Section F

Pennsylvania Convention Center
Room 123

Basic Research in Colloids, Surfactants & Nanomaterials

Nanomaterial Applications

R. Nagarajan, *Organizer*

Y. Mao, *Presiding*

8:30 COLL **584.** Preparation, growth mechanism and uses of one-dimensional nanostructures. **S. Hunyadi Murph**

8:50 COLL **585.** Bio-inspired synthetic giant clam system for solar energy applications. **H. Kim**, S. Vahidinia, A. Holt, A. Sweeney, S. Yang

9:10 COLL **586.** Tunable optical properties of 2D nanowire lattices. **S.J. Boehm**, L. Kang, D. Werner, C.D. Keating

9:30 COLL **587.** Design, synthesis, and characterization of mixed ionic/electronic conducting surface layers adsorbed on metal oxide particles. **J. Richards**, N.J. Wagner, P. Butler

9:50 COLL **588.** Hydrogen storage by nanostructured graphene and metal hybrids enhanced with spill-over mechanism. **Y. Mao**, L. Wei

10:10 COLL **589.** Graphene origami for 3D functional structures and devices. **W. Xu**, H. Kwag, A. Sarkar, K. Kwok, C. Yoon, J. Liu, T.D. Nguyen, D.H. Gracias

10:30 COLL **590.** Self-organization of organic molecules on graphite for photovoltaics. **J.M. Espinosa Duran**, D. Ashley, H. Castillo, J. Dobscha, B. Hirsch, Y. Liu, Y. Sereda, M. Baik, A.H. Flood, S.L. Tait, P. Ortoleva

10:50 COLL **591.** Designing hierarchical supramolecular interactions for organic 2D crystal assemblies at the liquid-solid interface. **H.D. Castillo**, J.R. Dobscha, Y. Liu, J.M. Espinosa Duran, D. Ashley, Y.V. Serada, B. Hirsch, M. Baik, P. Ortoleva, A.H. Flood, S.L. Tait

11:10 COLL **592.** *In situ* synthesis of single-molecule electronic components. **M.S. Inkpen**, L.M. Campos, Y.R. Leroux, P. Hapiot, L. Venkataraman

11:30 COLL **593.** Withdrawn.

11:50 COLL **594.** Assembling and aligning multicomponent nanowires with van der Waals forces. **B.D. Smith**, D. Kirby, X. Kong, Z. Gobert, C. Albright, K.A. Fichthorn, C.D. Keating

Section G

Pennsylvania Convention Center
Room 124

Basic Research in Colloids, Surfactants & Nanomaterials

Bio-Nano Materials

R. Nagarajan, *Organizer*

S. A. Claridge, *Presiding*

8:30 COLL **595.** Self-assembling extracellular matrix proteins as materials for the condensation of silica nanostructures. **C.M. Gomes**, L.F. Deravi

8:50 COLL **596.** Study of *in vivo* efficacies of antibody dependent cell cytotoxicity of antibody functionalized gold nanoparticles. **M. Ahmed**

9:10 COLL **597.** Dimensional control of orthogonal chemical interfaces using polymerizable amphiphiles. **S.A. Claridge**

9:30 COLL **598.** Thermophilic ferritin: A versatile nanocontainer for the encapsulation of nanoparticles and other useful cargo. **K.W. Pulsipher**, I.J. Dmochowski

9:50 COLL **599.** Optimizing the bio-nano interface via a multi-coordinating polymer coating. **W. Wang**, X. Ji, A. Kapur, H.M. Mattoussi

10:10 COLL **600.** Toward single-molecule biophysical surface-enhanced Raman spectroscopy with nanostar-liposomes bioconjugates. **W. Lum**, I. Bruzas, L. Sagle

10:30 COLL **601.** Bio-orthogonal coupling on hydrophilic quantum dots. **N. Zhan**, G. Palui, J. Merkl, H.M. Mattoussi

10:50 COLL **602.** Increased oxidation in lipid membranes from Cu^{2+} bound to phosphatidylethanolamine. **A.M. Sendecki**, M.F. Poyton, X. Cong, P.S. Cremer

11:10 COLL **603.** Nanocomposites hydroxyapatite: Polysaccharide hydrogels for bone regeneration. M. Kowaleff, G. Nunez, D. Akpatsu, M. Jitianu, N. O'Connor, **A. Jitianu**

Polymer Science at the Interface of Industry, Government & Academics

Industry/University Collaborations

Sponsored by POLY, Cosponsored by COLL, PMSE and SCHB

COMP

Division of Computers in Chemistry

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

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

SUNDAY MORNING

Section A

Sonesta Philadelphia Downtown
Whistler A

Modeling Water & Solvation in Biochemistry: Developments & Applications

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

W. Yang, *Presiding*

8:30 COMP **1.** Simulating biomolecules with implicit solvent models: GB, PB and 3D-RISM. **D.A. Case**

9:00 COMP **2.** Solvation vs. aggregation in dense protein solutions. **M. Feig**

9:30 Intermission.

9:45 COMP **3.** Solvent exchange in liquid water and rate theory. **L.X. Dang**

10:15 COMP **4.** Integration of electrostatics and solvation into statistical machine learning approaches for the quantitative modeling of protein-DNA binding affinities. T. Chiu, **R. Rohs**

10:45 COMP **5.** Quantifying uncertainty in biomolecular solvation. **N.A. Baker**, H. Lei, X. Yang, G. Wei

Section B

Sonesta Philadelphia Downtown
Hopper

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Cosponsored by PHYS and POLY

H. Nguyen, J. Shen, *Organizers*

B. H. Morrow, *Presiding*

8:30 Introductory Remarks.

8:40 COMP **6.** Using computation and experiment to explore the sequence space for short peptide self-assembly. **R. Ulijn**, T. Tuttle

9:10 COMP **7.** Using molecular tuning to design functional polypeptides. **T.J. Deming**

9:40 COMP **8.** Pattern formation of confined periodically sequenced polypeptides. **R.S. Tu**

10:10 Intermission.

10:25 COMP **9.** Materials construction through peptide computational design and solution assembly. **D.J. Pochan**

10:55 COMP **10.** Using theory and computation to guide the design of proteins, protein assemblies, and bimolecular materials. **J.G. Saven**

11:25 COMP **11.** Structure and properties of bioinspired, conductive coiled-coil fibers from *de novo* peptides. R.K. Spencer, N. Ing, **A. Hochbaum**

Section C

Sonesta Philadelphia Downtown
Warhol

Quantum Mechanics

Cosponsored by PHYS

S. E. Wheeler, *Organizer*

R. Bhattacharjee, *Presiding*

8:30 COMP **12.** Self-consistent implementation of meta-GGA exchange-correlation functionals within the ONETEP linear-scaling DFT code. **J.C. Womack**, C. Skylaris

9:00 COMP **13.** CAM-LDA0: The reincarnation of the local density approximation. **C.H. Borca**, M.A. Mosquera, M.A. Ratner, G. Schatz

9:20 COMP **14.** Principles and applications of a new Koopmans' theorem like range-separated density functional theory. **Y. Jin**, R.J. Bartlett

9:40 COMP **15.** London-dispersion corrected SCAN: hybrid-level accuracy with a non-empirical meta-generalized gradient approximation. J.G. Brandenburg, **J.E. Bates**, A. Ruzsinszky, J. Sun, J.P. Perdew

10:00 Intermission.

10:15 COMP **16.** Exciton coupled-cluster theory for large-scale electronic structure calculations. **A.D. Dutoi**, Y. Liu

10:45 COMP **17.** Convergence of ground and excited state properties in solution using combined quantum/classical methods. **M.R. Provorse**, X.S. Vazquez, J. Milanese, C. Isborn

11:15 COMP **18.** Efficient implementation of molecules-in-molecules fragment-based approach for chiroptical vibrational spectra of large molecules. **K. Jose**, K. Raghavachari

11:45 COMP **19.** Using agent-based modeling to bridging the length scales between DFT molecular level calculations and continuum scale modeling. **L.E. Achenie**

Section D

Sonesta Philadelphia Downtown
Benton

Designing Chemical Libraries for Screening

S. Das, *Organizer*

A. Shelat, *Organizer*, *Presiding*

8:30 Introductory Remarks.

8:45 COMP **20.** Strategies for the identification of scaffold families in chemical libraries and their application in a compound stability study. **C. Laggner**, Y. Shayo, C. Johnson, C. Loomis

9:15 COMP **21.** Novel methods for predicting and prioritizing design ideas from SAR matrices. **L. Zhang**, K. Johnson, J. Starr, J. Milbank, A. Kuhn, C. Poss, V. Shanmugasundaram

9:45 COMP **22.** Profile-QSAR Gen 2: Deep learning kinase IC_{50} predictions for novel compounds as accurate as 4-pt IC50s. **E.J. Martin**, V. Polyakov, L. Tian

10:15 Intermission.

10:30 COMP **23.** What can your library do for you? **R. Guha**, D. Nguyen, A. Jadhav

11:00 COMP **24.** ChemLG – A smart and massively parallel molecular library generator. **M. Afzal**, J. Hachmann

11:30 COMP **25.** Compound evolution taken by STORM: First ideas turn into genuine possibilities. **C. Detering**

12:00 Panel Discussion.

Section E

Sonesta Philadelphia Downtown
Wyeth Gallery C

Drug Discovery

Case Studies in SBDD

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

S. K. Lakkaraju, *Presiding*

8:30 COMP **26.** HRD motif as the central hub of the signaling network for activation loop autophosphorylation in Abl kinase. G. La Sala, L. Riccardi, R. Gaspari, A. Cavalli, O. Hantschel, **M. Devivo**

9:00 COMP **27.** Comparative analysis of the structural determinants of endogenous cannabinoids. **V.K. Yadav**, K.M. Elokely, M.L. Klein

9:30 COMP **28.** Structural basis for antagonist selectivity in orexin receptors. **K. Babaoglu**

10:00 Intermission.

10:15 COMP **29.** Lovastatin lactone may improve constipation in irritable bowel syndrome (IBS) by inhibiting enzymes in the archaeal methanogenesis pathway. **S.M. Muskal**, D. Sliman, D. Kokai-Kun, D. Pimentel, D. Wacher, D. Gottlieb

10:45 COMP **30.** Examination of hydroxyethylamino sulfonamide derivatives as anti-HIV-1 protease inhibitors using molecular dynamics and free energy calculations. **D. Das**, H. Hayashi, Y. Takamatsu, M. Aoki, R. Yedidi, A.K. Ghosh, H. Mitsuya

‡ *Cooperative Cosponsorship*

11:15 COMP **31.** Structure-based approach to identify selective JAK1 inhibitors for treatment of autoimmune diseases. **R. Unwalla**, M.L. Vazquez, N. Kaila, J.W. Strohbach, S. Han

11:45 COMP **32.** Development of new oxindole-based PI3K-δ inhibitors using structure-based drug design. **X. Fradera**

Advanced Potential Energy Surfaces

Classical Simulation Models & Methods

Sponsored by PHYS, Cosponsored by COMP

WCC Merck Research Award Symposium

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

SUNDAY AFTERNOON

Section A

Sonesta Philadelphia Downtown
Whistler A

Modeling Water & Solvation in Biochemistry: Developments & Applications

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

M. Feig, *Presiding*

1:30 COMP **33.** MN15: A new density functional for covalent and noncovalent interactions. **D.G. Truhlar**, H.S. Yu, X. He, S.L. Li

2:00 COMP **34.** Quantum chemical framework for next-generation force fields: the explicit polarization model for water. **J. Gao**

2:30 COMP **35.** Exploring water penetration in proteins and its functional implications. **Q. Cui**

3:00 Intermission.

