4:45 456. Silica and silica coated magnetite nanoparticles modified with 1,8-naphthalimide-trimethoxypropylsilane: A PET fluorescent sensor for Zn^{2+}. **S. K. Rastogi**, P. Pal, D. Newcombe, J. Branen, T. E. Bitterwolf, A. L. Branen

Section E

Salt Palace Convention Center
151 G

Applications in Nanoscience
Novel Structures Cosponsored by POLY, INOR, and NANO

R. Ragan, *Presiding*

2:00 457. Boron-containing polymer-silica hybrids for use in neutron capture therapy of cancer. **A. H. A. Mollard**, I. Zharov
2:20 458. Chemical assembly of colloidal gold nanoparticles on templates for the generation of localized electromagnetic fields. R. Ragan, **S. M. Adams**
2:40 459. Molecular patterning of solid-liquid interfaces with foldamers. **C. Gobbo**, J. H. van Esch, S. De Feyter
3:00 460. Novel aqueous sol-gel approach for hybrid barrier coatings. **M. Asuka**, W. M. Sigmund
3:20 Intermission.
3:30 461. Novel structures of transition metals and transition metal oxides through low temperature solution synthesis. **L. C. Fernández-Torres**
3:50 462. Organometallic dendrimers: New precursors in the synthesis of silica-supported iron-oxide nanoparticles. **E. Mitran**, R. L. McCarley
4:10 463. Photobleaching resistant pH sensing nanoreactors. **A. E. Ostafin**, Y-C. Chen
4:30 464. Responsive polymer brush nanosponges. **D. J. Dyer**, V. N. Wong, B. Mitrovic, G. R. Kinsel, S. Zauscher
4:50 465. Synthesis of functionalized superparamagnetic iron oxide nanoparticles from a common precursor and their application as heavy metal and actinide sorbents. **M. G. Warner**, C. L. Warner, R. S. Addleman, T. C. Droubay, M. Engelhard, J. D. Davidson, A. D. Cinson, M. A. Nash, W. Yantasee

COMP

Division of Computers on Chemistry

J. D. Madura, E. X. Esposito, and A. E. Roitberg, *Program Chairs*

SUNDAY MORNING

Section A

Salt Palace Convention Center
257

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Scaling Molecular Dynamics Applications Cosponsored by PHYS

S. T. Brown, R. C. Walker, and T. E. Cheatham III, *Organizers*

8:30 1. Docking performance accelerated 30-50 fold on the Cell/BE processor. **Z. Zsoldos**
9:10 2. Large-scale computational approaches: New tools to enable biomass conversion to ethanol. **M. F. Crowley**, M. Nimlos, Y. Bomble, J. Matthews, G. Beckham
9:50 3. Accurate modeling of biomolecular structure and dynamics using atomic-detail simulations. **C. L. Simmerling**
10:30 Intermission.
10:45 4. Multiscale simulation of cellular cytoskeleton proteins and their assemblies. **G. A. Voth**
11:25 5. Insights into the activation pathway of the adenovirus protease enzyme: Large scale nudged elastic band simulations on NSF supercomputers. **R. C. Walker**, J. V. Stern, W. J. McGrath, W. Mangel
12:05 6. Elucidating protein function through high-performance molecular dynamics simulation. **R. O. Dror**

Section B

Salt Palace Convention Center
258

Molecular Mechanics
Making Dreams into Methodologies

E. X. Esposito, *Organizer*

D. J. Sindhikara, *Presiding*

8:30 7. Lessons learned from predicting binding free energies in model binding sites. **D. L. Mobley**, S. Boyce, G. Rocklin, B. K. Shoichet, K. A. Dill
9:00 8. MD study of origin of enantioselectivity in CPO-catalyzed epoxidation. **D. C. Chatfield**, C. D'Cunha, C. Alvarez, R. Zhang
9:30 9. Modeling glycine tautomerization and glycyl-glycine peptide bond formation using a reactive force field. **O. Rahaman**, A. C. van Duin, D. J. Doren
10:00 10. Multiscale approach to developing universal coarse-grained peptide force fields. **I. F. Thorpe**, R. D. Hills, G. A. Voth
10:30 Intermission.
10:40 11. Statistically optimal free energy estimates from sparsely chosen states. **M. Shirts**, J. D. Chodera
11:10 12. Stochastic thermostat induced synchronization of MD trajectories in biomolecules. **D. J. Sindhikara**, A. E. Roitberg, A. F. Voter, S. Kim
11:40 13. Synergistic regulation and ligand-induced conformational changes of tryptophan synthase. **M. Q. Fatmi**, C-E. A. Chang

Section C

Salt Palace Convention Center
259

Molecular Modeling in Chemical Processes

L. Achenie, *Organizer*

8:00 14. Coarse-grained models to reflect functional dynamics of large biomolecules obtained by an elastic network model. **Z. Zhang**, K. Y. Sanbonmatsu, G. A. Voth
8:30 15. Quantum chemical and detailed chemical kinetic modeling of methylamine oxidation: Applications to atmospheric and supercritical water chemistries. K. M. Benjamin, **J. Meyer**, F. Sefa, **S. Lane**
9:00 16. Force-field development for heavy elements using ab initio data and the force matching method. **A. Clark**, B. Waldher, M. C. F. Wander, N. J. Henson
9:30 17. Shot-noise-limited detection of conformational states and photoblinks in single-molecule FRET trajectories. **J. N. Taylor**, C. F. Landes
10:00 18. Path sampling for nonequilibrium processes in many-dimensional order-parameter spaces. **A. R. Dinner**
10:30 19. The relative entropy in multiscale modeling and coarse-grained model development. **M. S. Shell**, A. Chaimovich
11:00 20. Surfactant formulation multiscale modeling with CULGI. **J. Fraaije**, S. Nath
11:30 21. Molecular modeling as an important step in the multiscale study of the CVD process. **L. Achenie**

