Section D

Walter E. Washington Convention Center
Room 150A

Photoresponsive Nanoparticles: From Fundamentals of Excitation to Applications

Devices

Y. Han, *Organizer*

B. G. DeLacy, Y. Sun, *Organizers*, *Presiding*

8:30 COLL **599.** Low-threshold optical gain and lasing with colloidal semiconductor nanoplatelets. **M. Pelton**

9:00 COLL **600.** Metal halide perovskite nanocrystals: Doping and surface-engineering for efficient optoelectronics. J. Pan, R. Begum, L. Quan, I. Dursun, B. Ooi, E. Sargent, O.F. Mohammed, **O.M. Bakr**

9:30 COLL **601.** Solution-processed nanomaterials for efficient optoelectronic devices. **F. Garcia de Arquer**, E. Sargent

10:00 Intermission.

10:20 COLL **602.** Plasmonic detection of reactions on nanostructures. **E. Borguet**

10:50 COLL **603.** Optically-thin metallic films for high-radiative-efficiency plasmonics. **B. Zhen**, Y. Yang, O. Miller, C. Hsu, J. Joannopoulos, M. Soljacic

Section E

Walter E. Washington Convention Center
Room 209B

Basic Research in Colloids, Surfactants & Nanomaterials

Interfacial Interactions

R. Nagarajan, *Organizer*

V. Sharma, *Presiding*

8:30 COLL **604.** Prediction of membrane breakthrough pressure using multicomponent surface energy models. **N. Redeker**, K. Greeson, J.R. Alston, A.J. Guenthner

8:50 COLL **605.** Supramolecular structural forces influence drainage and stratification kinetics in stratifying foam films. S. Yilixiati, R. Rafiq, Y. Zhang, **V. Sharma**

9:10 COLL **606.** Surface tensions of frothers and oil at saltwater-air interfaces: A computational study. **L. Chong**, Y. Lai, F. Shi, M. Gray, Y. Soong, Y. Duan

9:30 COLL **607.** Viscosity of liquids from the transfer function of microcantilevers. **S.J. Eppell**, P.B. Abel, A.M. Walker, F. Zypman

9:50 COLL **608.** Mesoscale structuring of binary liquids and its impact on chemical reactivity probed by photocatalysis. **T. Buchecker**, S. Krickl, A.U. Meyer, I. Grillo, P. Bauduin, B. König, A. Pfitzner, W. Kunz

10:10 COLL **609.** New insights into nanoparticle-protein interactions through measurement of binding kinetics. A.L. Lira, R.S. Ferreira, R.J. Torquato, H. Zhao, M.L. Oliva, P. Schuck, **A.A. Sousa**

10:30 COLL **610.** Quantifying nanoparticle stability and aggregation dynamics as a function of organic coating structure and density. **C. Kim**, S. Lee, J. Fortner

10:50 COLL **611.** Functional groups on carbon nanotubes are not necessary for their covalent attachment to surfaces. **M. Williams**, F. Gao, I. Ben Dhiab, A.V. Teplyakov

11:10 COLL **612.** Withdrawn.

Section F

Walter E. Washington Convention Center
Room 209A

Frontier of the Interface of Materials & Biology: Click Chemistry Approaches to Bio-Inspired Materials

V. O. Rodionov, Q. Wang, *Organizers*, *Presiding*

8:30 COLL **613.** X-ray excited optical luminescence of surface functionalized, hybrid LSO:Ce-fluorophore particles. **M.K. Burdette**, I. Bandera, E. Zhang, J.N. Anker, J. Weick, S.H. Foulger

8:50 COLL **614.** Versatile single chain polymeric nanoparticles via thiol-Michael addition. **P. Kröger**, J.M. Paulusse

9:10 COLL **615.** Bio-functionalizable polymer colloids prepared by radical-mediated thiol-ene click polymerizations. D.V. Chapman, M.N. Arguien, R.D. Beltran, O.Z. Durham, S. Krishnan, **D.A. Shipp**

9:30 COLL **616.** Fluorescent dye loaded resorcinarene cavitand nanocapsules. **B. Ramjee**, S. Allmon, K. Mahadevan

9:50 COLL **617.** Fluorescent functionalization across the quaternary structure of virus-like particles. **Z. Chen**, J.J. Gassensmith

10:10 COLL **618.** Analysis of noble polymer micelle by double hydrophilic block glycopolymer. **T. Oh**, M. Nagao, Y. Hoshino, Y. Miura

10:30 COLL **619.** Solid phase assisted split & combine approach towards branched precision glycomacromolecules. **M. Baier**, M. Giesler, L. Hartmann

Section G

Walter E. Washington Convention Center
Room 204C

Multimodal Imaging with Colloids

P. del Pino, L. Liz Marzan, W. Parak, *Organizers*

J. V. Jokerst, *Organizer, Presiding*

8:30 COLL **620.** Polymeric nanocapsules for theranostics. **B. Pelaz**

9:00 COLL **621.** Targeted delivery of zinc phthalocyanine (ZnPc) using liquid crystal nanoparticle for effective photodynamic therapy. **O.K. Nag**, J. Naciri, K. Burn, J. Delehanty

9:30 COLL **622.** Theragnostic approach for early diagnosis of Alzheimer's disease. M. Rodriguez-Perez, B. Pelaz, P. Aguiar, R. Iglesias-Rey, L. Vazquez-Vazquez, J. Pias-Peleteiro, J. Aldrey-Vazquez, F. Campos, J. Castillo, P. del Pino, **T. Sobrino**

10:00 Intermission.

10:30 COLL **623.** Cluster-nanocarrier MRI contrast agents. **S.L. Stoll**, V. Dahanayake, E. VanKeuren, O. Rodriguez, C. Albanese

11:00 COLL **624.** Colloidal tetrapyrroles as high contrast, multimodal biomedical imaging agents. **J. Lovell**

11:30 COLL **625.** Hybrid nanocomposites based on nanoMOFs and nanoparticles for theragnostic applications. **P. del Pino**

Nanoscale Sensing in Foods & Other Complex Media

Sponsored by AGFD, Cosponsored by AGRO, ANYL, COLL, ENVR and INOR

THURSDAY AFTERNOON

Nanoscale Sensing in Foods & Other Complex Media

Sponsored by AGFD, Cosponsored by ANYL, COLL, ENVR and INOR

COMP

Division of Computers in Chemistry

H. Woodcock, J. Shen and M. Feig, *Program Chairs*

BUSINESS MEETINGS:
Business Meeting, 3:00 PM: Sat

SUNDAY MORNING

Section A

Washington Marriott at Metro Center
Salon A

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

The Exascale Challenge

Cosponsored by PHYS

Y. Alexeev, G. S. Kedziora, P. Kent, A. F. Voter, *Organizers*

F. C. Hill, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 COMP **1.** Exascale applications: Opportunities and challenges. D.B. Kothe

9:10 COMP **2.** Seeking a sustainable model for scientific simulation in the exascale era. **R.J. Harrison**

9:40 COMP **3.** Molecular Sciences Software Institute. **T. Crawford**, C. Clementi, R.J. Harrison, T.L. Head-Gordon, S. Jha, A. Krylov, V.S. Pande, T.L. Windus

10:10 Intermission.

10:25 COMP **4.** NWChemEx: Opportunities and challenges in exascale computing. **T.H. Dunning**, **T.L. Windus, R.J. Harrison**

10:55 COMP **5.** Emerging systems and the super instruction architecture. **B.A. Sanders**, J. Byrd, B. Simons, A. Pathak, A. Peshne, R.J. Bartlett

11:25 COMP **6.** Solving the performance portability issue with Kokkos. **C. Trott**, S. Plimpton, A.P. Thompson

Section B

Washington Marriott at Metro Center
Salon B

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

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

X. Huang, *Presiding*

8:30 COMP **7.** Structure-based prediction of protein-protein and protein-ligand interactions on a genomic scale. J.I. Garzon, H. Hwang, F. Dey, D. Murray, D. Petrey, **B.H. Honig**

9:00 COMP **8.** Dock-and-coalesce mechanism for the association of a WASP disordered region with the Cdc42 GTPase. L. Ou, M. Matthews, X. Pang, **H. Zhou**

9:30 COMP **9.** Predicting protein-peptide interactions based on the peptide sequence and the protein structure. **X. Zou**

10:00 Intermission.

10:15 COMP **10.** Special role of the membrane in the allosteric mechanisms of transporter proteins. **H. Weinstein**

10:45 COMP **11.** Effects of homologous proteins on IAPP amyloid aggregation, fibril remodelling, and cytotoxicity. **Y. Xing**, E. Pilkington, B. Wang, F. Ding, P. Ke

11:15 COMP **12.** Structural characterization of the human KCNQ1 voltage-sensing domain by NMR. **K. Taylor**, H. Huang, C.R. Sanders

Section C

Washington Marriott at Metro Center
Salon C

Computational Studies of Water

Interface & Transport Properties

D. J. Sindhikara, *Organizer*

M. R. Jones, *Presiding*

8:30 COMP **13.** Withdrawn.

8:55 COMP **14.** Behavior of capillary wave fronts and their role in defining interfacial regions of water. **T. Zhou**, A. McCue, Y. Ghaadrghadr, I. Bakó, A.E. Clark

9:20 COMP **15.** Enhanced heterogeneous ice nucleation by special surface geometry. **Y. Bi**, B. Cao, T. Li

9:45 Intermission.

10:00 COMP **16.** Tuning proximal water diffusion via silanol patterning on quartz surfaces. **J. Monroe**, A. Schrader, S. Han, M. Shell

10:25 COMP **17.** Computational modeling tool for the assessment of lead levels in drinking water supply systems. **A.A. Abokifa**, P. Biswas

10:50 COMP **18.** Interfacial behavior of hydrotropes in aqueous solutions. A.A. Novikov, A.P. Semenov, V.N. Kuryakov, **V. Monje**, J.B. Klauda, M.A. Anisimov

11:15 COMP **19.** Coarse-grained modeling of polycrystalline ice in supercooled water. **H. Chan**, M. Cherukara, B. Narayanan, C. Benmore, S.K. Gray, S. Sankaranarayanan

Section D

Washington Marriott at Metro Center
Salon D

ACS COMP Symposium in honor of Peter Pulay

Gradients, Properties & Electron Correlation

Cosponsored by PHYS

F. Wang, *Organizer*

S. Hirata, *Organizer, Presiding*

M. Dupuis, F. Evangelista, *Presiding*

8:30 Introductory Remarks.

8:35 COMP **20.** Optimized van der Waals parameters for quantum/molecular mechanics calculations. **P. Pulay**, G. Fogarasi

9:05 COMP **21.** Implementation of analytic gradients for CCSD and EOM-CCSD using Cholesky representations of electron-repulsion integrals. **A. Krylov**

9:35 COMP **22.** Analysis of electronic structure by maximal orbital decomposition. **M. Dupuis**

10:05 Intermission.