3:15 COMP **36.** Towards a balanced implicit solvent force field for intrinsically disordered proteins. K. Lee, **J. Chen**

3:45 COMP **37.** Single-site multipole water and the hydrophobic effect. **T. Ichiye**

4:15 COMP **38.** Quantum mechanics / molecular mechanics method combined with resolution-adapted all-atomic and coarse-grained model. **L. Shen**, H. Hu, W. Yang

Section B

Sonesta Philadelphia Downtown
Hopper

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Cosponsored by PHYS and POLY

H. Nguyen, J. Shen, *Organizers*

A. Hochbaum, *Presiding*

1:30 COMP **39.** Experimental and computational design of stimuli-responsive diagnostic and therapeutic self-assembling peptide vehicles. **J.E. Goldberger**, C.J. Buettner, A. Wallace

2:00 COMP **40.** Functional materials from peptide amphiphiles: theory and experiment. **G.C. Schatz**

2:30 COMP **41.** Bioactive and bio-inspired supramolecular biomaterials. **S.I. Stupp**

3:00 Intermission.

3:15 COMP **42.** Controlling polysaccharide hydrogel structure, properties and function. **G.F. Payne**

3:45 COMP **43.** Modeling pH-sensitive biomaterials. **B.H. Morrow**

4:15 COMP **44.** Stimuli-responsive biomaterials utilizing superparamagnetic particles. **S. Minko**

Section C

Sonesta Philadelphia Downtown
Warhol

Emerging Technologies in Computational Chemistry

C. L. Simmerling, *Organizer*, *Presiding*

1:30 COMP **45.** Software ecosystem for the data-driven design of chemical systems and the exploration of chemical space. **J. Hachmann**, M. Haghighatlari, W. Evangelista, M. Afzal, C. Shih, B.A. Moore, M. Pechagin, Y. Tian

2:00 COMP **46.** Geometrical descriptors of time-dependent transition states. **G. Craven**

2:30 Intermission.

2:45 COMP **47.** Higher accuracy NMR crystallography at lower computational cost. J. Hartman, **G.J. Beran**

3:15 COMP **48.** Leveraging a computational chemistry app store to compute high accuracy lattice energies of molecular crystals. **R. Richard**, D. Sherrill

3:45 COMP **49.** Workflow development at Merck through Merck–Rutgers collaboration. **Y. Hu**, B. Sherborne, T. Lee, D.A. Case, D.M. York, Z. Guo

Section D

Sonesta Philadelphia Downtown
Benton

Designing Chemical Libraries for Screening

S. Das, *Organizer*

A. Shelat, *Organizer*, *Presiding*

1:30 Introductory Remarks.

1:45 COMP **50.** Predictive QSPR modeling of photochromic systems. **F. Jabeen**, M. Ossowski, P.R. Boudjouk

2:15 COMP **51.** Development of lower cost sampling methods to accelerate the discovery of CARM1 inhibitors. **Y. Zhang**, L. Du, C. Rupakheti, Q. Wang, D.N. Beratan

2:45 COMP **52.** Enriching chemical libraries with target binding site pharmacophore matching. **S. Das**, A. Singh, J.J. Bowling, E. Griffith, R.E. Lee, A. Shelat

3:15 Panel Discussion.

Section E

Sonesta Philadelphia Downtown
Wyeth Gallery C

Drug Discovery

Advances in Methods for Structure-Based Drug Design

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

N. Kumar, *Presiding*

1:30 COMP **53.** Relative binding free energy calculations to accelerate drug discovery. **W. Sherman**

2:00 COMP **54.** DOCK6 developments to assist in structure-based design. **R.C. Rizzo**

2:30 COMP **55.** Practicalities of molecular dynamics in ligand pose evaluation in a discovery workflow. **X. Zhu**, D. Langley, S. Johnson

3:00 Intermission.

3:15 COMP **56.** Turning binders into activators. **R.P. Pemberton**

3:45 COMP **57.** Peptide design challenges: a comparison and contrast to small molecule design. **D.J. Diller**, A.S. Bayden, J. Swanson, M. Jarosinski, J. Audie

4:15 COMP **58.** Conformational sampling of macrocycles: Recent progress. **P.C. Hawkins**

Advanced Potential Energy Surfaces

Classical Simulation Methods & Software

Sponsored by PHYS, Cosponsored by COMP

MONDAY MORNING

Section A

Sonesta Philadelphia Downtown
Whistler A

Modeling Water & Solvation in Biochemistry: Developments & Applications

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

T. Luchko, *Presiding*

8:30 COMP **59.** Constant pH molecular dynamics: From RNA to viral capsids and Bac. **C.L. Brooks**

9:00 COMP **60.** Water penetration determines the pKa of protein internal ionizable groups. **X. Wu**, A. Damjanovic, J. Lee, B. Brooks

9:30 Intermission.

9:45 COMP **61.** Use of Monte Carlo sampling and continuum electrostatics to derive energies of charge changes in proteins: Examples from cytochrome c oxidase and photosystem II. **M. Gunner**, C. Chenel, D. Matta, X. Cai, S. Salah, W. Szejgis

10:15 COMP **62.** Should I stay or should I go: Proton transfer revisited. **P. Czodrowski**

10:45 COMP **63.** pH regulates BACE1 enzymatic activity and inhibitor binding. **C.R. Ellis**

Section B

Sonesta Philadelphia Downtown
Whistler B

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Cosponsored by PHYS and POLY

H. Nguyen, J. Shen, *Organizers*

R. Mannige, *Presiding*

8:30 COMP **64.** Programming functional nanoscale DNA-based materials. **M. Bathe**

9:00 COMP **65.** Rational design of functional biomaterials and programmable assembly pathways. **H. Nguyen**

9:30 COMP **66.** Kinetic engineering of DNA self-assembly processes. **R. Schulman**

10:00 Intermission.

10:15 COMP **67.** Effect of oligonucleic acid (ONA) backbone design on the thermodynamics of ONA hybridization and melting. **A. Jayaraman**, A. Ghobadi

10:45 COMP **68.** Understanding the relationship between physical and electronic structure within biologically-inspired perylene diimide molecular array. N. Frey, A. Mazaheripour, C. Markegard, A. Bartlett, H. Nguyen, A.A. Gorodetsky, **S. Sharifzadeh**

11:15 COMP **69.** Thermodynamic model of heterochromatin formation through epigenetic regulation. Q. MacPherson, S. Mao, P. Mulligan, E. Koslover, **A. Spakowitz**

Section C

Sonesta Philadelphia Downtown
Warhol

Quantum Mechanics

Cosponsored by PHYS

S. E. Wheeler, *Organizer*

J. J. Shepherd, *Presiding*

8:30 COMP **70.** *Ab initio* propagator studies of the electronic structure of diffuse and valence anions: From fullerenes to double Rydbergs. **J.V. Ortiz**

9:00 COMP **71.** Fresh look at the shape and Feschbach resonances in the CO_2 anion using equation of motion coupled cluster (EOM-CC) and the stabilization method. **A. Bazante**, R.J. Bartlett

9:20 COMP **72.** Trapping transient species: Trianionic polyaromatic systems. **A.Y. Rogachev**

9:50 COMP **73.** Solvation and transport of carbon dioxide in molten carbonates: evidence of an oxo-Grotthuss mechanism via a pyrocarbonate anion. D. Corradini, **F. Coudert**, R. Vuilleumier

10:20 Intermission.

10:35 COMP **74.** Computational investigation of boronic and borinic acid interactions with poly-ols and saccharides. **J.D. Larkin**

11:05 COMP **75.** Iron porphyrin electrocatalysts for oxygen reduction: Mechanistic insight. **N. Kumar**, M. Pegis, B.A. McKeown, J.M. Mayer

11:35 COMP **76.** Composite approaches for accurate predictions of lanthanide and actinide chemistry. **C.C. Peterson**, D.A. Penchoff, A.K. Wilson

12:05 COMP **77.** Withdrawn.

Section D

Sonesta Philadelphia Downtown
Benton

Sharing Pharmaceutical Industry Data: Outlook & Opportunities

B. Sherborne, *Organizer*, *Presiding*

8:30 Introductory Remarks.

8:40 COMP **78.** New momentum in pre- and post-competitive pharma data sharing - getting the right data to drive the science. **B. Sherborne**, C. Peishoff, V.A. Feher, E.S. Manas, V. Shanmugasundaram, L. Shewchuk-Chapman, C.W. Hutchins

9:10 COMP **79.** Data sharing and beyond: Lessons learned from the life sciences industry. **C.I. Nitsche**

9:40 COMP **80.** ChEMBL database – Experiences as a data broker. **L. Bellis**

10:10 COMP **81.** D3R: Leveraging datasets to drive progress in protein-ligand modeling for computer-aided drug design. **V.A. Feher**

10:40 Panel Discussion.

Section E

Sonesta Philadelphia Downtown

Wyeth Gallery C

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

Cosponsored by PHYS

J. Gao, J. Pu, W. Yang, *Organizers*

Y. Shao, *Presiding*

8:30 Introductory Remarks.

8:35 COMP **82.** Studies of chemical reactions of organic molecules, enzymes, and metal-organic frameworks by means of QM/MM and QM/QM computational approaches. **H. Hirao**

9:05 COMP **83.** Redefining enzyme catalysis: Chemical control in the battle against fidelity in promiscuous terpene synthases. **D.T. Major**

9:35 COMP **84.** Multiple-environment single-system quantum mechanical molecular mechanical methods and their applications in reaction pathway studies. **Y. Shao**, E.R. Rosta, H.L. Woodcock, W. Yang, B. Brooks

10:05 Intermission.

10:20 COMP **85.** Mechanistic strategies in ribozymes: Catalytic roles of metal ions, nucleobases, and cofactors. **S. Hammes-Schiffer**, P.C. Bevilacqua

10:50 COMP **86.** Enzymatic chemical step mechanism coupled with artificial enzyme design from path sampling calculations. **S.D. Schwartz**

11:20 COMP **87.** Computational enzymology: from mechanistic studies to modulator design. **Y. Zhang**

Advanced Potential Energy Surfaces

QM with MM

Sponsored by PHYS, Cosponsored by COMP

Shedding Light on the Dark Genome: Methods, Tools & Case Studies

Sponsored by CINF, Cosponsored by BIOT, COMP and MEDI

MONDAY AFTERNOON

Section A

Sonesta Philadelphia Downtown

Whistler A

Modeling Water & Solvation in Biochemistry: Developments & Applications

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

A. V. Onufriev, *Presiding*

1:30 COMP **88.** Ras signaling: A challenge to the biological sciences. H. Jang, **R. Nussinov**

2:00 COMP **89.** Modeling intermolecular interactions and liquid-liquid phase equilibria in cell-like conditions. S. Qin, **H. Zhou**

2:30 Intermission.