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

SUNDAY AFTERNOON

Section A

Salt Palace Convention Center
257

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Scaling Molecular Dynamics Developments Cosponsored by PHYS

S. T. Brown, R. C. Walker, and T. E. Cheatham III, *Organizers*

1:00 22. Approaching petascale biomolecular simulation. **K. Schulten**, J. Phillips, J. E. Stone, L. Kale
1:40 23. Architectures and algorithms for millisecond-scale molecular dynamics simulations of proteins. **D. E. Shaw**
2:20 24. Folding@home: Scalable algorithms for computational biology, running today on a sustained-petaflop class cluster of processors. **V. S. Pande**
3:00 25. GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable molecular simulation. **B. Hess**
3:40 26. PMEMD: A high performance implementation of AMBER molecular dynamics. **R. E. Duke**, L. G. Pedersen

Section B

Salt Palace Convention Center
258

Connecting Computation to Experiment using Combined QM and MM Methods

B. P. Krueger and R. C. Walker, *Organizers, Presiding*

1:00 Introductory Remarks.
1:05 27. Combined QM and MM approaches for vibrational spectroscopy: Applications to water and proteins, including comparisons with experiment. **J. L. Skinner**
1:35 28. Shedding light on photochemical reactions: Computer simulation as a tool for time-resolved spectroscopy. **G. Groenhof**
2:05 29. Investigating biological spectroscopy with QM/MM methods. **I. R. Gould**
2:35 30. Multiscale modeling of electronic excitations at the nanoscale. **S. Tretiak**, C. Wu, S. V. Malinin, V. Chernyak
3:05 Intermission.
3:15 31. A quantum of common sense in crystallography. **X. Li**, K. M. Merz Jr.
3:45 32. Toward a fully quantum mechanical force field for simulations of biocatalysis. **D. M. York**
4:15 33. Fretting about FRET: Breakdown of the ideal dipole approximation. **B. P. Krueger**, A. Munoz-Losa, C. Curutchet, L. R. Hartsell, B. Mennucci

Section C

Salt Palace Convention Center
259

Molecular Modeling in Chemical Processes

L. Achenie, *Organizer*

1:00 34. Developing the promise of reactive molecular dynamics for performing kinetics experiments computationally. **P. R. Westmoreland**
1:30 35. Surface nanostructure, diffusion and catalysis: The role of confinement and surface chemistry. **K. E. Gubbins**
2:00 36. Using molecular simulation to understand wetting behavior. **J. R. Errington**
2:30 37. Identification of dynamical hinge points of L1 ligase using large scale molecular dynamics simulations. **G. M. Giambasu**, T-S. Lee, D. M. York
3:00 38. Simulating stimulating interfaces: Applications in adsorption and catalysis. **C. H. Turner**
3:30 39. Theoretical investigation of inverse spillover processes on alumina supported Pt catalysts. **J. Synowczynski**, J. W. Andzelm, D. G. Vlachos
4:00 40. Fatty acid induced toxicity: Interactions with the lipid bilayer. **A. K. Sum**
4:30 41. Molecular dynamics and structural studies of cyclopentane modified peptide nucleic acids. **A. K. Manukyan**, J. Radkiewicz-Poutsma

MONDAY MORNING

Section A

Salt Palace Convention Center
257

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Quantum Chemistry Developments Cosponsored by PHYS

S. T. Brown, R. C. Walker, and T. E. Cheatham III, *Organizers*

8:30 42. Electronic structure theory at the petascale: Progress and challenges. **M. S. Gordon**, T. L. Windus, M. H. Lamm, M. Sosonkina, A. Asadchev
9:10 43. Exposing more parallelism in quantum chemistry applications: Moving beyond the MPI and hybrid MPI/multithreaded programming models. **C. L. Janssen**
9:50 44. NWChem: Cutting-edge computational chemistry on large computing platforms. **W. A. de Jong**
10:30 45. Overcoming difficulties in density functional theory: Calculation of nondynamical correlation and dispersion interaction. **J. Kong**, E. Proynov, Y. Shao, Z. Gan, M. Freindorf, T. R. Furlani
11:10 46. Super instruction architecture of a parallel implementation of coupled cluster theory. **E. Deumens**, V. Lotrich, J. M. Ponton, R. J. Bartlett, B. A. Sanders

Section B

Salt Palace Convention Center
258

Molecular Mechanics
Applying Ideas

E. X. Esposito, *Organizer*

S. E. Nichols, *Presiding*

8:30 47. Catalytic mechanism of cyclophilin. **D. Hamelberg**, J. A. McCammon
9:00 48. Extended ensemble ligand binding affinities with OPLS-AA, AMBER99, and varying AM1-BCC charge sets. **M. Shirts**
9:30 49. Homogeneous ice nucleation: A coarse grain approach. **E. B. Moore**, V. Molinero
10:00 Intermission.
10:10 50. Roles of Mg2+ in hammerhead ribozyme. **T-S. Lee**, G. Giambasu, D. M. York
10:40 51. Thermostability of hydrogen bond network of cellulose. **T. Shen**, S. Gnanakaran
11:10 52. TraPPE-UA force field for acrylates and Monte Carlo simulations for their mixtures with alkanes and alcohols. **K. A. Maerzke**, J. L. Lewin, N. E. Schultz, R. B. Ross, J. I. Siepmann
11:40 53. Modeling conformation and toxicity of amyloid-forming peptides. **J. Zheng**, X. Yu, Q. Wang

Section C

Salt Palace Convention Center
259

Nanomaterials Modeling and Informatics
Nanotubes and Nanocomposites
Cosponsored by CINF and NANO

C. M. Breneman, *Organizer, Presiding*

9:00 Introductory Remarks.
9:05 54. Informatics for nanostructure discovery and design. **K. Rajan**

