Section F
Pennsylvania Convention Center
Room 123
Basic Research in Colloids, Surfactants & Nanomaterials

Nanomaterial Applications
R. Nagarajan, Organizer
Y. Mao, Presiding
8:30 COL 584. Preparation, growth mechanism and uses of one-dimensional nanostructures. S. Hunyadi Murph
8:50 COL 585. Bio-inspired synthetic giant clam system for solar energy applications. H. Kim, S. Vahidnia, A. Holt, A. Sweeney, S. Yang
9:10 COL 586. Tunable optical properties of 2D nanowire lattices. S.J. Boehm, L. Kang, D. Warner, C.D. Keating
9:30 COL 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 COL 588. Hydrogen storage by nanostructured graphene and metal hybrids enhanced with spill-over mechanism. Y. Mao, L. Wei
11:30 COL 593. Withdrawn.
12:30 COL 596. Polymer Science at the Interface of Industry, Government & Academics

Section G
Pennsylvania Convention Center
Room 112
Basic Research in Colloids, Surfactants & Nanomaterials

Bio-Nano Materials
R. Nagarajan, Organizer
S. A. Claridge, Presiding
8:30 COL 595. Self-assembling extra-cellular matrix proteins as materials for the condensation of silica nanostructures. C.M. Gomes, L.F. Deravi
8:50 COL 596. Study of in vivo efficiencies of antibody dependent cell cytotoxicity of antibody functionalized gold nanoparticles. M. Ahmed
9:10 COL 597. Dimensional control of orthogonal chemical interfaces using polymerizable amphiphiles. S.A. Claridge
9:30 COL 598. Thermophilic ferritin: A versatile nanocarrier for the encapsulation of nanoparticles and other useful cargo. K.W. Pulipher, I.J. Dmochowski
10:10 COL 600. Toward single-molecule biophysical surface-enhanced Raman spectroscopy with nanostar-liposomes biocongjugates. W. Lum, I. Brazis, L. Sajge
10:50 COL 602. Increased oxidation in lipid membranes from Cu(II) bound to phosphatidylthanolamine. A.M. Sendeski, M.F. Poyton, X. Cong, P.S. Cremer

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 & Solution in Biochemistry: Developments & Applications
Co-sponsored 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. Solution 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 solution into statistical machine learning approaches for the quantitative modeling of protein-DNA binding affinities. I. Chu, R. Rohs
10:45 COMP 5. Quantifying uncertainty in biomolecular simulation. N.A. Baker, H. Lei, X. Yang, G. Wei

Section B
Sonesta Philadelphia Downtown
Hopper
Designing Functional Biomaterials: Connecting Experiment with Theory & Simulation
Co-sponsored 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 structured polypeptides. R.S. Tu
10:10 Intermission.
10:55 COMP 10. Using theory and computation to guide the design of proteins, protein assemblies, and bimolecular materials. J.G. Savin

Section C
Sonesta Philadelphia Downtown
Warhol
Quantum Mechanics
Co-sponsored by PHYS

S. E. Wheeler, Organizer
R. Bhattacharjee, Presiding
8:30 COMP 12. Self-consistent implementation of meta-GGA exchange-correlation functional within the ONETEP linear-scaling DFT code. J.C. Womack, M. Skylaris
9:00 COMP 13. CAM-LDA4: The reincarnation of the local density approximation. C.H. Borca, M.A. Mosquera, M.A. Rainier, G. Schatz
10:00 Intermission.
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 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. Shelt, Organizer, Presiding
8:30 Introductory Remarks.
9:45 COMP 22. Profile-QSAR Gen 2: Deep learning mechanism IC50 predictions for novel compounds as accurate as 4-pIC50s. 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. Atal, J. Hiatt
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
Whistler B
Drug Discovery

Case Studies in SBDD

M. R. Landon, Y. Tseng, Organizers
S. K. Lakkaraju, Presiding
8:30 COMP 26. HDAC as the central hub of the signaling network for activation loop autophosphorylation in Abl kinase. G. L. Sala, L. Riccardi, R. Gaspari, A. Cavalli, C. Hantschel, M. Devivo
9:00 COMP 27. Comparative analysis of the structural determinants of endogenous cannabinoids. V.K. Yadav, K.M. Elskiey, M.I. Klein
9:30 COMP 28. Structural basis for antagonist selectivity in orexin receptors. K. Babaoglu
10:00 Intermission.
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. Jing, 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. Morz
3:15 COMP 91. Electrostatics and binding properties of G-protein coupled receptors. R. Abagyan, I. Kuterava