2:45 COMP **90.** Thermodynamics of virus capsid assembly in aqueous solution. **K.M. Merz**

3:15 COMP **91.** Electrostatics and binding properties of G-protein coupled receptors. **R. Abagyan**, I. Kufareva

3:45 COMP **92.** Interpreting thermodynamic profiles of aminoadamantane compounds inhibiting the M2 proton channel of influenza A by free energy calculations. N. Homeyer, H. Ioannidis, F. Kolarov, G. Gauglitz, C. Zikos, A. Kolocouris, **H. Gohlke**

Section B

Sonesta Philadelphia Downtown

Whistler B

Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation

Cosponsored by PHYS and POLY

H. Nguyen, J. Shen, *Organizers*

S. Sharifzadeh, *Presiding*

1:30 COMP **93.** Protein assemblies by design. **V.P. Conticello**

2:00 COMP **94.** Designing nanogel star polymers for drug delivery applications: Insight from simulations. **A.C. Carr**, W.C. Swope, V. Piunova, J.E. Rice, R.D. Miller, J.W. Pitera

2:30 COMP **95.** New class of highly stable and self-repairing membrane-mimetic 2D materials assembled from lipid-like peptoids. **C. Chen**

3:00 Intermission.

3:15 COMP **96.** Peptoid nanosheets exhibit a new secondary-structure motif. **R. Mannige**

3:45 COMP **97.** Grafted polymer layers for biomaterials. **I.A. Luzinov**

4:15 COMP **98.** Harnessing biomimetic cryptic bonds to form self-reinforcing gels. S. Biswas, V.V. Yashin, **A.C. Balazs**

Section C

Sonesta Philadelphia Downtown

Warhol

Molecular Mechanics

M. Feig, *Organizer*

S. Capponi, *Presiding*

1:30 COMP **99.** Using theory and experiment to elucidate the origin of product specificity in PRMT1. **O. Acevedo**, S. Gathiaka, B. Boykin, B. Caceres, J. Hevel

2:00 COMP **100.** Computational modelling structure-function relationships of tyrosylprotein sulfotransferase. **C. Christov**, T. Karabencheva-Christova, W. Singh

2:30 COMP **101.** Temperature effects on the dynamics of light harvesting complex II. **Y. Wang**, Y. Weng, J. Gao

3:00 COMP **102.** Cooperative motion of a key positively charged residue and metal ions for DNA replication catalyzed by Y-family polymerases. V. Genna, R. Gaspari, M. Dal Peraro, **M. Devivo**

3:30 Intermission.

3:45 COMP **103.** Description and assessment of common RNA dinucleotide conformations generated by different force field / water model combinations. **H.S. Hayatshahi**, T.E. Cheatham

4:15 COMP **104.** Delineating ion modulated conformational changes in ribosomal RNA using grand-canonical Monte-Carlo/molecular dynamics simulations. **S.K. Lakkaraju**, J.A. Lemkul, A.D. Mackerell

4:45 COMP **105.** Molecular dynamics studies of the effects of histone variant on nucleosome dynamics. **J. Wereszczynski**

Section D

Sonesta Philadelphia Downtown

Benton

Sharing Pharmaceutical Industry Data: Outlook & Opportunities

B. Sherborne, *Organizer*, *Presiding*

1:30 Introductory Remarks.

1:40 COMP **106.** Rapid, accurate and reproducible binding affinity calculation for drug discovery: A retrospective analysis of the Pfizer Pan-Trk Program. S. Wan, A. Bhati, **P.V. Coveney**, S. Skerratt, K. Gore, S.K. Bagal, V. Shanmugasundaram, K. Omoto

2:20 COMP **107.** Developing a community resource for the understudied kinome. **T.M. Willson**

2:50 COMP **108.** Advancing quantitative biophysical predictions: What can be gained from industry-academic data sharing? **J.D. Chodera**

3:30 COMP **109.** Beyond data sharing: Using real-world data for teaching real-world computational workflows and for benchmarking new methods. **J.M. Jansen**, R.E. Amaro, Y. Tseng, W.D. Cornell, E.X. Esposito, P. Walters

4:00 Panel Discussion.

Section E

Sonesta Philadelphia Downtown

Wyeth Gallery C

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

Cosponsored by PHYS

J. Gao, J. Pu, W. Yang, *Organizers*

L. V. Slipchenko, *Presiding*

1:30 COMP **110.** Quantum embedding method to simulate proton reduction reactions in transition-metal catalysts. **P. Huo**, J. Goodpaster, T.F. Miller

2:00 COMP **111.** Full embedding QM/MM with the effective fragment potential method. **L.V. Slipchenko**

2:30 COMP **112.** Studies of natural and artificial photosynthesis. **V.S. Batista**

3:00 Intermission.

3:15 COMP **113.** Simulating chemical and redox processes in solution and in enzymes. **W. Yang**

3:45 COMP **114.** QM/MM simulations of electron/proton transfer reactions and protein excited states. **M. Elstner**

4:15 COMP **115.** Photobiology in action: excited-state QM/MM simulations for understanding photodynamics in biological systems. **D. Morozov**, G. Groenhof

Advanced Potential Energy Surfaces

Excited State Surfaces & Spectroscopy

Sponsored by PHYS, Cosponsored by COMP

Tetrahedron Prize for Creativity in Organic Chemistry Symposium

Sponsored by ORGN, Cosponsored by BIOL, COMP and MEDI

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

MONDAY EVENING

Section A

Pennsylvania Convention Center

Halls D/E

Sci-Mix

H. L. Woodcock, *Organizer*

8:00 - 10:00

187-188, 191, 197, 206, 209, 211, 215, 227, 231, 237-239, 242-243, 246, 248, 251, 253, 255, 259-261, 264, 266-267, 272, 275-277, 283-284, 288, 292, 295, 297-303, 305-306. See subsequent listings.

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

‡ *Cooperative Cosponsorship*

TUESDAY MORNING

Section A

Sonesta Philadelphia Downtown
Whistler B

Modeling Water & Solvation in Biochemistry: Developments & Applications

Cosponsored by PHYS

E. Alexov, R. Luo, *Organizers*

X. Wu, *Presiding*

8:30 COMP **116.** Mathematical methods for solvation and binding free energy predictions. **G. Wei**

9:00 COMP **117.** Sampling protein functional dynamics via solvation force fluctuation. **W. Yang**

9:30 COMP **118.** Solvation free energy decomposition using the 3D-RISM theory of molecular solvation. **T. Luchko**

10:00 Intermission.

10:15 COMP **119.** Choice of water model matters. **A.V. Onufriev**

10:45 COMP **120.** Polarizable force fields for condensed phase simulation. **T.L. Head-Gordon**

11:15 COMP **121.** Determining polarizable force fields with electrostatic potentials from quantum mechanical linear response theory. **H. Wang**, W. Yang

Section B

Sonesta Philadelphia Downtown
Whistler A

Molecular Mechanics

M. Feig, *Organizer*

J. Huang, *Presiding*

8:30 COMP **122.** Development of TraPPE–UA2 models for ethane and ethylene and adsorption in all-silica zeolites. **M.S. Shah**, M. Tsapatsis, J.I. Siepmann

9:00 COMP **123.** Kirkwood-Buff derived force field for polyols. **N. Kariyawasam Manachchige**, P.E. Smith

9:30 COMP **124.** Development of torsional potentials for the KBFF model of peptides and proteins. **S. Karunaweera**, P.E. Smith

10:00 COMP **125.** Improved conformational sampling of intrinsically disordered proteins with the modified CHARMM36 protein force field. **J. Huang**, A.D. Mackerell

10:30 Intermission.

10:45 COMP **126.** Charge models for force fields from condensed phase quantum calculations. **W.C. Swope**, J.E. Rice

11:15 COMP **127.** Efficient and accurate pKa calculator using the QM-NBB method. **F.L. Kearns**, P.S. Hudson, S. Boresch, H.L. Woodcock

11:45 COMP **128.** Continuous constant pH molecular dynamics with particle mesh Ewald and titratable water. **Y. Huang**, W. Chen, J.A. Wallace, J. Shen

Section C

Sonesta Philadelphia Downtown
Warhol

Quantum Mechanics

Cosponsored by PHYS

S. E. Wheeler, *Organizer*

Y. Jin, *Presiding*

8:30 COMP **129.** Energy decomposition analysis with a well-defined charge-transfer term for interpreting intermolecular interactions. **J. Herbert**, K. Lao

9:00 COMP **130.** Energy decomposition analysis in an adiabatic picture – assessing the effect of different components of an intermolecular interaction on molecular properties. **Y. Mao**, P. Horn, M.P. Head-Gordon

9:20 COMP **131.** Insight into the locality of intermolecular interactions in organic crystals using conceptual density functional theory. **R. Bhattacharjee**, M. Zhang, T. Li

9:50 COMP **132.** Electron scattering in Liouville space: From coherence to decoherence to incoherence? **R. Jorn**

10:20 Intermission.

10:35 COMP **133.** Quantum chemistry strategies for the transition metals: Towards nondynamic electron correlation. **A.K. Wilson**

11:05 COMP **134.** Linear-response absorption spectra from explicitly time-dependent CC2. **A.E. DePrince**

11:35 COMP **135.** Exact Quantum Monte Carlo calculations for the H-H-H system at the sub-microhartree level. **J.B. Anderson**

Section D

Sonesta Philadelphia Downtown
Benton

Polypharmacology: How Little Can One Afford? How Much Can You Predict?

P. Walters, *Organizer*

P. Czodrowski, *Organizer*, *Presiding*

8:30 Introductory Remarks.

8:35 COMP **136.** Polypharmacology: Useful? C.G. Bologa, O. Ursu, J.J. Yang, **T.I. Oprea**

9:05 COMP **137.** Decoding polypharmacology from phenotypic screens. M.N. McCarroll, L. Gendelev, D. Kokel, **M.J. Keiser**

9:35 COMP **138.** BIOSEA: leveraging compound bioactivity data for prospective target identification and phenotypic screening. A. Cortes Cabrera, D. Lucena Agell, M. Redondo-Horcajo, I. Barasoain, F. Diaz, B. Fasching, **P. Petrone**

10:05 Intermission.

10:20 COMP **139.** Application of polypharmacology in daily research project work. **M. Bieler**

10:50 COMP **140.** Comprehensive analysis in drug target identification using protein sequence, structure, and ligand similarity approaches. Y. Chen, R. Tolbert, A.M. Aronov, G. McGaughey, P. Walters, **L. Meireles**

11:20 COMP **141.** Mapping the binding sites of the annotated structural proteome – Implications for polypharmacology. **N. Brown**

Section E

Sonesta Philadelphia Downtown
Wyeth Gallery C

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

Cosponsored by PHYS

J. Gao, J. Pu, W. Yang, *Organizers*

H. Lin, *Presiding*

8:30 COMP **142.** Graphical methods for systematic and predictive reaction exploration in complex systems and environments. **P.M. Zimmerman**

9:00 COMP **143.** Molecular kinetics from biased simulations. **E.R. Rosta**

9:30 COMP **144.** Adaptive-partitioning QM/MM for dynamics simulations. A. Duster, C. Garza, M. Zarecki, **H. Lin**

10:00 Intermission.

10:15 COMP **145.** Beyond QM/MM: Development of multistate density functional theory with explicit polarization for charge transfer processes. **J. Gao**

10:45 COMP **146.** Withdrawn.