9:30 55. Intelligent design of nanocomposites via informatics. **L. Brinson**, L. S. Schadler, C. M. Breneman, N. Sukumar, M. Kreim, R. Qiao
9:55 56. Quantitative structure property relationships of nanotube structural and mechanical properties. **T. L. Borders**, A. Rusinko III, K. Cho, A. F. Fonseca
10:20 Intermission.
10:35 57. Finite element modeling of CNT-nanocomposite interlaminar shear strength. **S. McHugh**
11:00 58. Interactions of epoxy-based polymers with carbon nanotubes studied by molecular modeling. **A. Bick**, L. Persiteras
11:25 59. Prediction and nanomechanics of interfacial strength between carbon nanotubes and resin. M. Garg, S. McHugh, **F. Abdi**

Library Design, Search Methods and Applications of Fragment-based Drug Design
Library Design and Search Methods
Sponsored by CINF, Cosponsored by COMP

MONDAY AFTERNOON

Section A

Salt Palace Convention Center
257

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Nontraditional Density Functional Methods
Cosponsored by PHYS

S. T. Brown, R. C. Walker, T. E. Cheatham III, and K. D. Jordan, *Organizers*

1:30 60. First-principles molecular dynamics on petascale computers: Algorithmic developments and applications. **F. Gygi**
2:10 61. Large-scale quantum mechanical simulations of materials under extreme conditions. **W. D. Mattson**, B. M. Rice, R. Balu
2:50 62. NEMO 3-D and OMEN: Nanoelectronic modeling tools for advanced semiconductor device studies and their deployment on nanoHUB.org. **G. Klimeck**, M. Luisier, R. Rahman, M. Usman, N. Kharche, H. Ryu, S. Lee, D. Vasileska
3:30 63. Scalable ab initio MD simulations for chemistry. **G. Martyna**
4:10 64. Toward petaflop computing for electronic structure calculations. **Y. Wang**, G. M. Stocks, A. Rusanu, D. M. C. Nicholson, M. Eisenbach

Section B

Salt Palace Convention Center
258

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Scaling Quantum Chemistry Applications
Cosponsored by PHYS

S. T. Brown, R. C. Walker, and T. E. Cheatham III, *Organizers*

1:30 65. Advances in density functionals for electronic structure calculations. J-D. Chai, **M. Head-Gordon**
2:10 66. Domain-specific languages for many-body molecular structure methods. **E. F. Valeev**
2:50 67. Generation of a database of hypothetical zeolite structures. **D. J. Earl**, M. W. Deem
3:30 68. Predictive chemical computing in condensed phases. **S. Hirata**, O. Sode, M. Keçeli, K. Yagi
4:10 69. Toward petascale applications with ACES III. **R. J. Bartlett**, V. Lotrich, T. Kus, T. Hughes, N. Flocke, A. Perera, E. Deumens

Section C

Salt Palace Convention Center
259

Nanomaterials Modeling and Informatics
Nanotubes and Nanocomposites
Cosponsored by CINF and NANO

C. M. Breneman, *Organizer*

M. Krein, *Presiding*

1:30 Introductory Remarks.
1:35 70. Multiscale modeling motivation, strategy, and approaches for nanoscale material and device design and development. **R. R. Barto**, T. L. Borders, C. M. Breneman, L. S. Schadler, K. Cho
2:00 71. New computational simulation techniques for nanosystems: Bridging the gap. **J. Maguire**, M. D. Benedict
2:25 72. Investigation of multiwalled carbon nanotube nanocomposites at multiple scale. **K. A. Morse**, C. L. Quartey, L. S. Schadler, T. Goren, M. Krein
2:50 Intermission.
3:05 73. Identification of critical parameters in continuum level modeling of nanocomposites through a multiscale study. **V. Flores**, M. J. Leamy, H. Zhang, A. F. Fonseca, K. Cho
3:30 74. Polymer nanophase multiscale modeling using CULGI. **J. Fraaije**, S. Nath
3:55 75. Multiscale simulation study of nanotube composite mechanics. **A. F. Fonseca**, H. Zhang, T. L. Borders, V. Flores, R. R. Barto, K. Cho
4:20 76. Withdrawn.

Section D

Salt Palace Convention Center
260

Quantum Chemistry
Theory, Methodology, and Application

A. E. Roitberg, *Organizer*

J. R. Hammond, *Presiding*

1:30 77. Computational chemistry investigation of spin traps using hybrid solvation models. **S. Sriharsha Konda**, S. J. Kirkby
2:00 78. Hypervalent vs. nonhypervalent carbon: Disk-between-balls model. S. C. A. H. Pierrefixe, J. Poater, C. Im, **F. M. Bickelhaupt**
2:30 79. Mechanism of efficient firefly bioluminescence via adiabatic transition state and seam of sloped conical intersection. **L. W. Chung**, S. Hayashi, T. Nakatsu, H. Kato, K. Morokuma
3:00 80. Modeling reactions in proteins. **J. J. P. Stewart**
3:30 Intermission.
3:40 81. Molecular dynamics simulations of carbon tetrachloride properties using quantum chemistry calculated potentials. **S. D. Chao**, A. H-T. Li
4:10 82. Theoretical exploration of sensing mechanisms of nitroaromatics. **B. Arman**, H. Fan, T. Cagin
4:40 83. Using data mining algorithms to develop semi-empirical quantum chemical methods: Polarizable solvent models. **V. Ediz**, A. C. Monda, R. P. Brown, D. J. Yaron

Photographing or recording meeting sessions and/or activities other than your own are prohibited at all official ACS events without written consent from ACS.

‡ Cooperative Cosponsorship

Library Design, Search Methods and Applications of Fragment-based Drug Design Sponsored by CINF, Cosponsored by COMP

MONDAY EVENING

Section A

Salt Palace Convention Center
Hall 5

Sci-Mix

E. X. Esposito, *Organizer*

8:00–10:00
135-136, 139, 142, 146, 149, 156-157, 162, 169, 176. See subsequent listings.