10:20 COMP **23.** Strategies for accurate computations on excited electronic states of complex molecules. **M.S. Gordon**, J. Mato, K. Keipert

10:50 COMP **24.** Quantum chemistry methods for ground and excited states with tunable accuracy. **F.A. Evangelista**, J.B. Schriber, T. Zhang

11:20 COMP **25.** Perturbative computation of ionization energies. **P.J. Knowles**

Merck Research Award Symposium

Sponsored by WCC, Cosponsored by BIOL, COMP, MEDI, MPPG, ORGN, PMSE and PROF

What do Synthetic Chemists Want from Their Reaction Systems?

Sponsored by CINF, Cosponsored by COMP, INOR, MEDI and ORGN

Electronic Structure Methods for Complex Chemical Systems

Many-body Perturbation Theory, Random Phase Approximation & Beyond

Sponsored by PHYS, Cosponsored by COMP

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Catalytic Promiscuity & the Emergence of New Proteins

Sponsored by PHYS, Cosponsored by BIOL and COMP

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

SUNDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Salon A

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

New Architectures

Cosponsored by PHYS

F. C. Hill, G. S. Kedziora, P. Kent, A. F. Voter, *Organizers*

Y. Alexeev, *Organizer, Presiding*

1:30 COMP **26.** Electronic structure theory on novel architectures. **M.S. Gordon**, K. Keipert, S. Leang, A. Rendell

2:00 COMP **27.** Modernizing quantum molecular and materials simulations. **J. Kim**

2:30 Intermission.

2:45 COMP **28.** Quantum chemistry on quantum computers? **J.E. Rice**

3:15 COMP **29.** Efficient seminumerical implementation of Coulomb and Hartree-Fock exchange matrix on Intel Phi coprocessor for density functional theory calculations. F. Liu, **J. Kong**

3:45 COMP **30.** Horizontal vectorization of electron repulsion integrals. **B. Pritchard**, E. Chow

Section B

Washington Marriott at Metro Center
Salon B

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

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

G. Li, *Presiding*

1:30 COMP **31.** Dynamic recognition in protein-DNA complexes. **C.L. Simmerling**, A.P. Grollman, D. Zharkov

2:00 COMP **32.** Modeling metal ion binding in RNA structure. **S. Chen**

2:30 COMP **33.** Structural analysis and quantitative modeling of protein-DNA interactions. **R. Rohs**, J.M. Sagendorf, T. Chiu

3:00 Intermission.

3:15 COMP **34.** Nucleosome: The very special protein-DNA complex. **A.V. Onufriev**

3:45 COMP **35.** Elucidating molecular recognition mechanisms of miRNA loading into the Argonaute protein by Markov state models. **X. Huang**

4:15 COMP **36.** Roles of noncovalent interactions in base recognition and catalysis in uracil DNA glycosylases. **W. Cao**

Section C

Washington Marriott at Metro Center
Salon C

Computational Studies of Water

Classical & Quantum Approaches

D. J. Sindhikara, *Organizer*

D. Janezic, *Presiding*

1:30 COMP **37.** Role of van der Waals interactions in models of liquid water. **R. Remsing**

1:55 COMP **38.** Solvation energy and entropy from 3D-RISM. **T. Luchko**, C.N. Nguyen, M.K. Gilson, T.P. Kurtzman

2:20 Intermission.

2:35 COMP **39.** Incorporating solvation thermodynamic mapping into docking. T.E. Balius, M. Fischer, R. Stein, A. Cruz-Balberdy, C.N. Nguyen, B. Shoichet, M.K. Gilson, **T.P. Kurtzman**

3:00 COMP **40.** Consistent multipole model for aqueous solvation of monovalent ions. **C.C. Dharmawardhana**, T. Ichiye

3:25 COMP **41.** PSO-assisted development of new polarizable and non-polarizable coarse-grained water models. K. Bejagam, S. Singh, Y. An, C. Berry, **S. Deshmukh**

3:50 COMP **42.** DFT investigation facilitating experimental fluorescence: Effect of substituent on photophysical properties of BTEX in water. **M.S. Khan**, J. Wu, B. Liu, C. Cheng, J. Tang

Section D

Washington Marriott at Metro Center
Salon D

ACS COMP Symposium in honor of Peter Pulay

Gradients, Properties & Electron Correlation

Cosponsored by PHYS

S. Hirata, *Organizer*

F. Wang, *Organizer, Presiding*

S. Li, T. Shiozaki, *Presiding*

1:30 COMP **43.** Symmetry projected coupled cluster theory. **G.E. Scuseria**

2:00 COMP **44.** QM/QM embedding scheme for strongly correlated problems. **D. Zgid**, L. Tran, A. Kananenka, A.R. Welden

2:30 COMP **45.** Predictive photodynamics from first principles. **T. Shiozaki**

3:00 Intermission.

3:15 COMP **46.** Some recent advances in energy decomposition analysis of electronic structure calculations. **M.P. Head-Gordon**

3:45 COMP **47.** Fragment-based models for calculating accurate potential energy surfaces and spectroscopic properties of large molecules and nanoscale systems. **K. Raghavachari**

4:15 COMP **48.** Recent developments and applications of generalized energy-based fragmentation approach for large molecules and condensed phase systems. **S. Li**

What do Synthetic Chemists Want from Their Reaction Systems?

Sponsored by CINF, Cosponsored by COMP, INOR, MEDI and ORGN

Electronic Structure Methods for Complex Chemical Systems

Extended Systems

Sponsored by PHYS, Cosponsored by COMP

Experimental & Computational Advances in Understanding Enzyme Specificity & Promiscuity

Computational Tools for Enzyme Evolution & Functional Annotation

Sponsored by PHYS, Cosponsored by BIOL and COMP

MONDAY MORNING

Section A

Washington Marriott at Metro Center
Salon A

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Large-Scale

Cosponsored by PHYS

Y. Alexeev, F. C. Hill, G. S. Kedziora, P. Kent, A. F. Voter, *Organizers*

W. D. Mattson, *Presiding*

8:30 COMP **49.** Large-scale MP2, RPA and GW calculations on pre-exascale HPC systems. **M. Del Ben**, J. Wilhelm, F.H. da Jornada, A. Canning, J. VandeVondele, J. Deslippe, J. Hutter

9:00 COMP **50.** Enabling hybrid density functional theory based *ab initio* molecular dynamics for large-scale condensed-phase systems. **R.A. Distasio**

9:30 COMP **51.** Linear scaling density functional theory in Daubechies wavelets basis: Towards paradigm shifts in large-scale electronic structure calculations. **L. Genovese**, S. Mohr, L.E. Ratcliff

10:00 Intermission.

10:15 COMP **52.** First-principles molecular dynamics: Computing more than a million atoms with over a million cores. **J. Fattebert**, D. Osei-Kuffuor, T. Ogitsu, E.W. Draeger

10:45 COMP **53.** Extreme-scale quantum and reactive molecular dynamics simulations. **A. Nakano**

11:15 COMP **54.** Large scale GW calculations at full scale on pre-exascale HPC systems. **J. Deslippe**

Section B

Washington Marriott at Metro Center
Salon B

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

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

H. Gohlke, *Presiding*

8:30 COMP **55.** Residue-specific protein force fields RSFF1 and RSFF2. **Y. Wu**

9:00 COMP **56.** IDP-specific force field ff14IDPSFF improves the conformer sampling of intrinsically disordered proteins. **H. Chen**, D. Song, R. Luo

9:30 COMP **57.** Correlating protein-ligand activity to quantum-mechanics/molecular-mechanics binding energies. **A. Crespo**

10:00 Intermission.

10:15 COMP **58.** Quantitative analysis of hot spots in protein-protein interaction. **J.Z. Zhang**

‡ *Cooperative Cosponsorship*

10:45 COMP **59.** Algorithms for discovering mutations that alter binding specificity. **B. Chen**

11:15 COMP **60.** Predicting binding free energy change caused by missense mutations in protein-DNA interactions using modified MM/PBSA method. **Y. Peng**, E. Alexov

Section C

Washington Marriott at Metro Center
Salon C

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Cosponsored by MEDI and PHYS

J. A. Morrone, *Organizer*

W. D. Cornell, *Organizer, Presiding*

8:30 COMP **61.** Drug-target residence time model: A 10-year retrospective. **R. Copeland**

9:05 COMP **62.** Modulating drug-target residence time, assessing target vulnerability, and predicting *in vivo* drug activity. **P.J. Tonge**

9:40 COMP **63.** *In silico* prediction of relative drug-protein residence times. **D.B. Kokh**, M. Amaral, J. Bomke, M. Dreyer, M. Frech, M. Lowinski, F. Vallee, M. Bianciotto, A. Rak, R.C. Wade

10:15 Intermission.

10:30 COMP **64.** Drug-target binding through molecular dynamics and enhanced sampling simulations. **A. Cavalli**

11:05 COMP **65.** Estimating ligand residence times from simulations and from structure. **A.T. Frank**, I. Deb

11:40 COMP **66.** Towards predictive drug unbinding simulations with full atomistic resolution. **P. Tiwary**

Section D

Washington Marriott at Metro Center
Salon D

ACS COMP Symposium in honor of Peter Pulay

Gradients, Properties & Electron Correlation

Cosponsored by PHYS

S. Hirata, *Organizer*

F. Wang, *Organizer, Presiding*

A. Szabados, E. F. Valeev, *Presiding*

8:30 COMP **67.** Model systems for examining the role of nodal surfaces in diffusion Monte Carlo calculations. **K.D. Jordan**, K. Gasperich

9:05 COMP **68.** Quantitative molecular orbital theory. **R.J. Bartlett**, D.S. Ranasinghe, Y. Park, P. Verma, Y. Jin, A. Perera

9:40 COMP **69.** Exploiting the pair function nature of UHF. **A. Szabados**, D. Földvári, Z. Tóth

10:15 Intermission.

10:30 COMP **70.** Reduced scaling and controlled precision: Extending the reach of many-body electronic structure. **E.F. Valeev**, C. Peng, F. Pavosevic

11:05 COMP **71.** Local correlation in molecules and condensed matter: Methods and applications. **E.A. Carter**

Electronic Structure Methods for Complex Chemical Systems

Noncolvalent Interactions, Nanosystems & Solvation

Sponsored by PHYS, Cosponsored by COMP

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Computational Approaches to Enzyme Design

Sponsored by PHYS, Cosponsored by BIOL and COMP

MONDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Salon A

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Electronic Structure

Cosponsored by PHYS

Y. Alexeev, F. C. Hill, G. S. Kedziora, P. Kent, A. F. Voter, *Organizers*

R. Pachter, *Presiding*

1:30 COMP **72.** Graph-based linear scaling electronic structure theory for Born-Oppenheimer molecular dynamics. **A.M. Niklasson**

2:00 COMP **73.** Accelerating large scale Kohn-Sham density functional theory calculations with semi-local functionals and hybrid functionals. **L. Lin**

2:30 COMP **74.** Some recent algorithmic developments in the large scale first principles simulations of complex materials. **A.S. Banerjee**, L. Lin, C. Yang, P. Suryanarayana, W. Hu, J. Pask

3:00 Intermission.