11:15 COMP **147.** Polarizable/multipolar and long-range corrected methods for QM/MM simulations. E.G. Kratz, R.E. Duke, **G.A. Cisneros**

Advanced Potential Energy Surfaces

Ab initio Molecular Dynamics

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

Sonesta Philadelphia Downtown
Whistler B

Drug Discovery

Novel Approaches in Ligand-Based Drug Design & Cheminformatics

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

A. Abbaspour Tamijani, *Presiding*

1:30 COMP **148.** Evaluation of the virtual screening performance and core-hopping potential of common pharmacophore hypotheses derived from phase's novel pharmacophore feature-based shape alignment. **M. Repasky**, S. Dixon, E. Mack, W. Duncan, C. Von Bargen

2:00 COMP **149.** *In silico* design of β-secretase 1 (BACE1) inhibitors. **R. Fraczkiewicz**, D. Miller, M.S. Lawless, R.D. Clark

2:30 Intermission.

2:45 COMP **150.** Structural diversity and potency range distribution of scaffolds in bioactive compounds and assessment of scaffold hopping versus activity cliff formation. **D. Stumpfe**, D. Dimova, J. Bajorath

3:15 COMP **151.** Extraction of structure-activity relationship information from activity cliff clusters via matching molecular series. **D. Dimova**, J. Bajorath

3:45 COMP **152.** Marvin Live: An integrated tool for knowledge driven/information rich live design sessions. **A. Strácz**, A. Costache

Section B

Sonesta Philadelphia Downtown
Whistler A

Molecular Mechanics

M. Feig, *Organizer*

N. Chen, *Presiding*

1:30 COMP **153.** Atomistic simulation of diblock-like peptoids forming membrane-mimetic 2D material. **M.D. Baer**, C. Chen

2:00 COMP **154.** Modeling anisotropy of vapor deposited films for OLED application. **D. Yu**, S.G. Arturo, D. Devore, K. Kearns, J. Kramer, S. Mulkhopadhyay, L. Spencer, P. Trefonas

2:30 COMP **155.** Utilizing Gibbs ensemble molecular dynamics and hybrid Monte Carlo/molecular dynamics simulations for efficient study of polymer-solvent phase equilibria. **T.E. Gartner**, T.H. Epps, A. Jayaraman

3:00 COMP **156.** Modeling ion specific effects: Toward correlations with hydrophobic solvation via aqueous interfacial fluctuations. **S.A. Patel**

3:30 Intermission.

3:45 COMP **157.** Understanding peptide self-assembly with multiscale modeling. **J. Li**

4:15 COMP **158.** Mapping the kinetic folding and binding networks of amyloid- and helix-forming peptides using coarse master equations. C.T. Leahy, R.D. Murphy, S.C. McCartan, B. Tywoniuk, Y. Yuan, A. Crowe, G. Sánchez-Sanz, D. Roy, **N. Buchete**

4:45 COMP **159.** Effect of lipids and cholesterol on the stability of the amyloid precursor protein (APP) homodimer. M. Audagnotto, **M. Dal Peraro**

Section C

Sonesta Philadelphia Downtown
Warhol

Material Science

H. L. Woodcock, *Organizer*

G. Leuty, *Presiding*

1:30 COMP **160.** Breaking badly: DFT-D2 gives sizeable errors for tensile strengths in bulk solids. **B.M. Wong**

2:00 COMP **161.** (110) Facet of rutile GeO_2 energetics: A dispersion-corrected DFT study. **A. Abbaspour Tamijani**

2:30 COMP **162.** Superhard borides: mechanism of hardness, its anisotropy, and ways to enhance it. **A. Alexandrova**

3:00 Intermission.

3:20 COMP **163.** Development of an improved intermolecular force field for MoS_2 adsorption simulations. **G.M. Leuty**, H. Turner, V. Varshney, C. Muratore, R.J. Berry

3:50 COMP **164.** Computational design of highly active Ir catalysts for water oxidation. **K. Yang**, V.S. Batista

4:20 COMP **165.** Oxygen reduction reaction catalysis in graphene-conjugated pyrazine with a cationic nitrogen. N. Ricke, **J.J. Shepherd**, M.G. Welborn, T.A. Van Voorhis

Section D

Sonesta Philadelphia Downtown

Benton

Polypharmacology: How Little Can One Afford? How Much Can You Predict?

P. Czodrowski, *Organizer*

P. Walters, *Organizer*, *Presiding*

1:30 COMP **166.** Predicting surprising polypharmacology. **A.N. Jain**, A.E. Cleves

2:00 COMP **167.** What is required for alchemical free energy methods to be useful in predicting drug polypharmacology? **J.D. Chodera**

2:30 COMP **168.** Kinome wide off-target prediction by mining structural and profiling data. **S. Fulle**, A. Volkamer, B. Merget, S. Turk, S. Eid, F. Rippmann

3:00 Intermission.

3:15 COMP **169.** Polypharmacology prediction with SPiDER for *de novo* designed compounds and natural products. **D. Reker**, G. Schneider

3:45 COMP **170.** Contrasting polypharmacology and pains. **A. Tropsha**, S. Capuzzi

4:15 COMP **171.** Understanding cytotoxicity in high-throughput screening collections using an *in silico* polypharmacological prediction protocol. **L. Mervin**, Q. Cao, I. Barrett, M. Firth, D. Murray, O. Engkvist, A. Bender

4:45 Concluding Remarks.

Section E

Sonesta Philadelphia Downtown

Wyeth Gallery C

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

Cosponsored by PHYS

J. Gao, J. Pu, W. Yang, *Organizers*

H. L. Woodcock, *Presiding*

1:30 COMP **172.** Interpreting solvent effects on chemical reactivity using QM/MM simulations. **O. Acevedo**

2:00 COMP **173.** Transition-tempered metadynamics accelerates the convergence of free energy surfaces in biomolecular systems from QM/MM simulation. **R. Sun**, O. Sode, J.F. Dama, G.A. Voth

2:30 COMP **174.** Recent advances in the development of QM/MM free energy methods to study biocatalysis. **D.M. York**

3:00 Intermission.

3:15 COMP **175.** QM/MM simulations of organic and enzymatic reactions in solution. J.Z. Vilseck, **W.L. Jorgensen**

3:45 COMP **176.** Understanding metalloenzyme catalysis with QM/MM free energy simulations. **Q. Cui**

4:15 COMP **177.** Obtaining accurate QM/MM free energies using novel sampling and reweighting approaches. P.S. Hudson, F.L. Kearns, S. Boresch, **H.L. Woodcock**

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

TUESDAY EVENING

Section A

Pennsylvania Convention Center

Hall E

NVIDIA GPU Award

Financially supported by NVIDIA Corporation

M. E. Berger, *Organizer*

6:00 - 8:00

COMP **178.** Extending excited state quantum chemistry to large-scale systems using graphical processing units. **B. Fales**, B. Levine

COMP **179.** Leveraging GPU-accelerated molecular dynamics simulations to compute and analyze the 4D chemical descriptor space of ERK2 kinase inhibitors. **J. Ash**, D. Fourches

COMP **180.** Atomic multipole polarizable model for nucleotides. **C. Lu**, J.W. Ponder

COMP **181.** Convolutional neural networks for protein-ligand scoring. **M. Ragoza**, J. Collins, D. Koes

COMP **182.** Cholesterol-enriched bilayers present a substantial barrier to oxygen permeation. C.R. Smith, K. Bueche, R. Dotson, G. Angles, **S.C. Pias**

Section A

Pennsylvania Convention Center

Hall E

OpenEye Outstanding Junior Faculty Award in Computational Chemistry

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **183.** Electronic excitation dynamics in liquid water under proton irradiation. **Y. Kanai**

COMP **184.** Elucidating heterogeneous ice nucleation mechanisms using large scale rare event simulations. **S. Sarupria**, B. Glatz, R. Defever, W. Hanger, L. Ngo, A. Apon

COMP **185.** Discovery of reaction mechanisms, catalysts, and materials by new quantum chemical simulation methods. **P.M. Zimmerman**

COMP **186.** Divide and conquer the electronic structure of condensed phases: Ground states and dynamics in real and imaginary time. **M. Pavanello**

Section A

Pennsylvania Convention Center

Hall E

Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

COMP **187.** Understanding the effect of amino acid conformation on binding affinity to Au(111) using quantum mechanical calculations. **M.C. Small**, J.L. Terrell, D.A. Sarkes, B.L. Adams, H. Dong, J. Jahnke, D.N. Stratis-Cullum, M. Hurley

COMP **188.** Multi-scale simulation of amyloid fibril growth: Trap states and main pathways. **Z. Jia**, A. Beugelsdijk, J.D. Schmit, J. Chen

COMP **189.** Structure and mode of action of organophosphate pesticides: A computational study. **L.K. Rathnayake**, S.H. Northrup

COMP **190.** AutoDock-GIST: Incorporating thermodynamics of active-site water into scoring function for accurate protein-ligand docking. **S. Uehara**, S. Tanaka

COMP **191.** Identification of rare oligosaccharide conformers using swarm-enhanced sampling molecular dynamics (sesMD). **I. Alibay**, K.K. Burusco, N.J. Bruce, R.A. Bryce

COMP **192.** De novo design of proteins to encapsulate nonbiological cofactors. **J. Blum**, J.G. Saven

COMP **193.** Modeling the structure and reactivity of Al^{3+}/Fe^{3+} substitution in kaolinite. **T. Hicks**, R.K. Szilagyi

COMP **194.** *In silico* modeling of dopamine transporter and design of novel neuroprotective agents. **T. Djikic**, K. Yelekci

COMP **195.** Design of orthogonal split inteins in silico. **S.C. Arbor**

COMP **196.** Challenges in generating bioactive small molecule conformation. **Q. Yang**, B.K. Rai, X.J. Hou

COMP **197.** What does it take to drive our prediction accuracy up? **Y. Gao**, A. Crespo, A. Verras, Y. Li, R. Wang, M. Holloway, Y. Hu, Z. Guo, B. Sherborne

COMP **198.** Exploring conformations of human fatty acid synthase inhibitors using replica exchange molecular dynamics. **N. Mele**, M. Miljak, R. Ward, J. W.Essex

COMP **199.** Comparative theoretical study of oxygen adsorption on neutral and anionic Ag_n and Au_n clusters (n = 2 - 25). **J.D. Watts**, M. Liao, M. Huang

COMP **200.** Surprisal-based adaptive sampling of all-atom simulations for rapid convergence of Markov state models. **G. Miller**, V. Voelz

COMP **201.** Probing the effects of N-methylation on peptide-protein interactions using alchemical free energy perturbation. **M. Hurley**, A. Wakefield, V.A. Voelz

COMP **202.** Assessment of actinide/lanthanide complexation using density functional theory. **A. Dinescu**, T. Weaver

COMP **203.** pH dependent NMR chemical shifts of model peptides. **E. Artikis**, C.L. Brooks

COMP **204.** Application of virtual screening and molecular dynamic simulations to the discovery of new antibiotics for LpxC in gram-negative bacteria. **V.K. Thilakarathne**

COMP **205.** Molecular dynamics investigation of the stability of sarcin/ricin domains: Towards using adaptively biased MD to find the full dynamic range of RNA. **J.M. Imamoto**, M.F. Bruist

COMP **206.** Modeling 10000 antibodies in about an hour: Leveraging the power of the Amazon Cloud. **E. Metwally**, A. Ajamian

COMP **207.** Hierarchical nanoparticles in photodynamic therapy. **N. Eldabagh**, J. Foley

COMP **208.** Constant pH molecular dynamics simulations of pH responsive polymers. **A. Sharma**

COMP **209.** Application of extended Huckel Theory to pharmacophore modeling. **A. Ajamian**

COMP **210.** Investigation of the role of metal ion in the active site of hammerhead ribozyme by Hamiltonian replica exchange molecular dynamics simulations. **H. Chen**, D.M. York

