theory of atoms-in-molecules (QTAIM) consideration of the electron density properties of ionic, covalent, and metallic bonds. **D.A. Clabo**

10:40 PHYS **573.** Multiscale modeling of the complete ligand binding pathways to influenza neuraminidase. **A.W. Van** Wynsberghe

11:20 PHYS **574.** Building a physical chemistry research program at a PUI. **T.C. Devore**

11:40 Concluding Remarks.

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Membrane Proteins: Structure, Activity & Drug Development

Structure & Dynamics of Membrane Proteins

M. J. Cocco, F. Marassi, *Organizers*

A. Kenworthy, J. Long, *Presiding*

8:00 PHYS **575.** Targeting proteins to membrane rafts: mechanisms and consequences. **A. Kenworthy**

8:30 PHYS **576.** Coherent vibrational imaging for living cells. **L. Wei**, W. Min

9:00 PHYS **577.** Withdrawn.

9:20 Intermission.

9:40 PHYS **578.** Structure-function relationships of host defense metallopeptides: When strong nuclease activity correlates with weak membranolyticity and high therapeutic index. **M. Cotten**, M. Libardo, E. Mihailescu, A.A. Bahar, B. Ma, A. De Angelis, J. Zhao, R. Rai, R. Fu, D. Ren, R. Nussinov, S. Opella, A.M. Angeles Boza

10:10 PHYS **579.** Microsecond simulations of antimicrobial peptides and mimetics of ApoA-I. **R. Pastor**

10:40 Intermission.

11:00 PHYS **580.** Peptide-mediated lipid organization, structure, and dynamics in pulmonary surfactant. **J. Long**, N. Tran, A. Smith, O. Braide

11:30 PHYS **581.** New method to study heterodimerization of membrane proteins and its application to fibroblast growth factor receptors. **K.A. Hristova**

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS Award in Experimental Physical Chemistry: Symposium in honor of Professor Kit Bowen

J. E. Shea, *Organizer*

W. C. Lineberger, D. R. Yarkony, *Presiding*

8:00 PHYS **582.** Geminate recombination of photodissociated anions in size-selected solvents. **W.C. Lineberger**

8:35 PHYS **583.** Characterization of reaction intermediates in homogeneous catalysis with cryogenic ion chemistry and spectroscopy. **M.A. Johnson**

9:10 PHYS **584.** Limits of Born-Oppenheimer dynamics. **D.R. Yarkony**

9:45 Intermission.

10:05 PHYS **585.** Adventures in anion photoelectron spectroscopy. **K.H. Bowen**

10:50 PHYS **586.** Photoelectron spectroscopy of negative ions: From planar boron clusters to borophenes and borospherenes. **L. Wang**

11:25 PHYS **587.** Microwave spectroscopic models for hydrogen storage in MOFs. **S.E. Novick**, D.A. Obenchain, G.S. Grubbs, H.M. Pickett

Molecular Mechanics

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THURSDAY AFTERNOON

Section F

Walter E. Washington Convention Center
Rooms 158A/B

Membrane Proteins: Structure, Activity & Drug Development

Structure & Dynamics of Membrane Proteins

M. J. Cocco, F. Marassi, *Organizers*

K. Gawrisch, S. Prosser, *Presiding*

1:00 PHYS **588.** Engineering nanodiscs for membrane protein studies. **G. Wagner**, M. Nasr, J. Ziarek, D. Baptista, H. Arthanari, Z. Sun, F. Hagn, A. Plückthun

1:30 PHYS **589.** Molecular underpinnings of GPCR pharmacology: An NMR and computational study of the adenosine A2 receptor. **S. Prosser**

2:00 PHYS **590.** *In silico* visioning of G protein-GDP complex communications with GPCR bound to different ligands using molecular dynamic simulations in explicit membrane. S. Sader, **C. Wu**

2:20 Intermission.

2:40 PHYS **591.** Endogenous cannabinoid ligand 2-arachidonyl glycerol (2-AG) and its interaction with cannabinoid type II cannabinoid receptor, CB_2. **T. Kimura**, A. Yeliseev, E. Mihailescu, D.L. Lynch, P. Reggio, K. Gawrisch

3:10 PHYS **592.** Probing membrane catalysis and ligand-receptor interactions in the apelinergic system. K. Shin, A. Pandey, D.N. Langelaan, S.K. Huang, C.A. Kenward, M. Sarker, D.M. LeBlanc, M. Alharbi, **J.K. Rainey**

3:40 Intermission.

4:00 PHYS **593.** NMR tools for drug discovery: Targeting membrane proteins. **M. Mesleh**

4:30 PHYS **594.** Membrane dependent allostery of oncoprotein RAS structure and function at biological membranes. Z. Feng, T. Gebregiworgis, K. Lee, M. Mazhab-Jafari, M. Smith, C. Marshall, **M. Ikura**

Section G

Walter E. Washington Convention Center
Room 151B

PHYS Awards Symposium

PHYS/Journal of Physical Chemistry Lectureship Award: Symposium in honor of Professor Benjamin Levine

J. E. Shea, *Organizer*

E. G. Hohenstein, *Presiding*

1:00 PHYS **595.** Recent progress in the electron-attached, ionized, and active-space equation-of-motion coupled-cluster methodologies. **P. Piecuch**, J. Shen, A.O. Ajala

1:35 PHYS **596.** Nonadiabatic dynamics using multiconfigurational wavefunctions with embedding corrections from density functional theory. **E.G. Hohenstein**

2:10 PHYS **597.** Quantum chemistry from molecules to materials. **A.K. Wilson**

2:45 Intermission.

3:05 PHYS **598.** Painless modeling of dynamics near conical intersections. G.A. Meek, **B.G. Levine**

3:40 PHYS **599.** *Ab initio* photodynamics in X-ray domain. **P. Slavicek**

4:15 PHYS **600.** Recent progress in density functional theories. **D.G. Truhlar**

POLY

Division of Polymer Chemistry

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

SUNDAY MORNING

Section A

Marriott Marquis Washington, DC
Marquis Ballroom Salon 6

8th Symposium on Controlled Radical Polymerization

Financially supported by Army Research Office, Anton Paar, Millipore-Sigma, Boron Molecular, Tosoh Bioscience, Kaneka, PPG

H. Gao, K. Matyjaszewski, B. S. Sumerlin, *Organizers*

N. V. Tsarevsky, *Organizer, Presiding*

M. J. Buback, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **1.** New macromolecular architectures and new ATRP initiating systems. **K. Matyjaszewski**

8:30 POLY **2.** Kinetics of radical polymerizations deduced via SP-PLP-EPR. **M.J. Buback**, H. Kattner

8:55 POLY **3.** Ionic auxiliaries for stereocontrolled radical polymerization. B. Noble, K. Fung, S. Ferrie, **M.L. Coote**

9:20 POLY **4.** RAFT 20 years later: Elements of RAFT navigation. **G. Moad**

‡ *Cooperative Cosponsorship*