3:15 COMP **75.** Quantum Monte Carlo in the exascale era: From algorithms to applications. **A. Benali**, Y. Luo, L. Shulenburger, A. Mathuryia, J. Kim, P. Kent

3:45 COMP **76.** Extending the accuracy and scale of first-principles molecular dynamics simulations. **F. Gygi**

4:15 COMP **77.** Enabling quantum modelling simulations for biological systems. A. Pozdneev, V. Weber, **T. Laino**, F. Zipoli

Section B

Washington Marriott at Metro Center
Salon B

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

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

C. Chang, *Presiding*

1:30 COMP **78.** New alchemical approaches for the calculation of protein – ligand binding free energies. **C.L. Brooks**

2:00 COMP **79.** Diffusional dynamics of proteins under crowded conditions. **M. Feig**, G. Nawrocki, I. Yu, P. Wang, Y. Sugita, T. Kigawa

2:30 COMP **80.** Polarizable force field development for cellular membrane lipids and their applications. **G. Li**, X. Peng, H. Chu, Y. Zhang

3:00 Intermission.

3:15 COMP **81.** High affinity interaction of calmodulin with K-Ras4B implicating membrane extraction. H. Jang, **R. Nussinov**

3:45 COMP **82.** Efficient approximation of configurational entropy changes upon binding to biomolecules. **H. Gohlke**, I.Y. Ben-Shalom

4:15 COMP **83.** Studying protein-ligand interactions by integrating data science with mechanism-based modeling. **L. Xie**

Section C

Washington Marriott at Metro Center
Salon C

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Cosponsored by MEDI and PHYS

W. D. Cornell, *Organizer*

J. A. Morrone, *Organizer, Presiding*

1:30 COMP **84.** Measuring drug-target residence time and binding kinetics: Why and how? **R. Zhang**

2:05 COMP **85.** Combining biophysical, structural and computational studies of GPCR-drug interactions to optimise kinetic parameters. **B. Tehan**, A. Dore, J. Errey, E. Segala, A. Zhukov, R. Cooke

2:40 COMP **86.** Toward high-throughput predictive modeling of protein binding/unbinding kinetics. **L. Xie**

3:15 Intermission.

3:30 COMP **87.** Modeling ligand-protein binding kinetics using molecular simulations and a novel pathway search method. **C. Chang**, W. You, Z. Tang

4:05 COMP **88.** Understanding the influence of drug-target binding kinetics on in vivo drug effects. **E.C. de Lange**

Section D

Washington Marriott at Metro Center
Salon D

Emerging Technologies in Computational Chemistry

C. L. Simmerling, *Organizer, Presiding*

1:30 COMP **89.** Gibbs sampler based λ-dynamics utilizing a Rao-Blackwell estimator for alchemical free energy calculation. X. Ding, J. Vilseck, R. Hayes, C.L. Brooks

1:50 COMP **90.** Pose prediction using 3D deep convolutional neural networks. **I. Wallach**, M. Dzamba, S. Schrödl, L. Rampasek

2:10 COMP **91.** Are we evaluating performance or just overfitting? How to assess the performance of ligand-based algorithms on virtual screening benchmarks. **A. Heifets**, I. Wallach

2:30 COMP **92.** Statistical learning of kinetic Monte Carlo models of high temperature chemistry from molecular dynamics. **Q. Yang**, C.A. Sing-Long, E. Chen, E. Reed

2:50 COMP **93.** Neural networks learning quantum chemistry: The rise of the machines. J. Smith, **O. Isayev**, A.E. Roitberg

Transformative Research & Excellence in Education Award

Sponsored by COMSCI, Cosponsored by BIOL, COLL, COMP, ENFL, INOR, PHYS and PRES

Electronic Structure Methods for Complex Chemical Systems

Emerging Directions in Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

Undergraduate Research Posters

Computational Chemistry

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Experimental & Computational Advances in Understanding Enzyme Specificity & Promiscuity

Discovery & Engineering of Industrially Relevant Enzymes

Sponsored by PHYS, Cosponsored by BIOL and COMP

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

H. L. Woodcock, *Organizer*

8:00 - 10:00

123, 158-159, 169, 172, 183, 187 197, 203, 206, 209-210, 216- 218, 222-223, 240, 242, 252-253, 266, 268, 270, 272-273, 275, 277, 280-281, 283, 286, 298-302, 304. See subsequent listings.

TUESDAY MORNING

Section A

Washington Marriott at Metro Center
Salon A

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Molecular Dynamics

Cosponsored by PHYS

Y. Alexeev, F. C. Hill, G. S. Kedziora, P. Kent, *Organizers*

A. F. Voter, *Organizer, Presiding*

8:30 COMP **94.** Leveraging the exascale to extend atomistic simulation timescales. **D. Perez**, A.F. Voter

9:00 COMP **95.** Overcoming large timescale problem of biological molecular dynamics simulations: Scalable ensemble algorithms on massively parallel computing. **W. Jiang**

9:30 COMP **96.** Describing peptide-protein and protein-protein interactions with molecular dynamics simulation. **J.A. Morrone**

10:00 Intermission.

10:15 COMP **97.** Recent algorithmic work in LAMMPS for extending accuracy and time scales for materials modeling. **S. Plimpton**, A.P. Thompson

10:45 COMP **98.** NAMD: Innovation towards exascale. **J. Phillips**, E. Tajkhorshid

11:15 COMP **99.** Atomic-level characterization of protein-protein association. **A.C. Pan**

Section B

Washington Marriott at Metro Center
Salon B

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

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

M. Feig, *Presiding*

8:30 COMP **100.** Are all enzymes molecular motors? An effect of binding and catalysis out of equilibrium. **M.K. Gilson**, D. Slochower

9:00 COMP **101.** Sampling long-timescale dynamics in biomolecular recognition. **W. Yang**

9:30 COMP **102.** Calculating protein-ligand binding affinities with MM/PBSA: Improvement and extension. **R. Qi**, C. Wang, L. Xiao, W.M. Botello-Smith, D. Greene, R. Luo

10:00 Intermission.

10:15 COMP **103.** Exploring variant nucleosomes: From experiments to modeling and back. A. Shaytan, D. Landsman, **A. Panchenko**

10:45 COMP **104.** New hallmarks of protein-small molecule binding: Interfacial rigidity and polarity. **L.A. Kuhn**, S. Raschka, A. Wolf, J. Bemister-Buffington

11:15 COMP **105.** Simulation study of integrin alpha-2 I domain activation. **Z. Jia**, E. Alexov

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

Section C

Washington Marriott at Metro Center
Salon C

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Cosponsored by MEDI and PHYS

J. A. Morrone, *Organizer*

W. D. Cornell, *Organizer, Presiding*

8:30 COMP **106.** Shifting the paradigm from *in vitro* potency to non-equilibrium time-dependent drug-target occupancy under *in vivo*-relevant conditions. **R.A. Pearlstein**, D. Mckay, G. Selvaggio, A. Golosov

9:05 COMP **107.** *In vitro* and *in vivo* target life for Immucillin transition-state analogs. **V.L. Schramm**, S. Gebre, S. Cameron

9:40 COMP **108.** What are the molecular interactions that govern ligand residence time? Insights from molecular dynamics. **A. Dickson**, S. Lotz

10:15 Intermission.

10:30 COMP **109.** Towards atomistic simulations of receptor-ligand unbinding kinetics. **L.T. Chong**

11:05 COMP **110.** How does benzene recognize the buried cavity in T4 Lysozyme L99A? **J. Mondal,** N. Ahalawat, P. Vallurupalli

11:40 COMP **111.** Rational modulation of the induced-fit conformational change for slow-onset inhibition in Mycobacterium tuberculosis InhA. **C.L. Simmerling**, P.J. Tonge, C. Lai

Section D

Washington Marriott at Metro Center
Salon D

New Directions in Conformational Sampling Methods

M. Feig, J. Shen, *Organizers*

R. C. Harris, *Presiding*

8:30 COMP **112.** New repulsive soft-core potential for accelerated alchemical free energy calculations. **K. Nam**

9:00 COMP **113.** Multisite λ dynamics enables accurate and efficient calculation of mutational changes in the folding free energy of T4 lysozyme. **R.L. Hayes**, J. Vilseck, T. Wymore, C.L. Brooks

9:30 COMP **114.** ForceGen 3D structure and conformer generation: From small lead-like molecules to macrocyclic drugs. **A.N. Jain**, A.E. Cleves

10:00 COMP **115.** How does PubChem generate computational 3-D structures of its compounds? **S. Kim, E. Bolton**

10:30 Intermission.

10:50 COMP **116.** Chain-of-states method based dynamical sampling. H. Zhou, **P. Tao**

11:20 COMP **117.** WExplore: An enhanced sampling method to study ligand release processes on timescales ranging from milliseconds to minutes. **A. Dickson**

11:50 COMP **118.** Coarse-grained directed simulations via adaptive linear biases. **G.M. Hocky**, T. Dannenhoffer-Lafage, G.A. Voth

Electronic Structure Methods for Complex Chemical Systems

Correlated Electronic Structure Methods for Complex Systems

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Salon A

Extending Accuracy & Scales with Emerging Computing Architectures & Algorithms

Data & Automation

Cosponsored by PHYS

Y. Alexeev, F. C. Hill, G. S. Kedziora, P. Kent, A. F. Voter, *Organizers*

R. Walker, *Presiding*

1:30 COMP **119.** Scalable *in situ* analysis for large-scale molecular dynamics simulations on supercomputers. **P. Malakar**, V. Vishwanath, C. Knight, T. Munson, M. Papka

2:00 COMP **120.** Use of dataflow-based execution to improve scalability and performance of coupled cluster codes. **T.L. Windus**, K. Kowalski, A. Danalis, H. Jagode

2:30 COMP **121.** Exploring reaction mechanisms with heuristics-aided quantum chemistry (HAQC). **D. Rappoport**

3:00 Intermission.

3:15 COMP **122.** Machine learnt models for accurate yet efficient materials design. **S. Sankaranarayanan**

3:45 COMP **123.** Enhancing QM/MM indirect free energy simulations with intramolecular force matching. P.S. Hudson, S. Boresch, D.M. Rogers, **H.L. Woodcock**

Section B

Washington Marriott at Metro Center
Salon B

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

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

A. V. Onufriev, *Presiding*

1:30 COMP **124.** Topological deep learning of biomolecular structure-function relationships. **G. Wei**

2:00 COMP **125.** Understanding the mechanisms of protein-ligand interactions through molecular dynamics simulations and free energy analysis. **J. Wang**

2:30 COMP **126.** Calculations of chemical ligand-receptor binding kinetics and thermodynamics using molecular mechanics. **C. Chang**, Z. Tang

3:00 Intermission.