COMP **211.** Identification and statistical analysis of structurally conserved waters via R. **E.X. Esposito**

COMP **212.** Nanoscale structure of lipid bilayers revealed by *in-silico* and experimental small angle neutron scattering. **M. Dorrell**, F. Heberle, J. Katsaras, E. Lyman

COMP **213.** Nonlinear onset of calcium wave propagation in cardiac cells. **O. Zavalov**

COMP **214.** Using Markov state models to better understand the effects of mutations on folding. **H. Wan**, V.A. Voelz

COMP **215.** Rationalizing non-standard interactions in ligand design: The duality of halogens. **A. Deschenes**

COMP **216.** Employing genetic algorithms to drive *de novo* design. **C.D. Singleton**, W.J. Allen, R.C. Rizzo

COMP **217.** Developing mutant-specific inhibitors of HER2 incorporating bridging water molecules. **J. Guo**, S. Collins, T. Miller, R.C. Rizzo

COMP **218.** Computational screening and selection of linear peptide hairpin mimetics by implicit solvent molecular simulation. **Y. Ge**, B. Kier, N.H. Andersen, V.A. Voelz

COMP **219.** Visible light-driven energy transfer: Hybrid engineered nanostructures versus plasmonic resonance in solar cell applications. **J. Codrington**, J. Foley

COMP **220.** Stirring a low Reynolds number MARTINI. **A. Zgorski**, E. Lyman

COMP **221.** Evaluation of multi-function scoring strategies for DOCK. **Y. Zhou**, R.C. Rizzo

COMP **222.** Computation calorimetry. **A. Webb**, C. Arnarez, E. Lyman

COMP **223.** MARTINI coarse-grained simulations of pH-driven aggregation of EAK16 peptides. L. Chong, **S. Mushnoori**, M. Dutt

COMP **224.** Ultra-coarse-grained models for geling-forming mucins. **P. Lin**, F. Ramezanghorbani, C.M. Colina

COMP **225.** Characterization of the binding pocket of FABP5 by docking studies and molecular dynamics simulations of ligands discovered by high throughput screening. **C.D. Bruce**, B. Brown, N. Hunter

COMP **226.** DMS: An equation-free multiscale molecular dynamics simulator. **A. Abi Mansour**, P. Ortoleva

‡ *Cooperative Cosponsorship*

COMP **227.** Computer aided discoveries: Predictive modeling for polymers, coating systems and drug like molecules. **F. Jabeen**, M. Ossowski, P.R. Boudjouk

COMP **228.** Early stage of acid-induced BBL unfolding. **Z. Yue**, J. Shen

COMP **229.** Study on the gas and heat-treated graphite edge planes using reactive forcefield. **H. Guk**, D. Chung, D. Kim, S. Choi

COMP **230.** Mechanism of diastereoselective encapsulation of tartaric acid by arylamide foldamers: a computational investigation. **M. Wujcik**, V. Pophristic, Z. Liu

COMP **231.** Relative importance of energy components in CMDwater – a computational tool for making decisions about displacing crystallographic waters during lead optimization. **A.S. Bayden**

COMP **232.** Computational filters for virtual screening of new battery electrolyte solvents. **D. Chung**, D. Kim, H. Guk, S. Choi

COMP **233.** Development of a general approach to study pH-reaction mechanism of nucleic acid systems. **J. Ouyang**, C. Gaines, D.M. York

COMP **234.** Density functional theoretical study on 2,7-carbazole and thieno[3,4-c]pyrrole-4,6-dione-based copolymers. **Y. Cho**, S. Hwang, H. Woo

COMP **235.** Density functional theoretical study on alkoxy- or alkylthio-substituted phenylene and benzothiadiazole containing photovoltaic polymers. **S. Hwang**, H. Woo

COMP **236.** Coarse-grained model for multiscale enhanced sampling of disordered protein conformations. **X. Liu**, **J. Chen**

COMP **237.** Exploring pH-modulated binding of BACE1 inhibitors by constant pH molecular dynamics. **C. Tsai**, C.R. Ellis, J. Shen

COMP **238.** New Ewald method for ab initio QM/MM molecular dynamics simulation. **T.J. Giese**, D.M. York

COMP **239.** Water dominates the specific antithrombin–heparin interaction. **P.D. Mosier**, W. Yu, U.R. Desai, A.D. Mackerell, A. Sarkar

COMP **240.** Ongoing developments in the CHARMM general force field. **G. Mukherjee**, K. Vanommeslaeghe, A.D. Mackerell

COMP **241.** Cation size effects on first electronic transition of proton-water cluster: electronic delocalization of hydrated proton in liquid water. **T. Goto**, K. Bec, Y. Ozaki

COMP **242.** Effect of fluorinated sugar on antiproliferation factor (APF) conformational properties. **A. Aytenfisu**, J.J. Barchi, A.D. Mackerell

COMP **243.** Democratizing the creation and application of machine learning models with AutoQSAR. **M. Repasky**, S. Dixon, J. Duan, C. Von Bargen

COMP **244.** Conformational sampling of intrinsically disordered peptides by enhanced sampling methods. **M. Miljak**, N. Mele, E. Haensele, D. Whitley, L. Banting, T.R. Clark, R. Ward, J.W. Essex

COMP **245.** N-heterocyclic carbene-based nickel and palladium complexes: A DFT comparison of the Mizoroki-Heck catalytic cycles. **V.H. Menezes da Silva**, A. A. C. Braga, T.R. Cundari

COMP **246.** Unified framework for computer-aided biologics design. R. Alvarez, **H. Shadnia**

COMP **247.** Molecular encapsulation of sugar alcohols by arylamide foldamers: a computational chemistry study. **E.C. Fluck**, Z. Liu, V. Pophristic

COMP **248.** Improved AMOEBA ions for aqueous salt solution simulation. **Z. Wang**, J.W. Ponder

COMP **249.** Action at a distance: How distal residues contribute to catalysis in human phosphoglucose isomerase. **S.C. Begay**, P.J. Beuning, M.J. Ondrechen

COMP **250.** *De novo* ligand design using DOCK6. **B.C. Fochtman**, W.J. Allen, R.C. Rizzo

COMP **251.** Seamless integration of 2D and 3D SAR to guide medicinal chemistry. J. Chisholm, M. Gastreich, E. Champness, C. Detering, P. Hunt, **T. Mansley**, C. Lemmen, M. Segall

COMP **252.** Evaluation of the solubility of cellulose in water: Free energy calculation using ER method. **K. Ueda**, M. Matsushita, K. Kataoka, Y. Matsubara

COMP **253.** Unique mechanistic characteristics of the *glmS* ribozyme. **K. Kostenbader**, D.M. York

COMP **254.** Molecular simulation study of the polycyclic aromatic small molecules as amyloid beta 40 modulators for treatment of Alzheimer's disease. C. Jin, J. Kim, J. Shin, E. Tumurbaatar, **S. Jee**, S.S. Jang

COMP **255.** Parametrization of halogen bonds in the CHARMM general force field. **F. Lin**, I. Soteras, K. Vanommeslaeghe, J.A. Lemkul, K. Armacost, A.D. Mackerell

COMP **256.** Classification of distinct conformers of $\beta_{<2}$-adrenergic receptor (β_2AR) based on binding affinity of ligands through docking studies. **E.D. Akten**, **G. Dilcan**

COMP **257.** Principal component analysis applied to jacobian matrices from structural kinetic modeling. **N.J. Carbonaro**, I.F. Thorpe

COMP **258.** Theoretical investigation of the relaxation energies and coupling constants in a series of pyrene derivatives fused with N-,S-, and O-containing heterocycles. **B. Wex**, M. Nakhoul, E. Challita, A. Merhi

COMP **259.** Post-transition state dynamics and micro solvation effects of F atom + $CH_3CN \rightarrow HF + CH_2CN$ exothermic reaction. **S. Pratihar**, X. Ma, R. Scott, W.L. Hase

COMP **260.** D3R 2015 and 2016 challenges: Evaluation of predictions for the grand and mini challenges. **S.M. Gathiaka**, M. Chiu, J. Grethe, S. Liu, H. Yang, S. Burley, R.E. Amaro, V. Feher

COMP **261.** Strategies for improving accuracy in carbohydrate NMR chemical shifts computations via free energy simulation. **P.S. Hudson**, B.C. Pollard, M.F. Crowley, H.L. Woodcock

COMP **262.** Application of wavelet transform for tumor/non-tumor classification of high-dimensional microarray data. **Z. Heidari**, A. Ardakani, J. Ghasemi

COMP **263.** Predicting properties of fuels using molecular dynamics. **B.H. Morrow**, M. Gustafson, J.A. Harrison

COMP **264.** Improving conformational sampling of RNA using the GB-Neck2 implicit solvent model. **K. Lam**, C.L. Simmerling

COMP **265.** Evaluation of natural enzymes for catalysis of Morita-Baylis-Hillman reaction. **N. Genccakir**, N. Celebi-Olcum, B. Akbulut

COMP **266.** Building up boron nanomaterials: From B to B_{24} and beyond. B. Catalano, G. Curtin, D. Vassileva, **J.R. Rocha**

COMP **267.** Monosubstituted phenylboronic acids, R–$B(OH)_2$ (R = C_6H_5, $C_6H_4CH_3$, $C_6H_4NH_2$, C_6H_4OH, and C_6H_4F): A computational investigation. **N.Z. Rao**, J.D. Larkin, C.W. Bock

COMP **268.** Molecular modeling of tertiary amines to forecast their CO_2 absorption properties. **M.A. Kuenemann**, D. Fourches

COMP **269.** Implementing experiment directed simulations. **D.B. Amirkulova**, A. White

COMP **270.** Investigation of allene oxide to cyclopentenone cyclization mechanism through a diradical oxyallyl intermediate. **S. Hebert**, J.K. Cha, A.R. Brash, H.B. Schlegel

COMP **271.** Mutational analysis of A1-domain interface residues that enhance the binding affinity of A2-domain of the blood coagulation factor VIIIa: A computational binding free-energy study. S. Shearin, **D. Venkateswarlu**

COMP **272.** Targeting viral receptors using binding free energy-based virtual screening and GPU-accelerated software. **B. Zhang**, D. Kilburg, R.P. Murelli, R.M. Levy, E. Gallicchio

COMP **273.** *In silico* approaches to design power conversion efficient organic dyes for dye-sensitized solar cells: Amalgamation of direct QSPR and first principles approach. **J.K. Roy**, S. Kar, J.R. Leszczynski

COMP **274.** Discovery of novel HIV-1 integrase by pharmacophore and structured-based virtual screening. A. Ardakani, **Z. Heidari**, J. Ghasemi

COMP **275.** Structural insight into agonist activity of cannabinoid receptor type-2 ligands using molecular dynamics simulation. **V.K. Yadav**, K.M. Elokely, M.L. Klein

COMP **276.** Investigating the fluorescence mechanism of boron-nitrogen based glucose chemosenors with QM/MM. **F.L. Kearns**, C. Robart, M.T. Kemp, J.D. Larkin, H.L. Woodcock

COMP **277.** Computational investigation of boronic acids with common antioxidant species. **D. Hobbis**, J.D. Larkin

COMP **278.** Computational application of Hartree-Fock theory: characterizing relationships between fundamental atomic properties. **L. VanLaar**, R.L. Dekock

COMP **279.** In silico profiling of activating mutations in cancer. **E.J. Jordan**, R. Radhakrishnan

COMP **280.** Binding of apolipoprotein-based nanoparticles to amyloid beta and the effect on amyloid beta misfolding for the treatment of Alzheimer's disease: a molecular simulation study. **S. Jee**, Y. Kim, S.S. Jang

COMP **281.** Inhibitory mechanism of a fullerene derivative against amyloid-β peptide aggregation: an atomistic simulation study. **Y. Sun**

COMP **282.** Synthesis, spectroscopic characterization, *in vitro* bioactivities, interaction with DNA and DFT study of aliphatic ferrocenyl ureas. **F. Asghar**, A. Badshah, I.S. Butler

COMP **283.** Effective Hamiltonian modeling of molecular water oxidation catalysts with multiple transition metal centers: Highly-scalable studies of catalyst stability for renewable energy applications. **J.R. Buchwald**, V. Meunier, P.H. Dinolfo

COMP **284.** Alchemical computational methodologies for the estimation of binding free energies of supramolecular complexes. **R. Pal**, L.B. Wickstrom, E. Gallicchio

COMP **285.** Luminescence properties of gold and silver nanoparticles. **K.M. Weerawardene**, C.M. Aikens

COMP **286.** Withdrawn.