TUESDAY MORNING

Section A

Salt Palace Convention Center
257

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Quantum Monte-Carlo Cosponsored by PHYS

S. T. Brown, R. C. Walker, and T. E. Cheatham III, *Organizers*

8:30 84. Massively parallel and multiscale simulations of strongly correlated electronic systems. **J. Mark**
9:10 85. Advances in quantum Monte Carlo: Topology of fermion nodes and pfaffian pairing wavefunctions. **L. Mitas**
9:50 86. Applications of the quantum Monte Carlo method to challenging electron correlation problems. **K. D. Jordan**, J. Xu, W. Lampart
10:30 87. Optimal wave functions for diffusion Monte Carlo. **C. J. Umrigar**, J. Toulouse, P. Nightingale
11:10 88. Quantum Monte Carlo for the electronic structure of molecular systems. **W. A. Lester Jr.**
11:50 89. Recent advances in quantum Monte Carlo for quantum chemistry: Optimization of wave functions and calculation of observables. **J. Toulouse**, C. J. Umrigar, R. Assaraf

Section B

Salt Palace Convention Center
258

Molecular Mechanics
QM + MM = QM/MM Wait! Is that Math Correct?

E. X. Esposito, *Organizer*

X. Cang, *Presiding*

8:30 90. Ab initio and hybrid QM/MM simulations on massively parallel supercomputers: Experience at ERDC. **O. Isayev**, J. Leszczynski, L. Gorb, F. Hill
9:00 91. A novel method for predicting ligand regioselectivity to metabolism by cyp p450 enzymes. **J. Zaretzki**, C. Bergeron, K. Bennett, C. M. Breneman
9:30 92. A QM/MM study of the cis-trans isomerism in peptide bonds. **G. D. M. Seabra**, R. C. Walker, A. E. Roitberg
10:00 93. Quantum mechanical/molecular mechanical studies of the reaction mechanism of human DNA polymerase λ with Mg^{2+} and Mn^{2+}. **G. A. Cisneros**, L. Perera, M. Garcia-Diaz, K. Bebenek, T. Kunkel, L. G. Pedersen
10:30 Intermission.
10:40 94. Theoretical insight into the nitroreductase mechanism. **O. Isayev**, L. Gorb, N. Cenas, M. Qasim, J. Leszczynski
11:10 95. Tuning the acidity of organic acids, and investigating their dissociation mechanism: A QM/MM approach. **R. Iftimie**, P. Maurer
11:40 96. Will polarizable MM force field improve the QM/MM method: A test of solvation free energy simulations. **H. Hu**

Section C

Salt Palace Convention Center
259

Nanomaterials Modeling and Informatics
Nanoparticles, Nanotoxicity and Molecular Machines Cosponsored by CINF and NANO

C. M. Breneman, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 97. Assessing the biological effects of nanoparticles using quantitative nanostructure – activity relationships. D. Fourches, L. Ye, R. J. Mumper, **A. Tropsha**
9:00 98. QSAR Analysis of nanoparticle formulation performance for a diverse set of drug and polymer systems. **M. D. Wessel**, T. L. Hayden
9:25 99. Identification of possible sources of nanotoxicity from carbon nanotubes. **A. J. Hopfinger**, J. Liu
9:50 Intermission.
10:05 100. Modeling of multiblade molecular turbines. J. Vacek, A. Prokop, **J. Chocholoušová**, J. Michl
10:30 101. Optical absorption and EPR spectra of gold and silver nanoparticles. **C. M. Aikens**, R. Jin
10:55 102. Understanding the molecular mechanisms underlying the nucleation and growth of nanoparticles. **J. Delhommelle**, C. Desgranges
11:20 103. Dissipative particle dynamics simulation of the formation and stabilization of iron nanoparticle. **H. Zhang**, G. Que

Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen
Crystal Form Analysis, Experiment and Prediction Sponsored by CINF, Cosponsored by COMP, CHAL, and MEDI

Library Design, Search Methods and Applications of Fragment-based Drug Design Sponsored by CINF, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

Salt Palace Convention Center
257

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of Mark S. Gordon Cosponsored by PHYS

M. S. Gordon, *Organizer*

D. G. Truhlar, *Presiding*

1:30 104. Physical understanding through variational reasoning: Electron sharing and covalent bonding. **K. Ruedenberg**, M. W. Schmidt
1:55 105. Reading bond orders from the density matrix. **M. W. Schmidt**, K. Ruedenberg
2:20 106. Mechanisms of reactions of $C_4H_4^+$ with pyridine. C. Q. Jiao, **J. A. Boatz**, C. A. DeJoseph Jr, A. Garscadden
2:45 Intermission.
3:00 107. Polarizability effects and dispersion interactions in complexed molecules: Computational considerations. **K. K. Baldridge**
3:25 108. Calculation of molecular properties of proteins. **J. H. Jensen**
3:50 109. High performance computational chemistry. **T. L. Windus**

4:15 110. Award Address (ACS Award for Computers in Chemical and Pharmaceutical Research, sponsored by Schrödinger). Toward a comprehensive method for intermolecular interactions. **M. S. Gordon**

Section B

Salt Palace Convention Center
258

Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium
Looking Toward the Future Cosponsored by PHYS

S. T. Brown, R. C. Walker, and T. E. Cheatham III, *Organizers*

1:30 111. Accelerating density functional theory calculations using graphical processing units. **Z. Gan**, R. Olivares-Amaya, L. Vogt, Y. Shao, A. Aspuru-Guzik, J. Kong
2:10 112. Biomolecular applications of graphics processors. **J. E. Stone**, J. Phillips, K. Schulten
2:50 113. First principles molecular dynamics simulation of proteins on graphical processing units. **I. S. Ufimtsev**, T. J. Martinez
3:30 Intermission.
3:45 114. Quantum computation for chemistry. **A. Aspuru-Guzik**
4:25 115. Meeting the challenge of petascale computing. **T. H. Dunning Jr.**
5:05 116. Computational chemistry at the petascale using NWChem and MADNESS. **R. J. Harrison**, E. Apra, W. A. Shelton