3:15 COMP **127.** Importance of protonation states and pH in structure-based drug design: The case of BACE1. **J. Shen**, C.R. Ellis, C. Tsai, R.C. Harris

3:45 COMP **128.** Fast, accurate pH dependent alchemical free energy calculations towards rational drug design. **R.C. Walker**, C. Lin, D. Mermelstein

4:15 COMP **129.** Martinizing the variational implicit solvent method (VISM): Solvation free energy for coarse-grained proteins. **C. Gravina Ricci**, B. Li, L. Cheng, J. Dzubiella, J.A. McCammon

Section C

Washington Marriott at Metro Center
Salon C

Quantum Mechanics

A. E. DePrince, *Organizer*

P. S. Hudson, *Presiding*

1:30 COMP **130.** Polarizabilities of π-conjugated chains revisited: Improved results from broken-symmetry, range-separated DFT. **B.M. Wong**, M.B. Oviedo, N.V. Ilawe

2:00 COMP **131.** Computational investigation of cell nitroxyl (HNO) fluorescent probe. H. Xu, A. Lippert, Y. Shao, **P. Tao**

2:20 COMP **132.** Ionization potential improved local density functional – QTP17-L. **Y. Jin**, R.J. Bartlett

2:40 COMP **133.** Note on accuracy of DFT density. **D.S. Ranasinghe**, A. Perera, R.J. Bartlett

3:00 COMP **134.** Mechanisms of excitation energy transfer in pigment-protein complexes. **D. Kosenkov**, Y. Kholod

3:20 Intermission.

3:35 COMP **135.** Electronic structure from Monte Carlo Green's function. **B. Winograd**

3:55 COMP **136.** Reduced scaling Green's function methods for local and non-local correlation. **A. Shee**, L. Tran, D. Zgid

4:15 COMP **137.** Calculating electronic g-tensors with density matrix renormalization group wavefunctions. **E. Sayfutyarova**, G. Chan

4:45 COMP **138.** Effect of electrode surface structure on electron transport in molecular junctions. **A. Becker**, S. Roy

Section D

Washington Marriott at Metro Center
Salon D

Material Science

Nanoparticles & 2D Materials

C. M. Aikens, *Organizer*

F. J. Irudayanathan, *Presiding*

1:30 COMP **139.** Electronic structure of silver nanocluster chromophores functionalized by DNA sequences. **Y. Small**, D. Nykypanchuk

1:55 COMP **140.** Atomistic scale investigation of plasmon decay in noble metal wires: The (eventually) catastrophic role of molecular vibration. **G. Donati**, D.B. Lingerfelt, C.M. Aikens, X. Li

2:20 COMP **141.** Quantum dot precursor design strategies from new first-principles discovery techniques. **J. Kim**, A.H. Steeves, H.J. Kulik

2:45 COMP **142.** Developing a nanoscale understanding of the growth mechanism of III-V quantum dots. **Q. Zhao**, H. Kulik

3:10 COMP **143.** Insights into nanoparticles-based NMR chemosensing via molecular dynamics simulations. **L. Riccardi**, L. Gabrielli, X. Sun, F. De Biasi, F. Rastrelli, F. Mancin, M. Devivo

3:35 Intermission.

3:50 COMP **144.** Surface reorganization and x-ray spectra of nitrogen-vacancy containing nanodiamonds. **A. Petrone**, D. Williams-Young, R. Beck, X. Li

‡ *Cooperative Cosponsorship*

4:15 COMP **145.** Inconsistencies in the electronic properties of phosphorene nanotubes: New insights from large-scale DFT calculations. **S. Allec**, B.M. Wong

4:40 COMP **146.** Structural, electronic and optical properties of 2H-TaSe2 in the charge density wave (CDW) phase. **S. Chowdhury**, J. Simpson, T.L. Einstein, F. Tavazza, A.R. Hight Walker

5:05 COMP **147.** Size and substrate induced phase stability of MoS2 nanoparticles under varying conditions. **A. Bruix**, J. Lauritsen, B. Hammer

Section E

Washington Marriott at Metro Center
Salon E

Computational Studies of Membranes & Membrane-Bound Systems

Membrane Bilayers

Cosponsored by PHYS

M. Feig, J. Shen, *Organizers*

J. Huang, *Presiding*

1:30 COMP **148.** CHARMM-GUI membrane builder with glycolipids and lipopolysaccharides. **W. Im**

2:00 COMP **149.** Asymmetric models for the trans-Golgi Network and plasma membranes of *S. cerevisiae*, insights from molecular dynamics. **V. Monje**, J.B. Klauda

2:30 COMP **150.** Transport and mechanical properties of membranes. **R. Pastor**

3:00 Intermission.

3:20 COMP **151.** All-atom simulation studies on lipid bilayers, composed of sphingomyelin, glycerophospholipids and cholesterol. **I. Bera**, J.B. Klauda

3:50 COMP **152.** Equilibration of the chemical potential between the lipid leaflets during molecular dynamics simulation. **F. Samarjeet**, T. Woolf, B. Brooks

4:20 COMP **153.** Intrinsic curvature and lipid sorting modulate dynamics of hemifusion diaphragm dissipation. **J. Gardner**, C.F. Abrams

Electronic Structure Methods for Complex Chemical Systems

Ultra-efficient Electronic Structure Methods & Molecular Dynamics

Sponsored by PHYS, Cosponsored by COMP

Experimental & Computational Advances in Understanding Enzyme Specificity & Promiscuity

Structure-Function Relationships in Enzyme Evolution

Sponsored by PHYS, Cosponsored by BIOL and COMP

TUESDAY EVENING

Section A

Walter E. Washington Convention Center
Hall C

Chemical Computing Group Graduate Student Travel Awards

K. N. Kirschner, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP **154.** First principles Monte Carlo simulations of reactive phase and sorption equilibria. **E. Fetisov**, M. Shah, C. Knight, J.I. Siepmann

COMP **155.** Role of graphene oxidation on physisorption of biomolecules using computational modeling. **H. Kim**, B.L. Farmer, A.M. Grant, V.V. Tsukruk, Y.G. Yingling

COMP **156.** Broadband absorption spectra from time-dependent coupled-cluster theory. **D. Nascimento**, A.E. DePrince

COMP **157.** Novel model reduction algorithm for the efficient evaluation of molecular response properties. **D.B. Williams-Young**, R. Van Beeuman, C. Yang, X. Li

COMP **158.** Environment-perturbed transition state sampling and its applications in chemical and biochemical reactions in condensed media. **Z. Yang**, C. Doubleday, K.N. Houk

Section B

Walter E. Washington Convention Center
Hall C

Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

COMP **159.** New computational methods for excited state time-resolved infrared and Raman scattering spectroscopies. **A. Petrone**, D. Williams-Young, D.B. Lingerfelt, X. Li

COMP **160.** Computational investigations of an unusual unimolecular decomposition pathway for CHF2CF3 forming :CF2 + HCF3 and analogous molecules of the form CF3CXFY that react to give XCF3 + :CFY. **B.E. Holmes**, B.R. Gillespie, C.A. Smith, G.L. Heard

COMP **161.** Computational studies on fluorescence and excited states of benzofuran derivatives. **A. Dinescu**, J. Jung

COMP **162.** Systematic investigation of 15N chemical shift prediction using density functional theory calculations. **D. Xin**, C.A. Sader, K. Wagner, U. Fischer, P. Jones, K. Fandrick, N.C. Gonnella

COMP **163.** Catalysis by montmorillonite on the synthesis of biological RNA polymer surrogates. **E. Gordon**, L. Tribe

COMP **164.** Environmental degradation of 2,4-dinitroanisole (DNAN): A computational investigation of excited state properties and structures. **H. McAlexander**, M.K. Shukla

COMP **165.** Theoretical study on pyrolysis of Jet Propellant-8 components: The behavior of aliphatic and non-aliphatic alkyl rings. **D. Belisario-Lara**, A.M. Mebel, J.L. Ribeiro

COMP **166.** From B atoms to small Bx clusters and beyond. **B.T. Catalano**, G.M. Curtin, E.K. Snyder, J.R. Rocha

COMP **167.** Grand canonical Monte Carlo simulation studies: Working mechanism of polyelectrolyte diode and transistor. **D. Lee**, R. Chang

COMP **168.** Withdrawn.

COMP **169.** Discovering polyimides with exceptional optical properties using first-principles modeling, virtual high-throughput screening, and machine learning. **M.F. Afzal**, **C. Cheng, J. Hachmann**

COMP **170.** Virtual high-throughput infrastructure for the accelerated discovery of organic materials. **M.F. Afzal**, J. Hachmann

COMP **171.** Computational bioluminescence. **Y. Liu**

COMP **172.** Diffusion processes of small hydrocarbons in MOF-74-Mg addressed via CI-NEB periodic calculations. **G.D. Degaga**, L. Valenzano

COMP **173.** Withdrawn.

COMP **174.** Molecular dynamics study of ligand-dendrimer interaction: A theoretical approach. **J. Stopinski**, B. Menot, S. Bouquillon, F. Allais, E. Hénon

COMP **175.** Improving workflows via a computational chemistry app store. **R. Richard**, B. Pritchard, C.D. Sherrill

COMP **176.** Consensus diversity plots: A free online web-server to analyze the global diversity of molecular data sets. M. González-Medina, F.D. Prieto-Martínez, J.R. Owen, **J.L. Medina-Franco**

COMP **177.** Zero-norm sparse coding in MSWI bottom ash. **L. Lang**

COMP **178.** Computer in microbiology. **T.D. Komolafe**

COMP **179.** Benefit of computerised in poultry (animal production). **T.O. Akinmusire**

COMP **180.** Automated geometric-based method for analysis of spectral data. **N. Sveshnikov**, V. Kirnosov

COMP **181.** Comparative DFT study on the metallocyclic ring size, stability, and global reactivity indexes of three phenanthrenedithiolato-diironhexacarbonyl complexes. **J.K. Agbo**, C.A. Mebi

COMP **182.** Withdrawn.