COMP **287.** Accelerated discovery of high-refractive-index polymers using first-principles modeling, virtual high-throughput screening, and data mining. **M. Afzal**, C. Cheng, J. Hachmann

COMP **288.** Effects of polarization and entropy on crystal polymorph free energies. **E. Dybeck**, N.P. Schieber, M.R. Shirts

COMP **289.** Withdrawn.

COMP **290.** Mechanistic design of chemically diverse polymers with applications on pharmaceutics. **L.I. Mosquera-Giraldo**, C.H. Borca, X. Meng, K.J. Edgar, L.V. Slipchenko, L. Taylor

COMP **291.** Biophysically inspired model for functionalized nanocarrier targeting to live cells. **R. Natesan**, D. Eckmann, P. Ayyaswamy, V. Muzykantov, R. Radhakrishnan

COMP **292.** Comparative study of chemically modified nucleosome core. **K. Chakraborty**

COMP **293.** Combinatorial approach to calculating binding free energies of HIV-RT and clinically relevant mutants using multisite lambda dynamics. **K. Armacost**, C.L. Brooks

COMP **294.** Advanced molecular simulations of reaction mechanisms and complex reaction environments in the methanol to olefins process. **K. De Wispelaere**, V. Van Speybroeck

COMP **295.** Dissociation mechanism for a dimeric photoreceptor protein from multiscale simulation. **H. Ren**, D. Zhong, J. Gao

COMP **296.** Mobility of Cu cations in the zeolite SSZ-13. **F. Goeltl**, A.M. Love, P. Sautet, I. Hermans

COMP **297.** Modeling activation states in the voltage-gated proton channel 1 (Hv1) as a strategy for drug discovery. **E. Gianti**, L. Delemotte, M.L. Klein, V. Carnevale

COMP **298.** Utilization of the AMOEBA force field to predict host-guest binding affinities. **M.L. Laury**, J.W. Ponder

COMP **299.** Molecular dynamics-based exploration of conformational space spanned by variably sulfated chondroitin disaccharides. **B. Nagarajan**, N. Sankaranarayanan, U.R. Desai

COMP **300.** Specific lipid binding sites identified by coarse-grained simulations. **C. Arnarez**, X. Periole, S. Marrink, E. Lyman

COMP **301.** Computational modeling of 2-*O*,3-*O*-desulfated heparin interaction with p300 histone acetyl transferase. **N. Sankaranarayanan**, D. Afosah, J. Voynow, U.R. Desai

COMP **302.** Interface-induced renormalization of electrolyte's energy levels in magnesium batteries. **N. Kumar**, D. Siegel

COMP **303.** Ethanol infiltration into demineralized dentin collagen fibrils via molecular dynamics simulations. **S. Jee**, F.R. Tay, D.H. Pashley, S.S. Jang

COMP **304.** From ionization of small acetylene clusters to the first aromatic ring: A different path for hydrocarbon growth. **T. Stein**, M.P. Head-Gordon, B. Bandyopadhyay, M. Ahmed

COMP **305.** Explanation not simulation: *Ad informatio* approaches to learning chemical principles. **P. Adler**, J. Schrier, A.J. Norquist, S. Friedler

COMP **306.** Predictive QSPR model leading to virtual screening of fullerene derivatives to evaluate key structural attributes critical for photoconversion efficiency as polymer solar cell acceptors. **S. Kar**, N. Sizochenko, L. Ahmed, V.S. Batista, J.R. Leszczynski

COMP **307.** Large-scale complete active space self-consistent field methods. **A.E. DePrince**

COMP **308.** Withdrawn.

COMP **309.** Computer-aided drug design and development of anti-tubercular agents as multi-target inhibitors. **K. Jani**, D. Savjani

COMP **310.** Using projection methods to explore transition metal chemistry. **H.P. Hratchian**

COMP **311.** Heterogeneous structure and dynamics of membranes at the nanoscale. **E. Lyman**

COMP **312.** Towards understanding the self-assembly of peptide-based nanotubes. **M.D. Mayes**

COMP **313.** Characterizing protein hydration to inform its solubility, interactions, and assemblies. E. Xi, R. Remsing, **A. Patel**

COMP **314.** Economic method for selecting high-quality receptor structures for target-based virtual screening. **Z. Huang**, C.F. Wong

COMP **315.** Integrative modeling of pre-initiation complex (PIC) assembles at the core promoter. **C. Yan**, Y. He, I.N. Ivanov, E. Nogales

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

COMP **316.** Assembling macromolecular complexes by evolutionary optimization. G. Tamo, **M. Dal Peraro**

COMP **317.** PB-SAM, a novel solution to the Poisson-Boltzmann equation for applications ranging from protein simulations to polymer membrane design. **L. Felberg**, M. Soniat, D. Brookes, E. Yap, T.L. Head-Gordon

COMP **318.** Scalable polarizable molecular dynamics using Tinker-HP. L. Lagardère, F. Lipparini, B. Stamm, Y. Maday, N. Gresh, G.A. Cisneros, E.G. Kratz, C. Narth, E. Polack, L. Jolly, J.W. Ponder, P. Ren, **J.A. Piquemal**

COMP **319.** Prediction of pKa shift in enzymes using quantum mechanical calculations and thermodynamic integration. **H. Chen**, T. Lee, B.L. Golden, D.M. York

COMP **320.** Development of Markov state models from molecular dynamics simulations: Allostery of PDZ case study. **K. Thayer**, B. Lakhani, D.L. Beveridge

COMP **321.** Quantum mechanical modeling of energy conversion in nanoscale. **Y. Zhang**

COMP **322.** Virtual screening of asymmetric selectivity in catalysis. E. Limé, **P. Norrby**, R. Munday, D. Buttar, S. Tomasi, E.C. Hansen, O. Wiest

COMP **323.** Predicting protein ligandability by quantifying desolvation of the binding sites. **S. Vukovic**, D.J. Huggins

COMP **324.** Computational study of a dinitrogen dicopper(I) complex from reaction of a mixed-valence dicopper hydride. S. Zhang, **H. Fallah**, T.R. Cundari, T.H. Warren

COMP **325.** Theoretical study of the ground and excited state tautomersim in curcumin using DFT based methods. **B.K. Grewal**, D. Ghosh

COMP **326.** Mechanistic investigation of palladium-catalyzed N-C bond formation with DFT methods. **Q. Jiang**, T.R. Cundari

COMP **327.** Accurate prediction of reaction enthalpies using density functional theory: Systematic error corrections via connectivity-based hierarchy (CBH). **A. Sengupta**, K. Raghavachari

COMP **328.** Exploring phase separation and domain formation in lipid bilayers through molecular simulation. **G.A. Pantelopulos**, T. Nagai, J.E. Straub

COMP **329.** Molecular interactions of complex biological systems in rare and orphan diseases. **K. Nguyen**, L. Tian, D. Li, M. March, R. Pellegrino, C. Kao, P. Sleiman, H. Hakonarson

COMP **330.** Virtual high-throughput screening methods testing at the small molecule screening facility of the University of Wisconsin-Madison. **S.S. Ericksen**, H. Wu, S.A. Wildman, F. . Hoffmann

COMP **331.** Transition tempered metadynamics and transition path sampling of ATP hydrolysis in actin filaments. **O. Sode**, R. Sun, S. Lee, G.A. Voth

Section A

Loews Philadelphia Downtown
Millennium Hall

The Chemical Computing Group Excellence Award for Graduate Students

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **332.** Optimal point charge approximation, from 3-atom water molecule to million-atom chromatin fiber. **S. Izadi**, R. Anandakrishnan, A.V. Onufriev

COMP **333.** Design of new theoretical and computational methods through the development of computer algebra systems. **C.H. Hector**, J.V. Ortiz

COMP **334.** Multiscale approach to designing drug-specific nanocarriers for anticancer drug delivery. **W. Jiang**, X. Wang, S. Nangia

COMP **335.** Predictive sampling of long-timescale protein functional motions in explicit solvent. **X. Li**, C. Lu, W. Yang

COMP **336.** Digging deep: A combined SAPT and NBO study towards the fundamental origin of CH...X^- and NH...X– interactions in receptor–anion complexes. **A. Sengupta**, A.H. Flood, K. Raghavachari, Y. Liu

Section A

Pennsylvania Convention Center
Hall E

Wiley Computers in Chemistry Outstanding Postdoc Award

K. N. Kirschner, *Organizer*

6:00 - 8:00

COMP **337.** Odd order dispersion interactions in the effective fragment potential method. **E. Guidez**, M.S. Gordon

COMP **338.** Polarizable force field for DNA and RNA based on the classical drude oscillator model. **J.A. Lemkul**, A.D. Mackerell

WEDNESDAY MORNING

Section A

Sonesta Philadelphia Downtown
Whistler B

Drug Discovery

Modeling ADME & Development Endpoints

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

H. S. Hayatshahi, *Presiding*

8:30 COMP **339.** Studying the interaction of cocaine with ceramide: insights into the blood brain barrier. **R.J. Gillams**, S.K. Callear, S.E. McLain

9:00 COMP **340.** Increasing the probability of success of hit series with *in silico* ADME profiles. **J. Sanders**, D.C. Beshore, T. Bueters, J.C. Culberson, J. Fells, H. Gunaydin, A. Haidle, J. Imbriglio, E. Joshi, B.E. Mattioni, K. Menzel, A. Rusinko, N. Sciammetta, R.P. Sheridan, A. Verras, A.M. Walji

9:30 COMP **341.** QSAR modeling of hERG inhibitors using a mix and match approach. **A. Zakharov**, N.J. Martinez, T. Zhao, D. Nguyen, N. Southall

10:00 Intermission.

