COMP

DIVISION OF COMPUTERS IN CHEMISTRY

Final Program, 237th ACS National Meeting, Salt Lake City, UT, March 22-26, 2009

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**

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

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

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

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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

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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

Submit Final Program