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. Haritazadeh, Presiding
1:30 COMP 93. Protein assemblies by design. V.P. Conticello
2:30 COMP 95. New class of highly stable and self-repairing membrane-mimetic 2D materials assembled from lipid-like peptides. C. Chen
3:00 Intermission.
3:15 COMP 96. Peptoid nanosheets exhibit a new secondary-structure motif. R. Mannig
3:45 COMP 97. Grafted polymer layers for biomaterials. L.A. Lubov
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. Gathala, B. Boykin, B. Caceras, J. Hevel
2:00 COMP 100. Computational modelling structure-function relationships of tyrosyl-protein sulfotransferase. C. Chrstov, T. Karabenchova-Chrstova, W. Singh
2:30 COMP 101. Temperature effects on the dynamics of light harvesting complex II. Y. Wang, Y. Wang, 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. Gaspar, M. Dal Peraro, M. Devio
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. Hayashitani, T.E. Cheatham
4:15 COMP 104. Delineting ion modulated conformational changes in ribosomal RNA using grand-canonical Monte-Carlo/molecular dynamics simulations. S.K. Lakaranau, J.A. Lennki, A.D. Mackern
4:45 COMP 105. Molecular dynamics studies of the effects of histone variant on nucleosome dynamics. J. Wereszczynski

Section D
Sonesta Philadelphia Downtown Bantam
Sharing Pharmaceutical Industry Data: Outlook & Opportunities
B. Sherborne, Organizer, Presiding
1:30 Introductory Remarks.
2:30 COMP 107. Developing a community resource for the under-studied kinome. T.M. Wilson
2:50 COMP 108. Advancing quantitative biophysical predictions: What can be gained from industry-academic data sharing? J.D. Chodera
4:00 Panel Discussion.

MONDAY EVENING

Section A
Pennsylvania Convention Center Halls D/E
Sci-Mix
H. L. Woodcock, Organizer
8:00 - 10:00

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

Sponsored by PHYS, Cosponsored by COMP

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 SODE
Section C  Sonesta Philadelphia Downtown  Warhol
Quantum Mechanics  Co-sponsored 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 intramolecular 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 H-H-H system at the sub-micro-hartree 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.
9:05  COMP 137. Decoding polypharmacology from phenotypic screens. N.M. McCarron, L. Gandeto, D. Kolek, M. Keiser
10:05 Intermission.
10:20  COMP 139. Application of polypharmacology in daily research project work. M. Bieler
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  Co-sponsored 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.
10:45  COMP 146. Withdrawn.

Advanced Potential Energy Surfaces Ab initio Molecular Dynamics  Co-sponsored by PHYS, Co-sponsored by COMP
8:30  COMP 148. Evaluation of the virtual screening performance and core-hopping potential of common pharmacophore hypotheses derived from phase’s screening performance and core-hopping for charge transfer processes. J. Gao
10:15  COMP 149. In silico design of 3-beta-secretase 1 (BACE1) inhibitors. R. Fraczewicz, D. Miller, M.S. Lawless, R.D. Clark
2:00  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
3:45  COMP 152. Marvin Live: An integrated tool for knowledge-driven/ information rich live design sessions. A. Stracz, A. Costache

Section B  Sonesta Philadelphia Downtown  Whistler A
Molecular Mechanics  M. Feig, Organizer  N. Chen, Presiding
1:30  COMP 153. Atomic simulation of diblock-like peptides forming membrane-mimetic 2D material. M.D. Blair, C. Chen
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

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 Tamjani

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137-TECH
Section D
Sonesta Philadelphia Downtown
Benton

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. Schroeder
2:30 COMP 168. Kinome wide off-target prediction by mining structural and profiling data. S. Fuller, A. Valkamer, B. Marget, S. Turk, S. Eit, F. Ripmann
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 pain. A. Troshpa, S. Capuzzi
4:15 COMP 171. Understanding cytotoxicity in high-throughput screening collections using an silico polypharmacological prediction protocol. L. Mervin, O. Tao, I. Barret, M. Fitth, D. Murray, D. Engkloft, 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 Co-sponsored by PHS
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. Asche

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


Section A
Pennsylvania Convention Center
Hall E

OpenEye Outstanding Junior Faculty Award in Computational Chemistry
C. L. Simmering, Organizer
6:00 – 8:00

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

COMP 184. Eliciting heterogeneous ice nucleation mechanisms using large scale rare event simulations. S. Sanpria, B. Gatt, P. Det愕or, W. Hanger, L. Ngi, A. Apir

COMP 185. Discovery of reaction mechanisms, catalysts, and materials by new quantum chemical simulation methods. PM. 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. Torrel, D.A. Sarkies, 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. Xia, A. Beugelsdijk, J.D. Schmidt, J. Chen


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 (swEMD). I. Alakby, K.K. Bunusu, N.J. Bruce, P.A. Bryce

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

COMP 193. Modeling the structure and reactivity of Al/Fc substitution in kaolinite. T. Hicks, R.K. Szilagyi

COMP 194. In silico modeling of dopamine transporter and design of novel neuroprotective agents. T. Dijkstra, K. Velec