Section C

Salt Palace Convention Center
259

Nanomaterials Modeling and Informatics
Nanostructure Modeling with Simulation and DFT Cosponsored by CINF and NANO

C. M. Breneman, *Organizer, Presiding*

1:30 Introductory Remarks.
1:35 117. Controlling C60 self-assembly via tethering of a single PEO chain: A simulation study. **J. B. Hooper**, D. Bedrov, G. D. Smith
2:00 118. Morphology and rheology of the blend of amphiphilic ABA and AB block copolymers: DPD simulation study. **Y. R. Sliozberg**, J. W. Andzelm, J. K. Brennan, M. VanLandingham, V. Pryamitsyn, V. Ganesan
2:25 119. Brownian dynamics modeling of charge mobility on single conjugated polymer chains in solution. **D. J. Yaron**, X. Cai
2:50 Intermission.
3:05 120. Effect of a Stone-Wales defect on Li+ binding with (6,6) armchair single-walled carbon nanotube and graphene sheet. **T. C. Dinadayalane**, T. M. Simeon, J. Leszczynski
3:30 121. Architecture of transition metal monatomic strings on boron-doped carbon nanotubes: A density-functional theory study. **W. An**, C. H. Turner
3:55 122. Ab initio and DFT studies of atomic hydrogen chemisorption on model graphite compounds. Y. Wang, **S. Irle**, K. Morokuma

Adaptive Scoring Functions Sponsored by CINF, Cosponsored by the CSA Trust and COMP

Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen

Please refrain from using cellular telephones and cameras during technical sessions.

Scientific and Regulatory Issues of Crystal Forms Sponsored by CINF, Cosponsored by COMP, CHAL, and MEDI

TUESDAY EVENING

Section A

Salt Palace Convention Center
Hall 1

Chemical Computing Group Excellence Award

C. L. Simmerling, *Organizer*

6:00–8:00
123. Calculation of protein-ligand binding free energy by a polarizable force field. **D. Jiao**, P. Ren
124. Constant pH replica exchange molecular dynamics simulation in biomolecules. **Y. Meng**, A. E. Roitberg
125. Estimating transition rate and free energy of Src kinase activation using Markov state model. **W. Gan**, B. Roux
126. Intramolecular electron transfer in two- and three-center mixed-valence triarylamines. **K. Lancaster**, S. A. Odom, S. C. Jones, S. Barlow, S. R. Marder, V. Coropceanu, J-L. Bredas
127. Investigating the properties of new water models capable of polarization and intermolecular charge transfer. **J. Chen**, T. J. Martínez

Section B

Salt Palace Convention Center
Hall 1

Hewlett-Packard Scholar Awards

C. L. Simmerling, *Organizer*

6:00–8:00
128. Practical many-body methods for computational thermochemistry, kinetics, and spectroscopy. **E. F. Valeev**
129. A new generation of analytical tools for biomolecular electrostatics. **A. Onufriev**
130. Enhanced sampling methods for molecular systems far from equilibrium. **A. R. Dinner**
131. Force-field development for heavy elements using ab initio data and the force matching method. **A. Clark**, B. Waldher, M. C. F. Wander, N. J. Henson