COMP **183.** Molecular rectification enhancement based on conformational and chemical modifications: Smart design of molecular devices. **J. Valdiviezo**, J.L. Palma

COMP **184.** Structure and phase change properties of confined metals. **K.E. Anderson**, N. Tran, F. Carlson, J. Davidson, J.I. Siepmann, A. Stein

COMP **185.** Density functional theory calculations of adsorption of phosphate to phosphate and phosphonate-rich surfaces for recovery from aqueous environments. C. Jakob, D.R. Talham, **L. Tribe**

COMP **186.** Read-across approach for predicting the toxicity of fragrance materials. **M.S. Date**

COMP **187.** Evidence for singlet fission driven by vibronic coherence in crystalline tetracene. **A. Morrison**, J. Herbert

COMP **188.** Theoretical studies of water splitting catalysts. **D. Perera**, J.C. Rasaiah

COMP **189.** Investigation on ionomer distribution of polymer electrolyte membrane fuel cells. J. Lee, S. Kwon, S. Choi, G. Doo, H. Kim, **S. Lee**

COMP **190.** GPU enabled molecular dynamics simulations of lipid nanodisc templated gold nanoparticle self-assembly. **H. Sharma**, E. Dormidontova

COMP **191.** Density functional theoretical study on the C-F oxidative addition reaction at an Al center. **S. Hwang**

COMP **192.** BS-GEP algorithm for prediction of variation of heavy metal morphology. **S. Sun**

COMP **193.** Deconstructing the confinement effect upon the organization and dynamics of water in hydrophobic nanoporous materials: Lessons learned from zeolites. **T. Zhou**, P. Bai, J.I. Siepmann, A.E. Clark

COMP **194.** Modeling of reactive oxygen species using ab initio methods. **U.A. Anene**, N. Matsunaga

COMP **195.** Hydration of end grafted PEO chains on gold surfaces of varying curvature: An extensive all-atom molecular dynamics simulation using GPU enabled GROMACS-4.6.5. **U.R. Dahal**, E. Dormidontova

COMP **196.** London dispersion contribute to the aggregations of organoplatinum(II) complexes: A theoretical study. **M. Xie**, W. Lu

COMP **197.** Hybrid peptide materials: Linking molecular architecture to nanostructure characteristics. **S. Mushnoori**, M. Dutt

COMP **198.** Effect of a DC electric field on the melting temperature, nucleation and ice growth rate of TIP4P water models. **J. Ramirez**, J.R. Espinosa, A. Zaragoza, R. Ramos, E. Sanz, C. Valeriani, C. Vega, J. Cobos

COMP **199.** Direct simulation of non-adiabatic dynamics in large-scale enzymatic systems. **J. Kretchmer**, T.F. Miller

COMP **200.** Withdrawn.

COMP **201.** New extremely efficient conformation search method based on energy evaluation for macrocyclic compounds including peptides size of greater than 10 residues. **A. Tomonaga**, A. Ueda, A. Matsuura

COMP **202.** CHARMM Drude polarizable force field for glycosidic linkages involving furanoses. **A. Aytenfisu**, A.D. Mackerell

COMP **203.** Elucidating product specificity in protein arginine methyltransferase 7 (PRMT7) using QM/MM/MD. **A. Thakur**, B. Caceres, J. Hevel, O. Acevedo

COMP **204.** Diffusive tracer dynamics in crowded environments. **B.D. Mahala**, R. Hernandez

COMP **205.** OPLS-AA force field parameters for ionic liquid molecular dynamic simulations. **B. Doherty**, X. Zhong, O. Acevedo

COMP **206.** New approach for detection and visualization of aggregation-prone regions. **C. Williams**

COMP **207.** Computer assisted study of the binding between translesion DNA polymerase zeta from *Dictyostelium discoideum* and DNA decamer containing a thymine-dimer. **D. He**, S.K. Mauldin

COMP **208.** Computational methods for elucidating mechanisms of substrate transport in membrane transporters. **D. Shukla**

COMP **209.** Dynamics of solute transport through the blood-brain barrier tight junction pores. **F.J. Irudayanathan**, S. Nangia

COMP **210.** Parametrization of the drude polarizable force field for halogenated compounds. **F. Lin**, A.D. Mackerell

COMP **211.** Conformational effects of threonine phosphorylation in proline-rich disordered motifs. **G.A. Lucero**, P.S. Nerenberg

COMP **212.** Effect of the number of points *n* on the accuracies of *n*-point water models. **Y. Xiong**, A.V. Onufriev

COMP **213.** Coarse-grained model for multiscale enhanced sampling of intrinsically disordered protein conformations. **X. Liu**, J. Chen

COMP **214.** OPLS-AA force field parameters for dicationic imidazolium-based ionic liquid simulations. **X. Zhong**, B. Doherty, O. Acevedo

COMP **215.** Metadynamics simulation studies of the interaction between TEX14 and CEP55. **Y. Cho**, R. Chang

COMP **216.** Explore the structural and dynamics differences between glucose transpoter-1 (GLUT1) and GLUT3. **S. Zhang**, C. Libby, C.E. Augelli-Szafran, A.B. Hjelmeland, W. Zhang

COMP **217.** Unravelling hemicellulose bio-synthesis using molecular simulations. **V.S. Bharadwaj**, M.F. Crowley

COMP **218.** Phospholipase A2: A unique paradigm of allosteric regulation by membranes. **V.D. Mouchlis**, J. McCammon, E.A. Dennis

COMP **219.** Phospholipase A2: An ideal system for studying protein-lipid binding and interactions. **V.D. Mouchlis**, J. McCammon, E.A. Dennis

COMP **220.** Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. **S. Ramsey**, C.N. Nguyen, R.C. Salomon, R. Walker, M.K. Gilson, T.P. Kurtzman

COMP **221.** ΔLogP o/w of between organic compound and corresponding perfluoro compound: A Monte Carlo simulation study. **H. Kim**

COMP **222.** Implicit solvent/explicit ions GB model for nucleic acid simulations. **I.S. Tolokh**, A.V. Onufriev

COMP **223.** Constant pH molecular dynamics reveals conformational selection in aspartyl proteases leading to inhibitor selectivity. **J.A. Henderson**, R.C. Harris, C.R. Ellis, J. Shen

COMP **224.** Development of a refined force field for *β*-hematin and molecular dynamics study. **J. Becker**, F. Wang, P. Sonnet, F. Dupradeau

COMP **225.** B-cell epitope discovery using molecular dynamics. **J.S. Grosch**, P. Ortoleva

COMP **226.** Molecular dynamics simulations of L-RNA involving complexes. M. Dudek, **J. Trylska**

COMP **227.** Empirical polarizable force field for RNA based on the classical Drude oscillator model. **J.A. Lemkul**, A.D. Mackerell

COMP **228.** Free energy calculation of the solubility of cellulose oligomers in water. **K. Ueda**, Y. Matsubara

COMP **229.** Making a splash in implicit solvent: Application of inhomogeneous solvation theory and continuum solvation to protein-ligand affinity predictions. **L.B. Wickstrom**, R. Pal, S. Ramsey, T.P. Kurtzman, E. Gallicchio

COMP **230.** Parametrization of dissipative particle dynamics: From bottom-up coarse graining to implicit-solvent modelling. **L. Gao**, M. Wan, C. Wen

COMP **231.** Phosphorylation of deubiquitinase affects its binding with ubiquitin. **L. Zhong**

COMP **232.** Withdrawn.

COMP **233.** RPIMapPr: A novel approach to predicting interfacing protein residues in RNA-protein complexes. **M.P. Beck**, H. Vashisth

COMP **234.** Modeling the atomistic structure and dynamics of the chloroplast signal recognition particles. **M. Benton**, M. Moradi

COMP **235.** Molecular dynamics simulation study of DNA mismatch recognition by thymine DNA glycosylase. **O. Yoluk**, A. Drohat, A.D. Mackerell

COMP **236.** Characterizing protein hydration to inform its interactions and assemblies. **A. Patel**

COMP **237.** NAMD/Q-Chem interface for *ab initio* QM/MM calculations under periodic boundary conditions. **X. Pan**, Y. Shao

COMP **238.** Correlating individual amino acid residues with protein allostery through rigid residue scan. **P. Tao**, H. Zhou, R. Kalescky, B. Zoltowski

COMP **239.** Protein evolution analysis integrating different levels of structures and simulations. Z. Dong, H. Zhou, **P. Tao**

COMP **240.** Structural, dynamic, and electrostatic influences on catalysis in wild type human phosphoglucose isomerase and the Q388A variant. **S.C. Begay**, P. Beuning, M.J. Ondrechen

COMP **241.** Custom solubility and partition ratio models for more quantitative agreement to experiment. **S.G. Arturo**

COMP **242.** Structural properties of disordered proteins: A molecular dynamics simulation study using OPC and TIP3P. **P. Seifpanahi, S. Izadi, A.V. Onufriev**

COMP **243.** Shedding light on the conformational changes leading to intrinsic activation of four night blindness mutations G90D, T94I, A292E, A295V on the human GPCR rhodopsin: A molecular dynamics simulation study. J. Mohen, **C. Wu**

COMP **244.** Computer modeling of cellulose-based polymers for applications on pharmaceutics. **C.H. Borca**, L.I. Mosquera-Giraldo, X. Meng, K.J. Edgar, L.V. Slipchenko, L. Taylor

COMP **245.** All-atomistic simulations of the interaction of the model hydrophobic drug camptothecin with phospholipid membranes. **P.K. Tang**, M. Kang, S. Loverde

COMP **246.** Hsp70's domains alternating flexibilities enable its chaperone action. **D.R. Merz**, R.I. Dima

COMP **247.** Conformational landscape of actin monomers and its implications for filament assembly. **G.M. Hocky**, B.J. Nolen, G.A. Voth

COMP **248.** Rationalization and visualization of non-bonded interactions using extended Hückel theory. **N. Li**

COMP **249.** Withdrawn.

COMP **250.** Docking-based virtual screening: Probing its applicability to GPCR models. **A. Cohen**, A. Danfora, M. Biederman, S. Costanzi

COMP **251.** Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **A. Deschenes**

COMP **252.** Unified framework for computer-aided biologics design. **A. Deschenes**

COMP **253.** RealityConvert: A tool for preparing 3D models of biochemical structures for AR and VR. **A. Borrel**, D. Fourches

COMP **254.** Enhancement of grid inhomogeneous solvation theory (GIST) by using polarizable force field: A cucurbit[7]uril study. **A. Cruz-Balberdy**, T.P. Kurtzman

COMP **255.** Understanding the interaction between graphene oxide and NDPK: A novel low cost approach to treating heart failure. **A. Ray**, I.G. Macwan, S. Singh, P.K. Patra, S. Silwal

COMP **256.** Analysis of allosteric and cryptic sites. **A. Wakefield**, S. Vajda

COMP **257.** *In silico* investigation into the structures of lysyl oxidase-like proteins. **L. Booysen**, C. Messier, F. Ryvkin

COMP **258.** Targeting the *Plasmodium falciparum* folate pathway: Molecular modelling of the affinity sulfonamide derivatives and isoforms of dihydrofolate reductase. **C.D. Mukinay**, N.Y. Forlemu

COMP **259.** Modeling ligand-protein binding: Explanation of the dynamic processes in the binding between CDK8/CycC and the inhibitors. **W. Chen**, Z. Tang, T. Cholko, C. Chang

COMP **260.** Small molecule inhibitor identification targeting fatty acid binding protein 5. **Y. Zhou**, M. Elmes, J. Sweeney, H. Li, I. Ojima, D.G. Deutsch, R.C. Rizzo

COMP **261.** Identification of Ebola virus inhibitors targeting viral-hots membrane fusion by glycoprotein GP2. **C.D. Singleton**, H. Yi, M.S. Humbly, R.C. Rizzo, A. Jacobs

COMP **262.** Exploring target flexibility for drug design. **D.B. Kokh**, A. Stank, M. Horn, E. Sizikova, R. Neil, J. Panecka, S. Richter, R.C. Wade

COMP **263.** Computational physics-based broadly neutralizing vaccine design-From epitope identification and assessment to predicted nanoparticle immunogenicity: Zika virus. **D. Biner**, J.S. Grosch, A. Ermel, D. Brown, P. Ortoleva

COMP **264.** Predicting protein drug binding sites using site identification by ligand competitive saturation method and Drude polarizable force field. **D. Sun**, A.D. Mackerell

COMP **265.** Withdrawn.