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

COMP 196. Challenges in generating bioactive small molecule conformations. Y. Yang, B.K. Rai, X.J. Hady


COMP 199. Comparative theoretical study of oxygen adsorption on natural and anionic Ag, and Au, clusters (n = 2 – 25). J.D. Watts, M. Liao, M. Huang

COMP 200. Surplus-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. Wakfeld, V.A. Voelz


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 a resistant strain. Y. Gao

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. Eldajah, 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 211. Identification and statistical analysis of structurally conserved water sites via R. E.K Esposito


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. P. Han, V.A. Voelz

COMP 215. Rationalizing non-standard interactions in ligand design: The duality of halogenos. 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 binding water molecules. J. Guo, S. Collins, T. Miller, R.C. Rizzo

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


COMP 220. Stimulating a low Reynolds number MARTINI. A. Zuporzn, E. Lyman

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

COMP 222. Computation calirimetry. A. Webb, C. Armero, 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 gel-forming mucins. P. Lin, F. Ramezanghorbani, C.M. Colina

COMP 225. Characterization of the binding pocket of FABPs 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. Orlova
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 A
Loeves Philadelphia Downtown
Millennium Hall
The Chemical Computing Group Excellence Award for Graduate Students
C. L. Simmering, Organizer
6:00 - 8:00

Section B
Sonesta Philadelphia Downtown
Whistler A

**Molecular Mechanics**
M. Feig, Organizer
V. K. Yadav, Presiding

**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

9:30 | **COMP 334.** Studying the interaction of cocaine with ceramide: insights into the blood brain barrier.
R. J. Giesen, T. F. Hughes, Y. Cao, J. Shen

10:00 | **COMP 335.** Odd order dispersion interactions in highly accurate density functional theory: new perspectives.
C. Kao, P. Sleiman, H. Hakonarson

10:30 | **COMP 336.** Solvent effects on initial reaction steps of AAAT (ADP/ATP translocase).
D. Granata, A. Sengupta

11:00 | **COMP 337.** Exploring the role of solvation and hydration on the structure and stability of water.
S. Tomasi, E. C. Hansen, O. Wiest

11:30 | **COMP 338.** Exploring the role of solvation and hydration on the structure and stability of water.
S. Tomasi, E. C. Hansen, O. Wiest

12:00 | **COMP 339.** Incorporating solvation effects in quantum chemical calculations: a comprehensive study.
Y. Zhang, W. Chen

**Section C**
Sonesta Philadelphia Downtown
Warhol

**Material Science**
H. L. Woodcock, Organizer
N. Kumar, Presiding

8:30 | **COMP 342.** Modeling materials and charge transfer for lithium-ion batteries:
L. Raguz, R. Jorn

9:00 | **COMP 343.** Charge transport mechanisms in solid phase redox end members: S and Li2S.
N. Kumar, H. Park, D. Siegel

9:30 | **COMP 344.** Ab initio study of charge carrier dynamics in polysulfonate clusters and fullerene-like polyelectrolyte systems.
A. Wang, D. Vostrov, O. C. Martin

10:00 | **COMP 345.** Exploring the role of solvation in ion channel folding.
D. Granata, P. O. Klein, C. Deutsch, V. Carnevale

10:30 | **COMP 346.** Exploring the role of solvation in ion channel folding.
D. Granata, P. O. Klein, C. Deutsch, V. Carnevale

11:00 | **COMP 347.** Exploring the role of solvation in ion channel folding.
D. Granata, P. O. Klein, C. Deutsch, V. Carnevale

11:30 | **COMP 348.** Exploring the role of solvation in ion channel folding.
D. Granata, P. O. Klein, C. Deutsch, V. Carnevale

12:00 | **COMP 349.** Exploring the role of solvation in ion channel folding.
D. Granata, P. O. Klein, C. Deutsch, V. Carnevale

**Technical Program**
Section D
Sonesta Philadelphia Downtown
Benton
Computational Study of Water
Methods & Biological Applications
D. J. Sridhikara, 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. Kasavhala, 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
10:00 Intermission.
11:15 COMP 363. Bridging disparate levels of theory in free energy simulation using non-equilibrium work. P.S. Hudson, H.L. Woodcock, S. Biresh

Section E
Sonesta Philadelphia Downtown
Wyeth Gallery C
QM/MM Simulation of Chemical & Biophysical Reaction Pathways: Recent Developments & Applications
Co-sponsored by PHSYS
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 field using QM/MM method. J. Pu
9:00 COMP 365. New methodological developments for the study of enzyme chemical reactions. I. Tufton
9:30 COMP 366. MMIC: A new multiscale interface for first-principles molecular. U. Rothlisberger
10:00 Intermission.
10:45 COMP 368. Recent advances in QM/MM simulations of enzymatic reactions. W. Thiel