10:15 COMP **342.** Using descriptors to address ADME/Tox challenges in peptide-based drug discovery. **A.S. Bayden**, J. Audie, J. Swanson, M. Jarosinski, D.J. Diller

10:45 COMP **343.** Computational support of process chemistry at Merck. **E.C. Sherer**

11:15 COMP **344.** Repeat manager as the bridge between data processing and data reporting. **S.E. Miller**, J. Feng, S. Arnstein, L. Wang

Section B

Sonesta Philadelphia Downtown
Whistler A

Molecular Mechanics

M. Feig, *Organizer*

V. K. Yadav, *Presiding*

8:30 COMP **345.** Adventures in the world of lipids: Towards the routine simulation of complex membranes and membrane bound proteins. **R.C. Walker**, B. Madej, C. Lin, C. Dickson, A. Skjevik, L. Yang, I.R. Gould

9:00 COMP **346.** Computational investigation of domain registration of membrane rafts. **N. Chen**, P.B. Moore

9:30 COMP **347.** Molecular modeling of structure and dynamics of K-Ras at a lipid membrane containing PIP_2. **Z. Li**, M. Buck

10:00 COMP **348.** Exploring the role of solvation in ion channel folding. **D. Granata**, P. Po, M.L. Klein, C. Deutsch, V. Carnevale

10:30 Intermission.

10:45 COMP 349. Weighted ensemble method reveals the *I-V* relationships in a K^+ ion channel. **S. Capponi**, J.L. Adelman, J.M. Rosenberg, M. Grabe

11:15 COMP **350.** pH-dependent mechanism of the M2 proton channel revealed by constant pH molecular dynamics. **W. Chen**, J. Shen

11:45 COMP **351.** Simulations of homo-oligomeric ion channels embedded within a lipid membrane. T.H. Nguyen, C. Moore, Z. Liu, **P.B. Moore**

Section C

Sonesta Philadelphia Downtown
Warhol

Material Science

H. L. Woodcock, *Organizer*

N. Kumar, *Presiding*

8:30 COMP **352.** Modeling materials and charge transfer for lithium-ion batteries. **L. Raguette**, R. Jorn

9:00 COMP **353.** Charge transport mechanisms in solid phase redox end members: S and Li_2S. **N. Kumar**, H. Park, D. Siegel

9:30 COMP **354.** Ab initio study of charge carrier dynamics in polyoxotitanate clusters and fullerene-like polyoxotitanium cage. **D. Vogel**, D. Kilin

10:00 Intermission.

10:20 COMP **355.** Ab initio study of charge carrier dynamics and fragmentation of gas–phase lanthanum cyclopentadienyl complexes. **Y. Han**, Q. Meng, B. Rasulev, P.S. May, M.T. Berry, **D. Kilin**

10:50 COMP **356.** Virtual screening and evaluation of highly efficient organometallic light-emitting materials. **S. Kwak**, D.J. Giesen, T.F. Hughes, Y. Cao, A. Goldberg, J. Gavartin, S. Dixon, M. Halls

11:20 COMP **357.** Electron dynamics at metal-organic interfaces: Triplet and singlet excitons. S. Zhang, **M. Pavanello**

‡ *Cooperative Cosponsorship*

Section D

Sonesta Philadelphia Downtown
Benton

Computational Study of Water

Methods & Biological Applications

D. J. Sindhikara, *Organizer*

R. Remsing, *Presiding*

8:30 COMP **358.** Improved generalized born water model for MD simulations of proteins and nucleic acids. **C.L. Simmerling**, H. Nguyen, K. Kasavajhala, H. Huang, K. Lam

9:00 COMP **359.** Recent applications of the WaterMap methodology to binding energy prediction and thermodynamic analysis of biomolecular recognition. **W. Sherman**

9:30 COMP **360.** Frustrated water networks on protein active site surfaces. **K. Haider**, M.K. Gilson, T.P. Kurtzman

10:00 Intermission.

10:15 COMP **361.** Water in dopamine receptors: Using solvation thermodynamics to modify a lead compound for specificity. **S. Ramsey**, T.P. Kurtzman, W. Harding, I.L. Alberts

10:45 COMP **362.** Making a splash in implicit solvent: Application of inhomogeneous solvation theory and continuum solvation to host-guest binding affinity predictions. **L.B. Wickstrom**, R. Pal, K. Haider, J. Xia, W. Flynn, T.P. Kurtzman, R.M. Levy, E. Gallicchio

11:15 COMP **363.** Bridging disparate levels of theory in free energy simulation using non-equilibrium work. **P.S. Hudson**, H.L. Woodcock, S. Boresch

Section E

Sonesta Philadelphia Downtown
Wyeth Gallery C

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

Cosponsored by PHYS

J. Gao, W. Yang, *Organizers*

J. Pu, *Organizer*, *Presiding*

8:30 COMP **364.** Toward quantitative understanding of how ABC-transporters hydrolyze ATP: Development of the reaction path force matching QM/MM method. **J. Pu**

9:00 COMP **365.** New methodological developments for the study of enzymatic chemical reactions. **I. Tuñon**

9:30 COMP **366.** MIMIC: A new multiscale interface for first-principles molecular dynamics. **U. Rothlisberger**

10:00 Intermission.

10:15 COMP **367.** New approaches to QM/MM: Anchor points reactive potentials and system-specific molecular mechanics with semiglobal internal coordinates and electrostatic screening. **D.G. Truhlar**, K.R. Yang, X. Xu, J. Zheng, S.L. Li, B. Wang

10:45 COMP **368.** Recent advances in QM/MM simulations of enzymatic reactions. **W. Thiel**

11:15 COMP **369.** Development and acceleration of multiscale QM/MM methods for simulations of complex biomolecular systems. **K. Nam**

Advanced Potential Energy Surfaces

Applications of Advanced Potential Energy Models & Methods

Sponsored by PHYS, Cosponsored by COMP

Computational Chemistry & Toxicology in Chemical Discovery & Assessment (QSARs)

Sponsored by AGRO, Cosponsored by COMP, ENVR and TOXI

WEDNESDAY AFTERNOON

Section A

Sonesta Philadelphia Downtown
Whistler B

Drug Discovery

Hybrid Methods in Computer-Aided Drug Design

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

L. Ahmed, *Presiding*

1:30 COMP **370.** Data-driven design of kinase inhibitors with controlled polypharmacology. C. Da, M. Stashko, S.V. Frye, X. Wang, **D. Kireev**

2:00 COMP **371.** Imbalance in chemical space: How to facilitate the identification of protein-protein interaction inhibitors. **M.A. Kuenemann**, C.M. Labbe, A. Cerdan, O. Sperandio

2:30 COMP **372.** Optimizing Surrogate AutoShim: Fast and accurate target-customized docking without a protein structure. **E.J. Martin**, B. Samudio

3:00 Intermission.

3:15 COMP **373.** Novelty score: Prioritising compounds that potentially form novel protein-ligand interactions and novel scaffolds using an interaction centric approach. **H.J. Patel**, G.M. Morris

3:45 COMP **374.** Whole-protein (holistic) scoring scheme for virtual screening achieves higher success rates than single-site scoring. S. Dadgar, D. Tesolin, R. Kamstra, **W.B. Floriano**

4:15 COMP **375.** Structural informatics modeling, drug discovery, and pharmacophore elucidation of novel synergy-based inhibitors for drug resistant bacterial infection. **J.H. Nettles**, E.K. Crispell, S. Chennamadhavuni, J.P. Snyder, D. Liotta, D.S. Weiss

Section B

Sonesta Philadelphia Downtown
Whistler A

Molecular Mechanics

M. Feig, *Organizer*

L. Raguette, *Presiding*

1:30 COMP **376.** Solving the macrocycle problem in silico. **D.J. Sindhikara**, T. Day, K. Borrelli

2:00 COMP **377.** Predicting PPI druggability using mixed-solvent simulations. **P. Ghanakota**, D. Lupyan, K.J. Lumb, H. Van Vlijmen, W. Sherman, T. Beuming

2:30 COMP **378.** Exploring protein-protein interactions using the site-identification by ligand competitive saturation (SILCS) method. **W. Yu**, A.D. Mackerell

3:00 COMP **379.** Computing absolute binding free energies for host-guest complexes. **F. Tofoleanu**, B. Brooks

3:30 Intermission.

3:45 COMP **380.** What makes enzymes work? Exploring life in *P-T-X*. **T. Ichiye**

4:15 COMP **381.** Conformational flexibility and ligand binding in *NiRE* SAM-dependent methyltransferase: A molecular dynamics study. **T. Karabencheva-Christova**, W. Singh, C. Christov

4:45 COMP **382.** Identification of a human thiol receptor highly responsive to thiols in the presence of Cu(I) and Ag(I) ions: QM/MM and mutagenesis studies. **L. Ahmed**, S. Li, R. Zhang, Y. Pan, H. Matsunami, E. Block, H. Zhuang, V.S. Batista

Section C

Sonesta Philadelphia Downtown
Warhol

Material Science

H. L. Woodcock, *Organizer*

J. E. Bates, *Presiding*

1:30 COMP **383.** Computational efforts to probe PEO-PS diblock copolymer assemblies. **K. Chakraborty**

1:50 COMP **384.** Impact of amorphous environment on the melting temperature of polyethylene envisioned by fine-grained simulation. **A. Shamloo**

2:10 COMP **385.** Computational design of di- and tripeptide aggregates. **S. Mushnoori**, M. Dutt

2:30 Intermission.

2:50 COMP **386.** Multicomponent diffusion of penetrant, solvent, and rubbery polymer ternary mixtures. **S.A. Bringuier**, M.J. Varady, T.P. Pearl, J.B. Cabalo, C.K. Knox, **B.A. Mantooth**

3:10 COMP **387.** Probing hydrogen-bonding and steric effects on multicomponent diffusion of small organic penetrants through solvated polyurethane and polyhydroxyurethane. **C.K. Knox**, J.B. Cabalo, M. Varady, S.A. Bringuier, T.P. Pearl, R. Lambeth, B.A. Mantooth

3:30 COMP **388.** Computational design of amphiphile-based nanoparticles. **X. Yu**, M. Dutt

3:50 COMP **389.** Predictive mix-QSAR modeling of antifouling surface coating systems containing quaternary ammonium salts. **F. Jabeen**, B. Rasulev, M. Ossowski, P.R. Boudjouk

Section D

Sonesta Philadelphia Downtown
Benton

Computational Study of Water

Models, Properties & Phenomena

D. J. Sindhikara, *Organizer*

P. S. Hudson, *Presiding*

1:30 COMP **390.** Timescale separation between energy contributions in the effective fragment potential. **C.H. Borca**, L.V. Slipchenko

2:00 COMP **391.** Electronically coarse grained model for water predicts water's signature properties from supercooled water to ice to the supercritical regime. **G.J. Martyna**

2:30 COMP **392.** Dissecting hydrophobic and ionic hydration. **R. Remsing**

3:00 Intermission.