COMP **266.** Modeling 10,000 antibodies in about an hour: Leveraging the power of the Amazon cloud. **E. Metwally**

COMP **267.** Incorporating the effect of water molecules into docking programs. **E. Chen**, S. Ramsey, T.P. Kurtzman

COMP **268.** Computational approach to energetically identify bridging water molecules and to incorporate them in virtual screens. **J. Guo**, R.C. Rizzo

COMP **269.** Withdrawn.

COMP **270.** Addressing challenges in drug design through novel computer simulations. **C. Tsai**, C.R. Ellis, R.C. Harris, J. Shen

COMP **271.** Allosteric modulation model of the mu opioid receptor by herkinorin via docking, molecular dynamics simulations and alchemical free energy calculations. **K. Martinez Mayorga**, A.F. Marmolejo-Valencia

COMP **272.** Water-based pharmacophore screening of DUD system. **K. Huang**, T. Kurtzman

COMP **273.** Tumor and organ uptake of Cu-64 labeled amatuximab, an anti-mesothelin antibody, in a nude mouse model bearing a shed antigen tumor by mathematical model simulation. **J. Lee**

COMP **274.** Computational *de novo* drug design applications: HIV gp41 and FABP. **L. Prentis**, R.C. Rizzo

COMP **275.** Rational design and evaluation of multi-target ligands at A1R, A2AR and PDE10A with therapeutic potential for neurodegenerative diseases. **L. Kalash**, I. Winfield, S. Carvalho, G. Ladds, A. Bender

COMP **276.** Computationally designed fluorinated phosphotriesterases for detoxification of chlorpyrifos. **L. Yin**, L.A. Halvorsen, A.J. Olsen, R.A. Bonneau, J.K. Montclare

COMP **277.** Molecular dynamics investigation in structure-based design of fatty acid synthase (FASN) inhibitors for cancer therapy. **M.A. Saeed**

COMP **278.** Improved structure-based virtual screening of estrogen receptor alpha with data fusion of pharmacophore and docking methods. **K. Cagasova**, J.S. Josan

COMP **279.** Discovery and identification of NPC1-derived peptides targeting the GPcl-NPC1 protein-protein interaction. **Q. Li**, L. Ma, J. Zhou, S. Cen

COMP **280.** *In silico* analysis of the interactions of CB ligands with their receptors: Towards the development of a consensus pharmacophore model for synthetic cannabinoids. **R.M. Sears**, C. McInnes

COMP **281.** Inclusion of halogens as probe molecules in the site-identification by ligand competitive saturation (SILCS) methodology. **W. Jiang**, W. Yu, S.K. Lakkaraju, S. Jo, A.D. Mackerell

COMP **282.** Homology modeling of class A GPCRs: Probing the impact of agonist-bound and blocker-bound templates. **S. Costanzi**, M. Biederman

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*

COMP **283.** Merck AcceSSible InVentory (MASSIV): In silico synthesis guided by chemical transforms obtained through bootstrapping reaction databases. **T. Knehans**, F. Klingler, H. Kraut, H. Saller, A. Herrmann, F. Rippmann, J. Eiblmaier, C. Lemmen, M. Krier

COMP **284.** Using the site-identification by ligand competitive saturation (SILCS) method to explore protein-protein interactions. **W. Yu**, S. Jo, S.K. Lakkaraju, A.D. Mackerell

COMP **285.** Withdrawn.

COMP **286.** Integrate bioinformatics, chemoinformatics and computational modeling methods to identify novel tiam1 inhibitors for prostate cancer therapy. **Z. Tan**, S. Zhang

COMP **287.** Aliphatic ferrocenylphenyl ureas: Synthesis, structural elucidation, pharmacological investigation and DFT calculations. **F. Asghar**, A. Badshah, I.S. Butler

COMP **288.** Building a library for combination screening starts with single agent profiles. **L. Chen**, K. Wilson, X. Zhang, C. McKnight, P. Shinn, C.J. Thomas, M. Ferrer, R. Guha

COMP **289.** Grid-based molecular surface generalized Born (GB) model for single-point calculations of electrostatic solvation free energies. **N. Forouzesh**, S. Izadi, A.V. Onufriev

COMP **290.** Rapid evaluation of relative change in binding affinity using single step free energy perturbation (SSFEP). **S.K. Lakkaraju**, S. Jo, A.D. Mackerell

COMP **291.** MetaTox: Web resource for prediction of the metabolic network for xenobiotics in the human organism. **A. Dmitriev**, A. Rudik, D. Filimonov, A. Lagunin, V. Poroikov

COMP **292.** Excipient-protein interactions for enhancing the stability of protein-based therapeutics using the site identification by ligand competitive saturation (SILCS) technology. **S. Jo**, **S.K. Lakkaraju, W. Yu, A.D. Mackerell**

COMP **293.** Application of structural bioinformatics in vaccine and antibody design. G. Chuang, R. Rawi, C. Shen, **P.D. Kwong**

COMP **294.** Collaboration in a competitive world: Sharing information for building models without sharing data. **P. Gedeck**, S. Skolnik, S. Rodde, R. Vianello

COMP **295.** Discovery of novel natural products as potent FXR antagonists by virtual screening. **Y. Diao**, S. Li, H. Li

COMP **296.** Discovery and rational design of natural product-derived analogs as novel and long-acting DPP-4 inhibitors for the treatment of type 2 diabetes. **S. Li**, Y. Diao, H. Li

COMP **297.** Importance of equilibration time, structure truncation, and membrane lipid type for simulations of ion channels. **N. Guros**, J.B. Klauda, A. Balijepalli

COMP **298.** Fe-S cluster-containing NAF-1: Promising target for breast cancer drugs. **F. Bai**, J. Onuchic

COMP **299.** Free tools for ligand discovery: An update. **J. Irwin**

Section C

Walter E. Washington Convention Center
Hall C

NVIDIA GPU Award

M. E. Berger, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP **300.** Efficient GPU/OpenMM implementation of the AGBNP solvation model for macromolecular binding. **E. Gallicchio**, D. Kilburg, B. Zhang

COMP **301.** Systematic analysis of plasmonic resonances using GPU-enabled real-time, time-dependent DFTB. **N.V. Ilawe**, M.B. Oviedo, B.M. Wong

COMP **302.** Deep learning on NVIDIA GPUs for QSAR, QSPR and QNAR predictions. **B. Sattarov**, A. Mitrofanov, A. Korotcov, V. Tkachenko

COMP **303.** GPU-accelerated molecular dynamics simulations of protein remodeling mediated by AAA+ biological nanomachines. **A. Javidialesaadi**, G. Stan

COMP **304.** Understanding the microscopic structure of lyotropic liquid crystal membranes using molecular dynamics simulations. **B. Coscia**, M.R. Shirts

Section D

Walter E. Washington Convention Center
Hall C

OpenEye Outstanding Junior Faculty Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **305.** Atomistic modeling of electromechanical spectroscopies in molecular junctions. **I. Franco**

COMP **306.** Large-scale complete active space self-consistent field methods. **A.E. DePrince**

COMP **307.** Replica exchange envelope distribution sampling (RE-EDS): A robust and accurate method to calculate multiple free energy differences from a single simulation. D. Sidler, M. Cristofol-Clough, A. Schwaninger, **S. Riniker**

COMP **308.** Determining dispersion coefficients for polarizable force fields using density functional theory. M. Mohebifar, E.R. Johnson, **C.N. Rowley**

Section E

Walter E. Washington Convention Center
Hall C

Wiley Computers in Chemistry Outstanding Postdoc Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **309.** Computational exploration of Pd(II)-catalyzed C-H activation and functionalization. **Y. Yang**, K.N. Houk

COMP **310.** Towards multiconfiguration quantum embedding methods for solids state. **S. Bernales Candia**, H. Pham, G.E. Scuseria, L. Gagliardi

WEDNESDAY MORNING

Section A

Washington Marriott at Metro Center
Salon A

Molecular Mechanics

Force Fields

Cosponsored by PHYS

M. Feig, *Organizer*

V. S. Bharadwaj, *Presiding*

8:30 COMP **311.** Benchmark free energy calculations using AMOEBA and an approximate non-iterative polarization scheme. **F.C. Pickard**, A.C. Simmonett, J. Rackers, J.W. Ponder, B. Brooks

9:00 COMP **312.** Conformational sampling of proteins with the fully polarizable Drude force field. **J. Huang**, A.D. Mackerell

9:30 COMP **313.** Evaluating molecular dynamics force fields using computed NMR chemical shifts. **D. Koes**

10:00 Intermission.

10:20 COMP **314.** Systematic improvement of ANI deep learned potentials through active learning in conformational and configurational space. **J.S. Smith**, R. Zubatyuk, O. Isayev, A.E. Roitberg

10:50 COMP **315.** Comparison and optimization of fixed-point charge and polarizable force fields for the simulation of water-alkane systems. **A. Krämer**, F.C. Pickard, J. Huang, R.M. Venable, D. Reith, K.N. Kirschner, R. Pastor, B. Brooks

11:20 COMP **316.** Ionic liquid OPLS-AA force field parameters for imidazolium-based simulations. **O. Acevedo**, B. Doherty, X. Zhong

Section B

Washington Marriott at Metro Center
Salon B

Drug Design

Cosponsored by CINF

M. R. Landon, Y. Tseng, *Organizers*

Y. Peng, *Presiding*

8:30 COMP **317.** Mathematics for drug design and discovery. **G. Wei**

9:00 COMP **318.** Insights into energetic contributions to SAR: Applications of fragment symmetry-adapted perturbation theory (F-SAPT) to drug-protein binding. **D. Sitkoff**, D.L. Cheney, X. Zhu, D. Langley, R.M. Parrish, B.W. Bakr, D. Sirianni, C.D. Sherrill

9:30 COMP **319.** Development and testing of *de novo* DOCK. W.J. Allen, B.C. Fochtman, T.E. Balius, **R.C. Rizzo**

10:00 Intermission.