Advanced Potential Energy Surfaces
Applications of Advanced Potential Energy Models & Methods
Sponsored by PHSYS, Co-sponsored by COMP
Computational Chemistry & Toxicology in Chemical Discovery & Assessment (QSARs)
Sponsored by AGRO, Co-sponsored by COMP ENVIR 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. Ma, M. Stankov, B.V. Fyfe, 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-custimized docking without a protein structure. E.J. Martin, B. Samulof
3:00 Intermission.
3:45 COMP 374. Whole-protein (holistic) scoring scheme for virtual screening achieves higher success rates than single-site scoring. S. Dazdar, T. Tesolin, R. Kamstra, W.B. Floriano
3:30 Intermission.
4:45 COMP 382. Identification of a human thioredoxin regulatory responsive to thios in the presence of Cu(II) and Ag(II) ions: QM/MM and mutagenesis studies. L. Ahmed, S. Li, F. Zhang, Y. Pan, H. Matsunami, E. Block, H. Zhuang, V.S. Batista

Section C
Sonesta Philadelphia Downtown
Warhol
Material Science
Sonesta Philadelphia Downtown
Whistler A

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. Sogal, I. Yudof, 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. Borbelyvich, L. Wastenhof

Advanced Potential Energy Surfaces
MM from QM
Sponsored by PHSYS
Co-sponsored by COMP

Computational Chemistry & Toxicology in Chemical Discovery & Assessment (QSARs)
Sponsored by AGRO, Co-sponsored by COMP ENVIR and TOXI

THURSDAY AFTERNOON

Section D
Sonesta Philadelphia Downtown
Benton
Computational Study of Water Models, Properties & Phenomena
D. J. Sridhikara, Organizer
P. S. Hudson, Presiding
1:30 COMP 395. Timescale separation in the effective fragment potential. C.H. Boro, L.V. Siponen
2:00 COMP 396. 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 397. 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. Wigen, P.B. Moore
Section B  
Sonesta Philadelphia Downtown  
Whistler A  
Molecular Mechanics  
M. Feig, Organizer  
F. L. Keams, 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. M. 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  

Section C  
Sonesta Philadelphia Downtown  
Warhol  
Material Science  
H. L. Woodcock, Organizer  
K. R. Yang, Presiding  

8:30  COMP 408. n-Stacking pancake bonding: computational challenges. M. Kartesz, Z. Mou  
9:00  COMP 409. Quantum chemical study of electrocatalytic in copper 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. Shattuck, M. Mustakimov  
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.  

SUNDAY MORNING  

Section A  
Pennsylvania Convention Center  
Room 109B  
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 storage materials. H. Li, Q. Li  
10:05  Intermission.  
10:50  ENFL 5. Integration of carbon capture and subsequent conversion. L. He  
11:40  ENFL 7. Reduction of CO2 into HCOOH with 5-pyrimidinolone under hydrothermal conditions. Y. Yang, F. Jin  
12:05  Concluding Remarks.  

Section B  
Pennsylvania Convention Center  
Room 109A  
Water-Energy Nexus  
Cosponsored by ENVR and MPPG  
D. Shuai, W. Zhang, Organizers, Presiding  
8:30  Introductory Remarks.  
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. Shashikumar, V.V. Krishnan, D. Panatulu  
10:05  Intermission.  
10:50  ENFL 12. Fabrication of Cu/Ti nanoelectrode for electrochemical denitrogenization of water. M. Li, X. Liu  
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 bimetallics for sintering and coking resistant dry reforming of methane. X. Guo  
10:10  ENFL 17. Demineralization pathways for oil shale seimcicke pyroconversion to a sorbent material. A. Suleimenov, J.L. Goldenfarb  
10:30  Intermission.  
11:45  ENFL 20. Influence of pore structure of the zeolite USY on catalytic cracking of Jetprobe Curcass oil. Q. Zheng, B. Shen  
12:05  ENFL 21. Preparation a shape-selective zeolite material and its application in heavy oil catalytic cracking. P. Zang  

Section D  
Pennsylvania Convention Center  
Room 109B  
Degradation of Materials for Energy & Fuel Production  
Cosponsored by ENVR and MPPG  
S. Nair, Organizer  
J. Baltrusatis, Z. Wu, Organizers, Presiding  
8:30  Introductory Remarks.  
8:35  ENFL 22. Controlled synthesis of sintering-resistant catalysts through nanostructured materials. S. Dai  
10:20  Intermission.  

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  
9:55  Intermission.  
10:05  ENFL 32. On establishing a consortium to print polymer photovoltaic cells. A. Holmes  

Technical program information known at press time.  
The official technical program for the 2522nd ACS National Meeting is available at: www.acs.org/Philadelphia2016  

‡ Cooperative Cosponsorship