Section C

Salt Palace Convention Center
Hall 1

Poster Session

E. X. Esposito, *Organizer*

6:00–8:00
132. A comparative study of B3LYP, X3LYP, and M06-class density functionals for predicting binding energies of neutral, protonated, and deprotonated water clusters. **V. S. Bryantsev**, M. Diallo, W. A. Goddard III
133. A single empirical expression for predicting protein-protein binding affinities and geometries. **J. Audie**
134. An ab initio and DFT study of the effects of water molecules on sulfur oxide reactions. **J. M. Standard**, M. C. Cafarelli, P. Gorczynski, R. A. Craigmile
135. Benchmark calculations of ammonium and nitrate ions in aqueous solution. **K. Range**
136. Binary QSAR model for classification of calpain inhibitors. **E. L. Mendonca**, G. Pieffet, I. Schiefer, V. Sinha, C. E. Ranepuradewage, S. Tapadar, T. W. Gihani, P. Edirisinghe, O. Arancio, G. R. J. Thatcher, P. A. Petukhov
137. BRICS: Breaking into retrosynthetically interesting chemical substructures. **C. Wegscheid-Gerlach**, J. Degen, H. Briem, M. Rarey, A. Zaliani
138. Comparative ligand binding characteristics of indoleamine 2,3-dioxygenase and tryptophan 2,3-dioxygenase. L. Capece, M. A. Martí, **M. Arrar**, D. A. Estrin
139. Conformational studies of bridgehead disubstituted bicyclo[m.m.m]alkane and bridgehead disubstituted bicyclo[8.8.n]alkane systems. **I. W. Jones**, E. Mash
140. Connecting experiment and principal mode analysis of QM/MM simulations to calculate vibrational frequency shifts for N-methylacetamide in water, a simple model for the peptide bond. **R. A. Wheeler**, K. R. Brorsen, S. E. Boesch
141. Crystalline structure of methyl 3-nitrosalicylate and properties comparison with methyl salicylate by experiments and calculations. Y. Liu, L. Zhang, X. Li, C. Qiu, **Y. Li**
142. Crystallization of charged nanoparticles in solution. **D. Zhang**, P. Gonzalez-Mozuelos, M. Olvera de la Cruz
143. Density functional theory and multiscale simulations combined with spectroscopic study of barium/strontium ferrate/cobaltate as a promising material for solid oxide fuel cell. **S. Gangopadhyay**, A. E. Masunov, T. Inerbaev, D. Altilio, N. Orlovskaya, J. Mesit, R. Guha, A. Sleiti, J. Kapat
144. Developing reweighting-based molecular dynamics with sights set on converged long-timescale biomolecular simulations. **D. Hamelberg**
145. Development of pharmacophore and CoMFA study for sigma 2 receptor ligands. **L. A. Wirpsza**, D. Jung, T. M. Gund
146. Effect of support, ZnO, on the structure and properties of Cu clusters. **C. B. Love**, L. Wang
147. Efficient methodologies for antibody homology modeling. **J. Maier**
148. Empirical corrections to density functional theory highlight the importance of nonbonded intramolecular interactions in alkanes. **M. D. Wodrich**, D. F. Jana, P. von Ragué Schleyer, C. Corminboeuf
149. Evidence for multilayer active sites in enzymes. **H. Brodkin**, W. R. Novak, A. C. Milne, A. D'Aquino, M. J. Ondrechen, D. Ringe
150. Investigating the binding mode of ligand of bcl-xL by steered molecular dynamics simulation. **F. Shah**, P. Mukherjee, M. A. Avery
151. Modeling nitrile-terminated polypropylene imine dendrimer fragmentation with DFT. **W. D. Price**, E. W. Martin
152. Modeling of PXR ligands. **L. Xiao**, C. Lesburg, W. Wang, E. Nickbarg, X. Cui, K-C. Cheng
153. Modeling the binding of CWAs to human AChE and BuChE compared to other species. **B. J. Bennion**, R. J. Law, J-L. Fattebert, E. Schwegler, F. C. Lightstone
154. Molecular dynamics and free energy calculations explain decreased inhibition of G-actin by oxalatrunculin B and semisynthetic analogs of latrunculin B. **P. R. Daga**, S. Odde, M. T. Hamann, R. J. Doerksen
155. Molecular modeling of the dra snf2 intein for the investigation of the atypical splicing mechanism. **L. E. Brace**, F. B. Perler, **F. Ryvkin**
156. Moving domain QM/MM method to describe polarization effects in protein electrostatics. **L. C. Menikarachchi**, J. A. Gascon
157. MSMM-CoMFA, a novel 3-D-QSAR method for ligands with multiple species and multiple binding modes. **S. Natesan**, S. Balaz
158. New protocol for efficient and accurate ab initio prediction of thermodynamic parameters. **A. Furmanchuk**, O. Isayev, L. Gorb, J. Leszczynski
159. Optimization of pattern recognition and classification by combinatorial QSAR modeling of the carcinogenic potency database. **K. Wang**, A. Golbraikh, A. Tropsha
160. Pair-wise property-encoded shape distributions for comparing binding sites in proteins. **S. Das**, A. Kokardekar, C. M. Breneman
161. Prediction of thermal cycloreversion and fatigue-resistance. A. E. Masunov, **P. D. Patel**, I. A. Mikhaylov, K. D. Belfield
162. Predictive statistical model building for hERG liability based on pharmacophore fingerprint descriptors. **T-Y. Wu**, D. Fourches, S. Marron, Y. Liu, A. Tropsha, Z. Yang
163. Q-Chem 3.2: Reaching higher ground. **J. Kong**
164. Qstr analysis of mixtures toxicity to Daphnia magna. **V. E. Kuz'min**, E. Muratov, E. Varlamova, A. G. Artemenko, N. Kovdienko, A. Tropsha
165. Quantitative predictions of protein-ligand binding affinities. **D. L. Mobley**
166. Quantitative structure – activity relationship study of organophosphorus pesticides, nerve agents and their derivatives. **Y. Paukku**, E. N. Muratov, V. E. Kuz'min, A. G. Artemenko, N. A. Kovdienko, J. Leszczynski
167. Quantum calculations on the regioselectivity of nitration reaction of methyl salicylate with iron nitrate. Y. Liu, X. Li, L. Zhang, C. Qiu, **Y. Li**
168. Reactivity and stereospecificity in the Wittig reaction: A molecular modeling study of the Wittig reaction of 9-anthraldehyde with the benzyltriphenylphosphonium ylide. **R. Shaw**, F. Colon, A. P. Kennedy
169. Relativistic calculations of the xenon – transition metal cation systems (XeM+, M=Ni, Pd, Pt, Cu, Ag, Au, Zn, Cd, Hg). **H. G. Nguyen**, E. M. Eyring, D. B. Hunter, T. N. Truong
170. Residual reactive curves construction using spreadsheet and Aspen Properties® complement for Excel®. **C. A. Trujillo H**, D. F. Mendoza, H. R. Zea, H. Rangel
171. Scanning the potential energy surface of furanosyl oxocarbenium ions: Models for reactive intermediates in carbohydrate reactions. J. S. Rhoad, **B. A. Cagg**, P. Carver
172. Simulations of a tethered p53 peptide in aqueous salt solutions. **J. Feng**, B. M. Pettitt
173. Study of the active site of inosine monophosphate dehydrogenase. **S. Braun-Sand**, R. Schultz, A. Cook, D. E. Mendes
174. Substrate induced population shifts and stochastic gating in the PBCV-1 mRNA capping enzyme. **R. V. Swift**
175. The gem-dimethyl effect revisited: Elucidation of rate acceleration for epoxidation reactions of chlorohydrins in water from QM/MM simulations. **J. Kostal**, W. L. Jorgensen
176. Theoretical investigations on interactions between L-lactic acids and terpenoid mosquito repellents. A. Findlater, S. Hyde, Z. Wang, **J. Song**
177. Weighted ensemble path sampling simulations of conformational transitions in lymphotactin. **D. Bhatt**, D. M. Zuckerman
178. Ligand conformational free energy change and its contribution toward improvement of binding affinity prediction between the XIAP BIR3 domain and its inhibitors. **C. Y. Yang**, H. Sun, J. Chen, Z. Nikolovska-Coleska, J. Meagher, J. Stuckey, S. Wang
179. Molecular dynamics simulation of the interactions of Aß oligomers with lipid bilayers: Implication for toxicity of Alzheimer's disease. **X. Yu**, Q. Wang, M. Hosseini, J. Zheng
180. DFT study of the explosive tetraacetone tetraperoxide. **J. N. Woodford**, G. S. Harbison, P. Goodman, J. G. Redepenning