10:15 COMP **320.** Fast screening of chemical libraries with solvent mapping derived fake ligands. **D. Hall**, I.J. Enyedy

10:45 COMP **321.** New computational tools at the molecular scale for protein-ligand binding in drug discovery. **D. Janezic**, J. Konc

11:15 COMP **322.** Study on the efficacy of mesothelin targeting recombinant immunotoxins in a nude mouse model bearing shed antigen tumors by mathematical model simulation. **J. Lee**

Section C

Washington Marriott at Metro Center
Salon C

Quantum Mechanics

A. E. DePrince, *Organizer*

J. Larkin, *Presiding*

8:30 COMP **323.** Mapping transition metal chemical space with continuous descriptors – feature selection and implications for machine learning models. **J. Janet**, H. Kulik

8:50 COMP **324.** Withdrawn.

9:20 COMP **325.** Renaissance of semi-empirical methods: Fast computation of 2-electron integrals. P.E. Lopes

9:40 COMP **326.** Temperature dependent QM/QM embedding using Green's functions. **A.R. Welden**, D. Zgid

10:00 COMP **327.** Regional DMET: Efficient and accurate single-fragment embedding of wave functions in Kohn-Sham DFT. **G. Knizia**, J.E. Klein

10:30 Intermission.

10:45 COMP **328.** Ring-polymer surface-hopping: Incorporating nuclear quantum effects into non-adiabatic dynamics simulations. **F.A. Shakib**, P. Huo

11:05 COMP **329.** Conical intersections found in silicon nanoparticles with a dangling bond defect. **W. Peng**, B. Fales, B.G. Levine

11:25 COMP **330.** Understanding entropy of metal-ligand complexes. **A.L. Dewyer**, P.M. Zimmerman

11:45 COMP **331.** Toward the accurate simulation of vibrationally-resolved phosphorescence spectra. **J. Bloino**, A. Baiardi, F. Egidi, M. Fusè, V. Barone

Section D

Washington Marriott at Metro Center
Salon D

Material Science

Methods for Property Prediction & Computational Screening

C. M. Aikens, *Organizer*

G. D. Degaga, *Presiding*

8:30 COMP **332.** Breaking badly: DFT-D2 gives sizeable errors for tensile strengths in bulk solids. **B.M. Wong**, N.V. Ilawe

8:55 COMP **333.** Composite thermochemical approach to tin alkyl precursors in hybrid molecular beam epitaxy. **R. Harkins**, W.L. Gladfelter, C.J. Cramer, B. Jalan, T. Wang, A. Prakash

9:20 COMP **334.** High pressure phases of cylo-para-phenylenes: Aromatic vs. quinonoid structures and polymer formation. L. Qiu, **M. Kertesz**

9:45 COMP **335.** Improved isotropic and anisotropic thermal gradient approaches for the quasiharmonic approximation to predict thermodynamic properties of organic crystals. **N.S. Abraham**, E. Dybeck, N.P. Schieber, M.R. Shirts

10:10 Intermission.

10:30 COMP **336.** High-throughput identification and characterization of two-dimensional materials using density functional theory. **K. Choudhary**

10:55 COMP **337.** Data-driven prediction of materials properties in an automated fashion. **S. Kwak**, T.J. Mustard, D. Giesen, T.F. Hughes, A. Goldberg, S. Dixon, M. Halls

11:20 COMP **338.** Chemical and radiation stability of ionic liquids: A computational screening study. **N.V. Ilawe**, J. Fu, S. Ramanathan, B.M. Wong, J. Wu

11:45 COMP **339.** Prediction of regulation toxicological tests applied to high energy molecules. **R. Terreux**, C. Alliod, R. Denis, J. Chemelle, G. Jacob

Section E

Washington Marriott at Metro Center
Salon E

Computational Studies of Membranes & Membrane-Bound Systems

Biology in the Membrane

Cosponsored by PHYS

M. Feig, J. Shen, *Organizers*

L. Riccardi, *Presiding*

8:30 COMP **340.** Interplay between lid domain plasticity and lipid flexibility modulates specificity of human monoacylglycerol lipase. **L. Riccardi**, J.M. Arencibia, L. Bono, A. Armirotti, S. Girotto, M. Devivo

9:00 COMP **341.** Connecting molecular structure with cellular function: Membranes allosterically regulate phospholipases A2. **V.D. Mouchlis**, A.M. Vasquez, J. McCammon, E.A. Dennis

9:30 COMP **342.** How do special lipids influence the structures, dynamics, and functions of multi-domain proteins? **J. Li**

10:00 COMP **343.** Photosynthetic energy transfer in purple bacteria: A multiscale view through the computational microscope. **A. Singharoy**, C. Maffeo, E. Tajkhorshid, K. Schulten

10:30 Intermission.

10:50 COMP **344.** Bacterial membrane disruption mechanism of defensins. **A. Cho**

11:20 COMP **345.** Interaction of amyloid β peptides with lipid membrane. **N. Xiang**, Y. Lyu, X. Zhu, G. Narsimhan

11:50 COMP **346.** Modeling the nano-bio interface: Cytochrome *c* on lipid bilayers. **C.R. Allen**, E. Melby, R. Hernandez, C.J. Murphy, R.J. Hamers, J.A. Pedersen

Drug Discovery: Cheminformatic Approaches

Sponsored by CINF, Cosponsored by COMP

Experimental & Computational Advances in Understanding Enzyme Specificity & Promiscuity

New Strategies to Expand the Scope of Enzyme Engineering

Sponsored by PHYS, Cosponsored by BIOL and COMP

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

WEDNESDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Salon A

Molecular Mechanics

Nucleic Acids

Cosponsored by PHYS

M. Feig, *Organizer*

L. Prentis, *Presiding*

1:30 COMP **347.** Asymmetric breathing motions of nucleosomal DNA and the role of histone tails. **K. Chakraborty**, S. Loverde

2:00 COMP **348.** Computational simulations of RNA containing modified bases. **M.C. Nagan**

2:30 COMP **349.** Improving force field accuracy and structure determination of RNA by a combined computational and experimental approach. **C. Bergonzo**, R. Acevedo, C.W. Lawrence, A. Grishaev, T.E. Cheatham

3:00 COMP **350.** Effect of nucleotide state on the protofilament conformation of tubulin octamers. **A. Manandhar**, M. Kang, S. Loverde

3:30 Intermission.

3:50 COMP **351.** Probing the binding mechanism of BRACO19 to parallel quadruplexes from human telomeric DNA using molecular dynamics simulation with a free ligand. **C. Wu**, B. Machireddy

4:20 COMP **352.** Withdrawn.

4:50 COMP **353.** Combining structure-based models and enhanced sampling methods to probe RNA conformational dynamics. R. Jacobs, **H. Vashisth**

Section B

Washington Marriott at Metro Center
Salon B

Drug Design

Cosponsored by CINF

M. R. Landon, Y. Tseng, *Organizers*

A. Thakur, *Presiding*

1:30 COMP **354.** Striking the right balance between speed, accuracy and reliability in quantitative ligand binding free energy calculations: A case study of a FXa protein-ligand system. **Z. Guo**

1:55 COMP **355.** Multisite lambda dynamics can compute precise free energies of binding in combinatorically large chemical spaces featuring ligand and protein perturbations. **J. Vilseck**, K. Armacost, R. Hayes, C.L. Brooks

2:20 COMP **356.** Modeling molecular recognition: Free energy calculations for inhibitors binding to protein kinases. **W. Chen**, Y.M. Huang, Z. Tang, C. Chang

2:45 Intermission.

3:00 COMP **357.** Molecular dynamics fingerprints (MDFP): Machine-learning from MD data to predict free-energy differences. **S. Riniker**

3:25 COMP **358.** Large-scale QSAR modeling: Proteochemometrics vs. multitask deep learning. **A. Zakharov**, T. Zhao, D. Nguyen, N. Southall

3:50 COMP **359.** Exploiting submodel diversity in ensemble prediction. **P. Daga**, M. Waldman, R.D. Clark

4:15 COMP **360.** Energy minimization and pose generation with convolutional neural network scoring. **D. Koes**

Section C

Washington Marriott at Metro Center
Salon C

Quantum Mechanics

A. E. DePrince, *Organizer*

D. Chaves Claudino, *Presiding*

1:30 COMP **361.** Computational and theoretical studies on electron excitations in several oxyluciferin and curcumin derivatives. V.B. Satalkar, **Y. Shao**

2:00 COMP **362.** Quantum-based refinement. **M. Waller**

2:20 COMP **363.** Efficient computational screening of transition metal centered dyes. **L.A. Fredin**, T. Allison

2:40 COMP **364.** Improved quantum mechanical model of P450-mediated aromatic oxidation. **R. Leth**, P. Hunt, M. Segall

3:00 Intermission.

3:15 COMP **365.** Effect of ancillary ligands (A) on oxidative addition of CH4 to MIII complexes: M = Ta, Re; A = B, Al, CH, SiH, N, P using DFT, MP2, CCSD(T) and MCSCF methods. **R. Parveen**, T. Cundari

3:35 COMP **366.** Digging deep: A SAPT study towards a quantitative understanding of non-covalent interactions in receptor–anion complexes. **A. Sengupta**, A.H. Flood, K. Raghavachari

3:55 COMP **367.** Initial applications of a computational chemistry app store to understanding basis-set superposition error. **R. Richard**

4:25 COMP **368.** Correlated Gaussian primitive sets based on energy deviations per electron. **D. Chaves Claudino**, R.J. Bartlett

Section D

Washington Marriott at Metro Center
Salon D

Material Science

Adsorption, Diffusion & Catalysis

C. M. Aikens, *Organizer*

M. F. Afzal, *Presiding*

1:30 COMP **369.** Predictive modeling of adsorption and diffusion for zeolite nanosheets and hierarchical zeolites. **J.I. Siepmann**

1:55 COMP **370.** Adsorption and diffusion mechanisms of C1-C4 hydrocarbons in MOF-74-Mg/Zn: A quantum chemical study for selective gas separation applications in petroleum refining industries. **G.D. Degaga**, L. Valenzano

2:20 COMP **371.** Molecular orientation and water transport in carbon nanotube reinforced aromatic polyamide membranes. **R. Cruz Silva**, T. Araki, Y. Takizawa, J. Ortiz-Medina, A. Morelos-Gomez, S. Inukai, S. Tejima, K. Takeuchi, T. Noguchi, T. Hayashi, T. Kawaguchi, M. Terrones, M. Endo

2:45 COMP **372.** Computational investigation of acid-gas induced degradation mechanism of zeolitic imidazolate frameworks. C. Han, C. Zhang, **N. Tyminska**, D. Sholl, J.R. Schmidt

3:10 Intermission.