3:15 COMP **393.** Activity coefficients of tetra-n-butyl ammonium chloride at varying concentrations and temperatures calculated using molecular dynamics simulations. R.L. Napoleon, R. Wigent, **P.B. Moore**

3:45 COMP **394.** Surface tension of NaCl solution: Molecular dynamics simulation on the concentration and temperature dependence. **X. Wang**, H. Su, U. Pöschl, Y. Cheng

4:15 COMP **395.** Neutralization of water self-ions via 3D H-bond networks vs. 1D H-bond wires: a Lewis study. **J. Herzfeld**, C. Bai

Section E

Sonesta Philadelphia Downtown
Wyeth Gallery C

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

Cosponsored by PHYS

J. Gao, J. Pu, W. Yang, *Organizers*

G. S. Kedziora, *Presiding*

1:30 COMP **396.** Investigation of RNase A 2'-O-transesterfication mechanisms via a series of 1D, 2D and 3D QM/MM simulations. **M. Huang**, T.D. Dissanayake, D.M. York

2:00 COMP **397.** Quantum mechanics on the fly for bond breaking in molecular dynamics simulation of strained polymers. **G.S. Kedziora**, S. Barr, J. Moller, G. Leuty, R. Berry, T. Breitzman

2:30 COMP **398.** Investigation of the reaction mechanism of the twister ribozyme supports a new twist on general acid catalysis. **C. Gaines**, D.M. York

Advanced Potential Energy Surfaces

MM from QM

Sponsored by PHYS, Cosponsored by COMP

Computational Chemistry & Toxicology in Chemical Discovery & Assessment (QSARs)

Sponsored by AGRO, Cosponsored by COMP, ENVR and TOXI

THURSDAY MORNING

Section A

Sonesta Philadelphia Downtown
Whistler B

Drug Discovery

Consider the Data

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

E. Gianti, *Presiding*

8:30 COMP **399.** Avoiding missed opportunities by analysing the sensitivity of our decisions. M. Segall, I. Yusof, E. Champness, **P. Hunt**

9:00 COMP **400.** 3D-RISM driven method to establish the complete solvent site structure in macromolecular crystallographic refinement: Implications for structure based drug design. **O. Borbulevych**, L. Westerhoff

9:30 COMP **401.** Optimal decomposition of hydrogen-bonded water clusters for drug design. **E. Gianti**, R.J. Zauhar, M.L. Klein, G. Fiorin

Section B

Sonesta Philadelphia Downtown
Whistler A

Molecular Mechanics

M. Feig, *Organizer*

F. L. Kearns, *Presiding*

8:30 COMP **402.** Withdrawn.

9:00 COMP **403.** Inferring perturbed Markov state model kinetics upon thermodynamic reweighting. **V.A. Voelz**, G. Zhou, H. Wan

9:30 COMP **404.** Efficient molecular dynamics of biomolecules using a swarm-enhanced sampling scheme. **R.A. Bryce**

10:00 Intermission.

10:15 COMP **405.** Mixing machine learning with experiment: Nonlinear learning of assembly landscapes and mechanisms from particle tracking data. A. Long, J. Zhang, S. Granick, **A. Ferguson**

10:45 COMP **406.** Correlation analysis of molecular dynamics simulation: Beyond the assumption of stationarity. **K. Ho**, D. Hamelberg

11:15 COMP **407.** Compression of molecular dynamics (MD) simulation trajectories using wavelet transform. **Z. Heidari**, D.R. Roe, C. Bergonzo, J. Ghasemi, T.E. Cheatham

Section C

Sonesta Philadelphia Downtown
Warhol

Material Science

H. L. Woodcock, *Organizer*

K. R. Yang, *Presiding*

8:30 COMP **408.** π–Stacking pancake bonding: computational challenges. **M. Kertesz**, Z. Mou

9:00 COMP **409.** Quantum chemical study of electronic coupling in carbon nanostructures. **M. Kim**, J. Klos, M.H. Alexander, Y. Wang

9:30 COMP **410.** Correlated calculations of magnetic and optical properties of trigonal zigzag graphene nanodisks. **H. Chakraborty**, A. Shukla

10:00 Intermission.

10:20 COMP **411.** Fingerprint functions and graph theory as complimentary techniques for high-throughput crystal structure comparison. **K. Ryan**, M. Shatruk, M. Mustyakimov

10:40 COMP **412.** Hierarchical multiscale simulation of materials: Application to Taylor Anvil and Steven impact tests of RDX. **B.C. Barnes**, K. Leiter, R. Becker, J. Knap, J.K. Brennan

11:00 COMP **413.** Withdrawn.

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

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ENFL

Division of Energy and Fuels

X. Wang and D. Heldebrant, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

CO_2 Reduction: Electrocatalysis (see *CATL*, Wed)

Catalysts & Catalytic Technologies for Conversion of Biomass & Its Derivatives (see *CATL*, Mon, Tue, Wed)

Applied Catalysis for Environmental Applications (see ENVR, Tue, Wed)

Chemistry of Biomass Wastes Conversion to Energy & Chemicals (see *ENVR*, Tue, Wed)

Nanoparticles: Synthesis, Characterization & Their Application in Catalysis (see *COLL*, Sun, Mon)

Chemistry of Materials: Nanomaterials (see *INOR*, Sun, Tue)

SOCIAL EVENTS:

ENFL Business/Social Hour, 12:00 PM: Mon

ENFL Dinner (Tickets Required), 6:00 PM: Tue

BUSINESS MEETINGS:

ENFL Program & Executive Committee Meeting, 3:00 PM: Sun

SUNDAY MORNING

Section A

Pennsylvania Convention Center
Room 108B

USA-China Symposium on Energy

Cosponsored by ENVR

Y. H. Hu, *Organizer*

F. Jin, *Organizer*, *Presiding*

Q. Li, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **1.** Effect of interfacial interaction on catalytic and electrochemical reduction of CO_2. **Q. Ge**

9:10 ENFL **2.** New strategy for highly efficient CO_2 reduction by water spilling with solar biomass energy-driven two-step process. G. Yao, **F. Jin**

9:45 ENFL **3.** Modified Chou Model for negative temperature dependence in the hydrogenation of hydrogen storage materials. **H. Long**, **Q. Li**

10:05 Intermission.

10:15 ENFL **4.** Shape and surface engineering of monodisperse nanocrystals for photocatalysis and electrocatalysis. **C.B. Murray**, M. Cargnello, S. Zhang, V.V. Doane-Nguyen, T.R. Gordon, M. Cui, H. Yun, J. Luo, S. Najmr, P. Fornasiero, R.J. Gorte

10:50 ENFL **5.** Integration of carbon capture and subsequent conversion. **L. He**

11:25 ENFL **6.** Novel method for converting carbon dioxide into carbon under mild conditions. **Y. Chen**, Z. Jing

11:45 ENFL **7.** Reduction of CO_2 into HCOOH with 2-pyrrolidinone under hydrothermal conditions. **Y. Yang**, F. Jin

12:05 Concluding Remarks.

Section B

Pennsylvania Convention Center
Room 108A

Water-Energy Nexus

Cosponsored by ENVR and MPPG

D. Shuai, W. Zhang, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **8.** Effect of operating parameters in a high rate activated sludge A-stage system on carbon capture for methane production. **M. Kinyua**, W. Thomas, M. Elliott, B. Wett, S. Murphy, K. Chandran, C. Bott

9:05 ENFL **9.** Highly active Pt-Ni and Ni catalysts for catalyzing the decomposition of hydrogen iodide, as part of the sulfur iodine cycle for hydrogen production from water. A. Singhania, A.N. Bhaskarwar, **V.V. Krishnan**, D. Parvatalu

9:35 ENFL **10.** Photoelectrochemical hydrogen generation using multi-band III-nitride nanowire arrays. **H.P. Nguyen**

10:05 Intermission.

10:20 ENFL **11.** Probing nanoscale characteristics of hydrophilized polyethersulfone membranes. **W. Fu**, S. Mitra, W. Zhang

10:50 ENFL **12.** Fabrication of Cu/Ti nanoelectrode for electrochemical denitrification of groundwater. **M. Li**, X. Liu

11:20 ENFL **13.** Enhanced desalination and kinetics using cyclopentane hydrates in water-in-oil emulsions. **L. Yining**, G. Jing, G. Chen

11:50 Concluding Remarks.

Section C

Pennsylvania Convention Center
Room 113A

Unconventional Energy on Heavy Oil & Shale Gas

Cosponsored by ENVR and MPPG

E. Hensen, *Organizer*

B. Shen, Z. Wu, *Organizers*, *Presiding*

F. Xiao, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **14.** Light olefin synthesis from shale gas feedstock by catalytic routes. **A. Bhan**

9:10 ENFL **15.** Hollow zeolite encapsulated Ni-Pt bimetals for sintering and coking resistant dry reforming of methane. **X. Guo**

9:40 ENFL **16.** Nanoscale design of bifunctional catalysts and its impact on hydroconversion. **J. Zecevic**, G. Vanbutsele, K. De Jong, J. Martens

10:10 ENFL **17.** Demineralization pathways for oil shale semicoke byproduct conversion to a sorbent material. **A. Suleimenov**, **J.L. Goldfarb**

10:30 Intermission.

10:40 ENFL **18.** Engineering the H_2S splitting cycle for oil sands bitumen upgrading: Can we recover hydrogen from H_2S too? **H. Wang**, W. Zhang, M. Liang, A. Moniri

11:15 ENFL **19.** Controllable synthesis of ZSM-5/EU-1 co-crystalline zeolite. L. Sun, Y. Zhang, **Y. Gong**

11:45 ENFL **20.** Infulence of pore sructure of the zeolite USY on catalytic cracking of Jatropha Curcasl oil. **Q. Zheng**, B. Shen

12:05 ENFL **21.** Preparation a shape-selective zeolite material and its application in heavy oil catalytic cracking. **P. Zeng**

Section D

Pennsylvania Convention Center
Room 109B

Degradation of Materials for Energy & Fuel Production

Cosponsored by ENVR and MPPG

S. Nair, *Organizer*

J. Baltrusaitis, Z. Wu, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **22.** Controlled synthesis of sintering-resistant catalysts through nanostructured materials. **S. Dai**

9:10 ENFL **23.** Strategies for protecting the active site in chemical conversion on Ni-CeO_x catalysts: Insights from *in-situ* studies over models and powders. **S.D. Senanayake**, Z. Liu, D. Grinter, D. Vovchok, C. Guild, S.L. Suib, J. Rodriguez

9:45 ENFL **24.** Cascade aldolization and self-deoxygenation over $Zn_xZr_yO_z$ mixed oxides: The effect of surface acidity on the catalyst deactivation. **J. Sun**, R. Baylon, D. Mei, K.J. Martin, P. Venkitasubramanian, Y. Wang

10:20 Intermission.

10:30 ENFL **25.** *Operando* IR investigations on catalysts for fuel synthesis and conversion: Reaction mechanisms and deactivation. **M. Daturi**, P. Bazin, O. Marie, A. Roger, S. Thomas

11:05 ENFL **26.** Assessing deactivation processes of supported vanadium oxide catalysts at a molecular-level; an *operando* Raman methodology approach. M.V. Martínez-Huerta, M. Guerrero-Perez, **M.A. Banares**

11:40 ENFL **27.** Formation of platinum oxide films on the surface of platinum nanoparticles during propane oxidation. **C. O'Brien**, G. Jenness, D.G. Vlachos, I. Lee

12:00 ENFL **28.** Effect of surface structure on CO_2 adsorption on TiO_2 nanoparticles: Experimental and theoretical investigations. U. Tumuluri, J. Howe, W. Mounfield, M. Li, K. Walton, D. Sholl, S. Dai, **Z. Wu**

Section E

Pennsylvania Convention Center
Room 107B

Solar Fuels: Power to the People

Cosponsored by ENVR and MPPG

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

Y. Ng, H. Wang, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **29.** Exciton dissociation and plasmon induced hot electron transfer in semiconductor/metal quantum rod heterostructure. **T. Lian**

9:05 ENFL **30.** Plasmonic metal-semiconductor heterojunctions for solar energy conversion. **N. Wu**, S. Cushing, J. Li, D. Chu

9:35 ENFL **31.** Co/TiO_2 catalysts for photocatalytic CO_2 reforming of methane. **W. Wei**, Y.H. Hu

9:55 Intermission.

10:05 ENFL **32.** On establishing a consortium to print polymer photovoltaic cells. **A. Holmes**