WEDNESDAY MORNING

Section A

Salt Palace Convention Center
257

Drug Discovery

I. Visiers, *Organizer*

Z. Yang, *Presiding*

8:30 181. Peptide to potent compounds by structure-based design techniques. **B. J. Burke**, M. Melnick, K. Lewis, L. Mitchell

9:00 182. Development and characterization of cyclic analogs of apelin-13 through replica-exchange molecular dynamics and experimental validation. **N. J. M. Macaluso**, S. L. Pitkin, P. N. Sanderson, A. P. Davenport, R. C. Glen
9:30 183. E-Novo automated workflow for structure-based lead optimization. **B. C. Pearce**, D. R. Langley, J. Kang, H. Huang, A. Kulkarni
10:00 184. Hepatitis B virus DNA polymerase inhibition: Computational insight into resistance development. **P. R. Daga**, R. J. Doerksen
10:30 Intermission.
10:40 185. Good BREEDing, techniques for generating hybrid molecules. **J. M. Leonard**
11:10 186. Ro5.1: Pfizer rules revisited. **T. I. Oprea**
11:40 187. Graph representation of molecular datasets: Applications to dataset visualization and comparison using graph indices. **D. Fourches**, A. Tropsha

Adaptive Scoring Functions Sponsored by CINF, Cosponsored by the CSA Trust and COMP

WEDNESDAY AFTERNOON

Section B

Salt Palace Convention Center
257

Drug Discovery

I. Visiers, *Organizer*

A. Tropsha, *Presiding*

1:30 188. Accurate prediction of logD and hERG liability by pharmacophore fingerprint QSAR (pFPQSAR) for drug discovery in GSK. **Z. Yang**, T-Y. Wu
189. Withdrawn.
2:00 190. A novel mehod for generating structure-based pharmacophores using energetic analysis. **N. K. Salam**, B. W. Sherman
2:30 191. Alignment and overlay of protein surfaces using shape and chemical features: Application to detect local similarity among ligand binding sites. **B. K. Rai**, G. A. Bakken
3:00 Intermission.
3:10 192. Automated QSAR modeling to guide drug design. **O. Obrezanova**, M. D. Segall
3:40 193. Combination of amide hydrogen/deuterium-exchange mass spectrometry and computational chemistry: Applications to study protein dynamics, protein-ligand interactions, and protein-protein interactions. **Y. Hamuro**, **D. Pandit**
4:10 194. Detecting conserved patterns of shape and property distributions on ligand binding site surfaces of proteins using property-encoded shape distributions. **S. Das**, A. Kokardekar, C. M. Breneman

Section C

Salt Palace Convention Center
258

Quantum Chemistry
Making the Difficult Attainable

A. E. Roitberg, *Organizer*

K. Shahrokh, *Presiding*

1:30 195. Accurate calculation of explicit water molecule free energies: Applications to PDZ binding domains. **T. Beuming**, B. W. Sherman, R. Farid
2:00 196. Statistics and physical origins of ionization state changes upon protein-ligand binding. **A. Onufriev**
2:30 197. A solution structural model for human intrinsic blood coagulation tenase complex (fVIIIa:fIXa) derived from protein docking and MD simulations: Implications for factor X activation. **D. Venkateswarlu**
3:00 Intermission.
3:10 198. Definition of chemical reactivity parameter and its validation. **S. Yao**
3:40 199. Cross Pharma High Performance Computing Forum: Collaboration to optimize HPC capabilities to accelerate drug discovery. **Z. Yang**
4:10 200. Lemniscular phyrins as calibrants of electron correlation fidelity in hybrid DFT methods. **H. S. Rzepa**

Adaptive Scoring Functions Sponsored by CINF, Cosponsored by the CSA Trust and COMP

THURSDAY MORNING

Section A

Salt Palace Convention Center
257

Quantum Chemistry
The Quantum and Physical Worlds Meet

A. E. Roitberg, *Organizer*

R. J. Doerksen, *Presiding*

8:30 201. Acidity modeling of arsenic and arsenous oxide and sulfide acids using ab initio model chemistries. **M. D. Zimmermann**, J. A. Tossell
9:00 202. Red shift vs. blue shift of C-H stretching frequency of C-H . . . pi interactions in benzene dimer: Influence of counterpoise correction in the frequency calculations at the MP2 method. **T. C. Dinadayalane**, J. Leszczynski
9:30 203. Density functional calculations of 15N chemical shielding in peptides and proteins. **L. Cai**, D. Fushman, D. Kosov
10:00 204. Nonlinear dimensionality reduction for reaction path discovery in ab initio multiple spawning dynamics. **A. M. Virshup**, J. Chen, T. J. Martinez
10:30 Intermission.
10:40 205. Spin decoherence in carbon and boron-nitride nanoribbons. **A. F. Izmaylov**, M. J. Frisch
11:10 206. Theoretical study of the anharmonicity of molecular vibrations of Li^+–H_2, Na^+–H_2, B^+–H_2 and Al^+–H_2 complexes. **N. De Silva**, B. Njegic, M. S. Gordon
11:40 207. Calculation of quantum mechanical vibrational energy relaxation rates in liquids via semiclassical methods. **F. X. Vázquez**, E. Geva

Section B

Salt Palace Convention Center
258

Drug Discovery

I. Visiers, *Organizer*

Z. P. Yang, *Presiding*

8:30 208. eHiTS: Docking and scoring ligand/target interactions to give good score-rmsd and ic50 correlations in in silico high throughput screening. **D. Harris**, Z. Zsoldos
9:00 209. Mining public databases for structure-activity relationships. **B. Wendt**, U. Uhrig, L. Wang
9:30 210. Protein ensemble generation for improved ligand-protein docking. **A. Nayeem**, K. A. Rossi, S. R. Kimura, S. R. Krystek Jr.
10:00 Intermission.
10:10 211. Screening tools and results for inhibitors of human tyrosyl DNA phosphodiesterase (Tdp1). **I. E. Weidlich**, T. Dexheimer, Y. Pommier, C. Marchand, M. C. Nicklaus
10:40 212. Structure-based discovery and biological evaluation of novel selective TRAF6 inhibitors. **S. Zhang**, L. Du-Cuny, B. Darnay
11:10 213. Understanding the potential role of hydrogen bonding in drug discovery. **D. C. Reuter**, K. Brameld, S. Connolly

