

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 Withdrawn.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 Cu²⁺ bound to phosphatidylethanolamine. A.M. Sendeck, 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. Uljin, 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 biomolecular 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-LDAO: 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. Provorso, X.S. Vazquez, J. Milaneso, C. Isborn

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

11:45 COMP 19. Using agent-based modeling to bridge 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 IC₅₀ 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. Devisio

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. Wachter, 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

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. Ichiiye**

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. Goldberg, 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. Haghghatari, 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. Jabene, 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 CO₂ 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 CINP, 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. Plunova, 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 tyrosyl-protein 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. Devoio

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. Mackereil

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

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. Jörn
- 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-microhertz 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. Gendeleev, 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. Fraczekiewicz, 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. Strącz, 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. Mukhopadhyay, 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. Tywoniuik, 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 GeO₂ energetics: A dispersion-corrected DFT study. A. Abbaspour Tamijani

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- 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 MoS₂ 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. Cleaves**
- 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**

Technical program information known at press time.

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

- 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**

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 Al³⁺/Fe³⁺ 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. Shama**
- 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. Amarez, 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 gelling-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**

- COMP 227.** Computer aided discoveries: Predictive modeling for polymers, coating systems and drug like molecules. **F. Jabeen, M. Ossowski, P.R. Boujdjouk**
- 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. Wujiak, 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. Matsuubara**
- COMP 253.** Unique mechanistic characteristics of the *glnS* 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 $\beta_{2\text{-adrenergic}}$ receptor ($\beta_2\text{-AR}$) 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 + $\text{CH}_3\text{CN} \rightarrow \text{HF} + \text{CH}_2\text{CN}$ 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. Gencckakir, 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 ($\text{R} = \text{C}_6\text{H}_5$, $\text{C}_6\text{H}_4\text{CH}_3$, $\text{C}_6\text{H}_4\text{NH}_2$, $\text{C}_6\text{H}_4\text{OH}$, and $\text{C}_6\text{H}_4\text{F}$): 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 oxallyl 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 structure-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. Elkely, M.L. Klein**
- COMP 276.** Investigating the fluorescence mechanism of boron-nitrogen based glucose chemosensors 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 pharmaceuticals. **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. Muzykantor, 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**

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

- 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. Arnez**, X. Periole, S. Marrink, E. Lyman
- COMP 301.** Computational modeling of 2-O,3-O-desulfated heparin interaction with p300 histone acetyltransferase. **N. Sankaranarayanan**, D. Afosah, J. Voinow, 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 informatico* 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) assemblies at the core promoter. **C. Yan**, Y. He, I.N. Ivanov, E. Nogales
- 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: Allosteric 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 tautomers 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. Paterlopoulos**, 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
- 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. Culbertson, 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 PIP₂. **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. Deusch, 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. Jörn

9:00 COMP 353. Charge transport mechanisms in solid phase redox end members: S and Li₂S. **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

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

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-cus-tomized 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. Beumung

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. Boucjouk

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-transesterification 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. Yusuf, 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. Borbuluych, 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 complementary 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

‡ Cooperative Sponsorship

ENFL

Division of Energy and Fuels

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

OTHER SYMPOSIA OF INTEREST:

CO₂ 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 CO₂. Q. Ge

9:10 ENFL 2. New strategy for highly efficient CO₂ 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 CO₂ 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. Singhan, 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 bimetal 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 H₂S splitting cycle for oil sands bitumen upgrading: Can we recover hydrogen from H₂S 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. Influence of pore structure of the zeolite USY on catalytic cracking of Jatropha Curcas 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,Zr₂O₇ mixed oxides: The effect of surface acidity on the catalyst deactivation. J. Sun, R. Baylon, D. Mei, K.J. Martin, P. Venkatasubramanian, 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. Martinez-Huerta, M. Guerrero-Perez, M.A. Baneres

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 CO₂ adsorption on TiO₂ 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/TiO₂ catalysts for photocatalytic CO₂ 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