3:25 COMP **373.** Unveiling atomistic mechanisms of vanadium redox reactions on nitrogen-doped graphene from first principles simulations. **K. Klyukin**, N.N. Intan, Z. Jiang, V. Alexandrov

3:50 COMP **374.** Mechanistic study of oxygen reduction reaction in alkaline solutions: Importance of chemisorbed water. **S. Liu**, M.G. White, P. Liu

4:15 COMP **375.** Combined quantum mechanical and molecular mechanical method for catalyst design on the NU-1000 metal-organic framework. **X. Wu**, L. Gagliardi, D.G. Truhlar

4:40 COMP **376.** Gas-phase hydrolysis of dimethyl methylphosphonate by the cyclic tetramer of zirconium hydroxide. **I. Schweigert**, L.D. Gunlycke

Section E

Washington Marriott at Metro Center
Salon E

Computational Studies of Membranes & Membrane-Bound Systems

Transport Across Membranes

Cosponsored by PHYS

M. Feig, J. Shen, *Organizers*

F. Samerjeet, *Presiding*

1:30 COMP **377.** Interactions between bioorganic molecules and membrane: Passive permeation, membrane defects, and phase behavior. **R. Sun**, J.M. Swanson, G.A. Voth

2:00 COMP **378.** Membrane permeability of gasotransmitters calculated using the solubility-diffusion model. **F. Sajadi**, E. Awoonor-Williams, C.N. Rowley

2:30 COMP **379.** Mechanism of substrate translocation in an alternating access transporter. **R.O. Dror**

3:00 COMP **380.** Binding free energy calculations for inhibitors and HCN ion channels. **F. Tofoleanu**, B. Brooks

3:30 Intermission.

3:50 COMP **381.** Atomistic simulation studies of synthetic channels in biomimetic membranes. **D. Barden**, H. Vashisth

4:20 COMP **382.** Transport of vitamin B12-peptide nucleic acid conjugates through the BtuB outer membrane receptor of E. coli. T. Pienko, **J. Trylska**

‡ *Cooperative Cosponsorship*

4:50 COMP **383.** Molecular mechanism of pH-dependent activation of sodium-proton antiporters. **Y. Huang**, W. Chen, J. Shen

Drug Discovery: Cheminformatic Approaches

Sponsored by CINF, Cosponsored by COMP

THURSDAY MORNING

Section A

Washington Marriott at Metro Center
Salon A

Molecular Mechanics

Cosponsored by PHYS

M. Feig, *Organizer*

E. Sayfutyarova, *Presiding*

8:30 COMP **384.** Testing for physical validity in molecular dynamics. **P.T. Merz**, M.R. Shirts

9:00 COMP **385.** MD-binding: Enabling fully dynamic simulation of binding for real-world drug-target systems. **W. Rocchia**, A. Spitaleri, S. Decherchi, A. Cavalli

9:30 COMP **386.** Direction-dependent protein remodeling by AAA+ biological nanomachines. **A. Javidialesaadi**, G. Stan

9:50 COMP **387.** Finding multiple reaction pathways via global optimization of action. **J. Lee**, I. Lee, I. Joung, J. Lee, B. Brooks

10:20 Intermission.

10:40 COMP **388.** Dynamic hydrogen bonding network in *E. coli* glycinamide ribonucleotide transformylase (GAR Tfase). **P. Gupta**, A.E. Roitberg

11:00 COMP **389.** Using constant pH molecular dynamics and free energy perturbation to compute ph-dependent binding free energies. **R.C. Harris**, C. Tsai, C.R. Ellis, J. Shen

11:30 COMP **390.** Structure, activity, and chemical recognition of pH and ionic strength induced protein-protein interactions. **M.R. Jones**, A.K. Wilson, B. Brooks

11:50 COMP **391.** Machine learning enabled approach to incorporate multi-state information in molecular modeling of dynamic allostery: A case study of the PDZ2 domain. M. Botlani, A. Siddiqui, **S. Varma**

Section B

Washington Marriott at Metro Center
Salon B

Drug Design

Cosponsored by CINF

M. R. Landon, Y. Tseng, *Organizers*

L. Kalash, *Presiding*

8:30 COMP **392.** Addressing phospholipase A2 selectivity towards phospholipids: An important step for developing potent and selective inhibitors. **V.D. Mouchlis**, A.M. Vasquez, J. McCammon, E.A. Dennis

9:00 COMP **393.** Benchmarking methods for virtual screening of match molecular pairs: A PDB-wide and ChEMBL-wide analysis. **M. Baumgartner**, D. Evans

9:30 COMP **394.** Duality of protein binding site similarity and cognate ligand similarity. **A.N. Jain**, A.E. Cleves

10:00 Intermission.

10:15 COMP **395.** Discovery of multiple fragments binding to different regions of the catalytic pocket of LP-PLA2 and the structure-based rational design towards leads. **V. Berdini**

10:45 COMP **396.** Investigating the importance of region1 in the small molecule CD4 mimics (SMCM) through QM/MM and pure QM methods. **F. Moraca**

11:15 COMP **397.** Withdrawn.

Section C

Washington Marriott at Metro Center
Salon C

Quantum Mechanics

A. E. DePrince, *Organizer*

D. Nascimento, *Presiding*

8:30 COMP **398.** MP2 hydration free energies of 20 different salts show excellent agreement with experiments. **F. Wang**, J. Li

9:00 COMP **399.** Role of the medium on the stereoselectivity in organic reactions. **V. Aviyente**

9:30 COMP **400.** Solubility prediction from first principles: A density of states approach. **S. Boothroyd**, A. Kerridge, J. Anwar

10:00 COMP **401.** Computational study of the Criegee intermediate through ozonolysis reaction. **M. Almatarneh**, I.A. Elayan, Z. Ahmed

10:30 COMP **402.** Robust Chebyshev filtering for SCF iteration. **A. Breuer**, X.C. Wang

Section D

Washington Marriott at Metro Center
Salon D

Material Science

Batteries, Bio-Based Materials & Beyond

C. M. Aikens, *Organizer*

Y. Xing, *Presiding*

8:30 COMP **403.** Analysis, design and simulation of nanobatteries: Silicon anodes and beyond. L.A. Selis, V.H. Ponce, D.E. Galvez-Aranda, L. Benitez, **J.M. Seminario**

8:55 COMP **404.** First-principles density functional theory modeling of redox potential of organic materials for lithium-ion batteries. K. Kim, T. Liu, S.W. Lee, **S. Jang**

9:20 COMP **405.** Theoretical insights into flavin-C60 complexes via molecular mechanics and molecular dynamics. **E. Karunaratne**, J. Gascon, F. Papadimitrakopoulos

9:45 COMP **406.** Design and insight into the electronic structure of power conversion efficient arylamine organic dyes for dye-sensitized solar cells (DSSCs): *In silico* approaches. **J.K. Roy**, S. Kar, J.R. Leszczynski

10:10 COMP **407.** Density functional theory study of the thermodynamic and mechanical properties of single crystal group (IV) diborides with boron vacancies. **M. Sun**, J. Liu

10:35 Intermission.

10:50 COMP **408.** Multiscale modeling of multicompartment micelle nanoreactors. **C.P. Callaway**, P. Sood, S. Jang

11:15 COMP **409.** Structure and chirality of supramolecular nanostructures with peptide-drug amphiphiles. **M. Kang**, K. Chakraborty, H. Cui, S. Loverde

11:40 COMP **410.** Coarse-grained and statistical mechanics modeling of dynamic, mechanically compliant DNA hinges. Z. Shi, C. Castro, **G. Arya**

12:05 COMP **411.** Hybrid peptide-based materials encompassing ultrashort peptides: Molecule to materials. S. Mushnoori, **M. Dutt**

ENFL

Division of Energy and Fuels

D. Heldebrant, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Advances & Challenges at the Food-Energy-Water Nexus (see *ENVR*, Tue, Wed)

Cooperative Catalysis at Surfaces & Interfaces: Impact on Chemistry & Energy Frontiers (see *CATL*, Sun Mon, Tue)

Emerging Catalytic Processes for Methane Conversion (see *CATL*, Mon, Tue)

How to get your First Industrial Job (see *YCC*, Tue)

Recent Advances towards the Bioeconomy (see *CELL*, Sun)

Understanding the Chemistry of Our Planet (see *PRES*, Tue)

SOCIAL EVENTS:

Dinner, 6:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting & Social, 12:00 PM: Mon

Executive Committee Meeting, 4:00 PM: Sun

Program Meeting, 1:00 PM: Sun

SUNDAY MORNING

Section A

Walter E. Washington Convention Center
Room 143A

Carbon Management: Advances in Carbon Efficiency, Capture, Conversion, Utilization & Storage

CO_2 Conversion

Y. H. Hu, P. K. Koech, *Organizers*

H. Lin, X. Wang, *Organizers*, *Presiding*

M. Hu, *Presiding*

8:00 ENFL **1.** CO_2 conversion to novel solid materials for energy conversion and storage. Y.H. Hu

8:50 ENFL **2.** Photo-initiated reduction of CO_2 by H_2 on silica. **C. Liu**, J.M. Notestein, E. Weitz, K.A. Gray

9:15 ENFL **3.** Bimetallic Fe-Cu catalysts for CO_2 hydrogenation to C_2^+ hydrocarbons. **W. Wang**, X. Wang, X. Jiang, C. Song

9:40 ENFL **4.** Progresses in CO_2 hydrogenation to methanol over In_2O_3 supported Pd catalysts. **C. Liu**, N. Rui

10:20 Intermission.

10:30 ENFL **5.** Perovskite nanocomposite as an exceptional CO_2 splitting agent in a hybrid solar-redox scheme. **F. Li**

11:10 ENFL **6.** Plasmonic CO_2 conversion to formic acid by cis-Rubpy complex with high selectivity and rate under mild condition. **H. Jun**, M. Yang, Y. Nam

11:35 ENFL **7.** Fe-based bimetallic catalysts supported on TiO2 for selective CO_2 hydrogenation to higher hydrocarbons. **N. Boreriboon**, W. Wang, X. Jiang, C. Song, P. Prasassarakich

Section B

Walter E. Washington Convention Center
Room 142

Solar Energy & Solar Cells

Y. H. Hu, R. T. Koodali, *Organizers*

N. Wu, *Presiding*

8:00 Introductory Remarks.

8:05 ENFL **8.** Charge transfer and energy transfer from plasmonic metals to semiconductors. **N. Wu**

8:45 ENFL **9.** Spectroscopic evolution of graphene oxide/perovskite interfaces for solar energy. **M. Acik**, R. Rosenberg

9:05 ENFL **10.** Withdrawn.

9:25 ENFL **11.** Imaging photovoltaic functionality of polycrystalline and perovskite solar cells at the nanoscale. **E.M. Tennyson**, M.S. Leite

9:45 Intermission.

9:55 ENFL **12.** Plasmon enhanced photocatalysis and solar cells. **D. Ma**

10:35 ENFL **13.** Incorporation of inequivalent neodymium cations into perovskite hybrids for boosting device performance of perovskite photovoltaics. **X. Gong**

10:55 ENFL **14.** Modelling materials and processes in perovskites solar cells. **F. De Angelis**

11:15 ENFL **15.** Progress towards the study of proton-coupled electron transfer reactions via the mixed quantum-classical Liouville approach. **F.A. Shakib**, G. Hanna

11:35 Concluding Remarks.