THURSDAY AFTERNOON

Section A

Salt Palace Convention Center
257

Drug Discovery

I. Visiers, *Organizer*

B. J. Burke, *Presiding*

1:00 214. Computational approaches to antibacterial and antimalarial hit finding. **A. P. Johnson**, C. W. G. Fishwick, G. A. McConkey, T. Heikkila, M. Davies, D. Cowan, A. Agarwal
1:30 215. Computer-aided design of [(biphenyloxy)propyl]isoxazoles – agents against coxsackievirus B3. **E. Muratov**, V. E. Kuz'min, A. G. Artemenko, E. Varlamova, A. Kuz'mina, A. Tropsha, V. Makarov, O. Riabova, P. Wutzler, M. Schmidtke
2:00 216. Docking and 3-D-QSAR studies on isatin sulfonamide analogs as caspase-3 inhibitors. **Q. Wang**, R. H. Mach, D. E. Reichert
2:30 Intermission.
2:40 217. Prediction of cytochrome P450 mediated oxidation using induced fit docking. **M. Shelley**
3:10 218. Protein modeling and virtual screening to discover novel GSK-3 inhibitors. **P. Sivaprakasam**, P. R. Daga, A. Xie, **R. J. Doerksen**
3:40 219. Targeting the acetylcholine binding protein: A relaxed-complex approach to virtual screening. **A. Babakhani**, T. T. Talley, P. W. Taylor, J. A. McCammon

Section B

Salt Palace Convention Center
258

Quantum Chemistry
Materials. It's Where it's At!

A. E. Roitberg, *Organizer*

Y. Meng, *Presiding*

1:00 220. First-principles studies of octacyclopropylcubane: A novel high-energy density material. **S. L. Richardson**, R. N. Allen, D. Finkenstadt, M. J. Mehl, M. R. Pederson
1:30 221. Mechanism of thermal decomposition of carbamoyl phosphate and its stabilization by aspartate and ornithine transcarbamoylases. **Q. Wang**, J. Xia, V. Guallar, G. Krilov, E. R. Kantrowitz
2:00 222. Theoretical studies of uranyl complexes. **G. E. Schoendorff**, W. A. deJong, M. S. Gordon, T. L. Windus
2:30 223. Theoretical study on the interaction between xenon and positive silver clusters in the gas phase and on the (001) chabazite surface. **H. G. Nguyen**, G. Konya, E. M. Eyring, D. B. Hunter, T. N. Truong
3:00 Intermission.
3:10 224. Interfacing the effective fragment potential with the reactive force field. **S. A. Nedd**, M. S. Gordon
3:40 225. Using pseudo atoms to model silicon and silicon oxide surface chemistries with electronic structure theory. **H. P. Hratchian**, U. Das, G. A. Ferguson, K. Raghavachari

Please refrain from using cellular telephones and cameras during technical sessions.

ENVR

Division of Environmental Chemistry

S. Al-Abed, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Catalysis in Fuel Chemistry (see *FUEL*, Mon, Tue, Wed, Thu)

Coal Chemistry (see *FUEL*, Wed)

Emissions from Combustion Processes: Environmental Issues, Assessment, and Control (see *FUEL*, Tue)

Methods and Techniques in Analytical Characterization for Fuel Nanoscience (see *FUEL*, Mon)

Coprecipitation of Metals during Chemically and Biologically Induced Mineral Precipitation (see *GEOC*, Sun, Tue)

Geochemistry Division Award Symposium in honor of Fred T. Mackenzie (see *GEOC*, Mon)

Multiscale Reactions Including Fe-oxides, Oxyhydroxides, and Hydroxides (see *GEOC*, Tue, Wed)

Speciation and Kinetics in Natural Waters in Honor of Frank J. Millero (see *GEOC*, Tue, Thu)

Nanoscale Materials in Chemistry: Environmental Applications: In Honor of Professor Klabunde, I&EC Division Fellow (see *I&EC*, Mon)

Nanotechnology and the Environment: Emphasis on Green Nanotechnology (see *I&EC*, Sun, Tue, Wed, Thu)

SOCIAL EVENTS:
Dinner: Tue
Social Hour: Tue

BUSINESS MEETINGS:
Executive Committee Meeting: Sun
Long Range Planning Subcommittee Meeting: Sun
Program Planning Subcommittee Meeting: Sun

SUNDAY MORNING

Section A

Hilton
Alpine Ballroom West

New Energy Technology
Low Energy Nuclear Reactions: Introduction and Overview

J. Marwan, *Organizer, Presiding*

8:30 1. Introducing low energy nuclear reactions. **J. Marwan**
8:55 2. Low-energy nuclear reaction research: 2009 ACS update. **S. B. Krivit**
9:20 3. Condensed matter nuclear science discoveries. **S. R. Chubb Sr.**, T. A. Chubb
9:45 4. From cold fusion to condensed matter nuclear science: 20 years of research. **M. C. H. McKubre**
10:10 5. Twenty year history of LENR research using Pd/D codeposition. **F. E. Gordon**, S. Szpak, P. A. Mosier-Boss, M. H. Miles, L. Forsley
10:35 6. From the proof of principle to a working prototype. **A. De Ninno**
11:00 7. Practical use of nuclear quadrupole and internal magnetic field augmented LENR. **D. Cravens**, R. Gimpel, V. Golubic

‡ Cooperative Cosponsorship