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.


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


10:30 — Intermission.

10:40 —11. Statistically optimal free energy estimates from sparsely chosen states. M. Shirts, J. D. Chodera


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


10:00 —18. Path sampling for nonequilibrium processes in many-dimensional order-parameter spaces. A. R. Dinner

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*


1:40 — 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**


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**


3:05 — Intermission.


3:45 —32. Toward a fully quantum mechanical force field for simulations of biocatalysis. **D. M. York**


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**


3:00 —38. Simulating stimulating interfaces: Applications in adsorption and catalysis. **C. H. Turner**


4:00 —40. Fatty acid induced toxicity: Interactions with the lipid bilayer. **A. K. Sum**


**MONDAY MORNING**
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_


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


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


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


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
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

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


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

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


3:30 —68. Predictive chemical computing in condensed phases. S. Hirata, O. Sode, M. Keçeli, K. Yagi

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.


2:00 — _71_. New computational simulation techniques for nanosystems: Bridging the gap. **J. Maguire**, M. D. Benedict


2:50 — Intermission.


3:30 — _74_. Polymer nanophase multiscale modeling using CULGI. **J. Fraaije**, S. Nath


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


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


11:10 —88. Quantum Monte Carlo for the electronic structure of molecular systems. W. A. Lester Jr.


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


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. Itimie, P. Maurer

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


9:50 — Intermission.


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


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
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


2:45 — Intermission.

3:00 — 107. Polarizability effects and dispersion interactions in complexed molecules: Computational considerations. **K. K. Baldridge**


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


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


5:05 — 116. Computational chemistry at the petascale using NWChem and MADNESS. R. J. Harrison, E. Apra, W. A. Shelton

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.


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


3:55 — 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


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


135. Benchmark calculations of ammonium and nitrate ions in aqueous solution. K. Range


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

http://oasys.acs.org/acs/237nm/comp/staff/program.cgi?format=expande...
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


144. Developing reweighting-based molecular dynamics with sights set on converged long-timescale biomolecular simulations. D. Hamelberg


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


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


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

160. Pair-wise property-encoded shape distributions for comparing binding sites in proteins. **S. Das**, A. Kokardekar, C. M. Breneman


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**


165. Quantitative predictions of protein-ligand binding affinities. **D. L. Mobley**


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


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


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. **http://oasys.acs.org/acs/237nm/comp/staff/program.cgi?format=expande...**
Findlater, S. Hyde, Z. Wang, J. Song

177. Weighted ensemble path sampling simulations of conformational transitions in lymphotactin. **D. Bhatt**, D. M. Zuckerman


**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


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**

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 method 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 — Intermision.

3:10 — 192. Automated QSAR modeling to guide drug design. **O. Obrezanova, M. D. Segall**


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**

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**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


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. Doerkson, 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


11:40 — 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


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


11:10 — 213. Understanding the potential role of hydrogen bonding in drug discovery. D. C. Reuter, K. Brameld, S. Connolly

THURSDAY AFTERNOON
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


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. Sivaparakasam, P. R. Daga, A. Xie, R. J. Doerksen


Quantum Chemistry

Materials. It's Where it's At!

A. E. Roitberg, Organizer
Y. Meng, Presiding

1:00 — 220. First-principles studies of octacyclopropylocubane: 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 transcarbamoylase. Q. Wang, J. Xia, V. Guallar, G. Krilov, E. R. Kantrowitz


2:30 — 223. Theoretical study on the interaction between xenon and positive silver clusters in the gas phase

**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