COMP

DIVISION OF COMPUTERS IN CHEMISTRY

Final Program, 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007

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

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

I

C. F. Wong and R. A. Friesner, *Organizers*
D. Murray, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:40 —1. Reminiscing about chemical and biological applications of continuum electrostatics. **B. H. Honig**

9:25 —2. Proton and chloride pumping in bacterio and halo-rhodopsin. **M. R. Gunner**, Y. Song

9:55 —3. Binding entropies and free energies. **M. K. Gilson**

10:25 — Intermission.

10:40 —4. A modest proposal for the use of physical quantities in continuum electrostatics. **A. Nicholls**

11:10 —5. Interactions of cationic-hydrophobic peptides with lipid bilayers: A coarse-grained Monte Carlo simulation method. **N. Ben-Tal**

11:40 —6. Modeling protein-protein interactions with continuum electrostatics. **E. G. Alexov**

Section B

Unknown Site -- Unknown Room

Computer Assisted Drug Design: Reminiscing about the Future. A Symposium Honoring Yvonne C. Martin

Computer Assisted Drug Design: Reminiscing about the Future

Cosponsored with Abbott Laboratory. (NOTE: Coffee breaks and end of symposium reception sponsored by J. Computer-Aided Molecular Design) Other co-sponsors are, CINF, and WCC
O. F. Guner, *Presiding*
A. Tropsha, *Organizer, Presiding*

8:15 — Introductory Remarks.

8:30 —7. Using knowledge on chemical reactions for drug design. **J. Gasteiger**

9:00 —8. Experimental and computational approaches to measuring compound reactivity. **P. Hajduk**

9:30 —9. Drug Guru: A new kind of computational tool for medicinal chemists. **K. Stewart**

10:00 — Intermission.

10:20 —10. Pushing the boundaries of 3D-QSAR. **R. D. Cramer**

10:50 —11. Outliers in SAR and QSAR: What are the possible sources? **K. H. Kim**

11:20 —12. Do multi-conformer queries enhance three-dimensional lead hopping? **S. W. Muchmore**, Y. C. Martin

11:50 —13. Advances in conformational sampling. **D. K. Agrafiotis**, F. Zhu, S. Izrailev, A. Gibbs, E. Martin

Section C

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session I

A. E. Roitberg, *Organizer*
G. D. M. Seabra, *Presiding*

8:30 —14. Coupled-cluster and explicitly-correlated perturbation-theory calculations of the uracil anion. **M. S. J. Gutowski**, R. Bachorz, W. Klopper

9:00 —15. Ab initio study of the interaction of the phospolipid head-group with representative quartz and aluminosilicate structures. **J. Snyder**

9:30 —16. Quantum chemistry calculations of the methane dimer potentials. **S. D. CHAO**, A. H. -T.Li

10:00 —17. Density Functionals for Noncovalent Interaction Energies of Biological Importance. **Y. Zhao**, D. G. Truhlar

10:30 — Intermission.

10:45 —18. Validation of density functionals, semiempirical methods, and SCC-DFTB for Zn coordination chemistry. **E. A. Amin**, D. G. Truhlar

11:15 —19. TDDFT studies of 3-hydroxykynurenine and its photoproducts in primate eyes. **B. C. Dutmer**, T. M. Gilbert

11:45 —20. Accurate quantum chemical calculations of NMR chemical shifts and application to protein structure refinement. **Y. Zhang**, E. Oldfield

Measures of Accuracy and Reliability in Molecular Simulation

Materials Simulation

Sponsored by PHYS, Cosponsored with COMP

SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

II

C. F. Wong, R. A. Friesner, and D. Murray, *Organizers*
M. Gunner, *Presiding*

1:30 —21. Probing pH dependent conformational landscapes. **C. L. Brooks III**

2:00 —22. Prediction of long loops in proteins: improved sampling and continuum solvation model. **R. Friesner**

2:30 —23. Macromolecular simulations using continuum solvent models. **D. A. Case**

3:00 — Intermission.

3:15 —24. Protein folding using mechanism-based searching and implicit solvent models. **K. A. Dill**

3:45 —25. Implicit modeling of complex cellular environments. **M. Feig**

4:15 —26. Hybrid solvation model for MM–PB/SA free energy calculations. **H. Gohlke**, A. Metz

Section B

Unknown Site -- Unknown Room

ACS Award for Computers in Chemistry and Pharmaceutical Research

Session I

Cosponsored with WCC
J. D. Madura, *Organizer*
T. M. Chang, *Presiding*

1:30 —27. A new paradigm for high-temperature superconductors. **W. A. Goddard III**, J. Tahir-Kheli

2:00 —28. How ab initio calculations can help in the microscopic understanding of sensors and charge transport through molecules. **A. J. R. da Silva**

2:30 —29. Dopants in engineering materials – atomic effects on stability and structure. **K. M. Carling**

3:00 —30. First principles calculations of the widths of atomic resonances near surfaces. **P. Nordlander**, K. Niedfeldt, E. A. Carter

3:30 — Intermission.

3:45 —31. Embedded configuration interaction theory view of the many-body Kondo state. **P. Huang**, E. A. Carter

4:15 —32. The chemical reactivity of a nano graphene ribbon's zigzag edge. **D -E. Jiang**, B. G. Sumpter, S. Dai

4:45 —33. Insights into high temperature evolution of thermal barrier coatings from first principles. **B. Hinnemann**, E. A. Carter

Section C

Unknown Site -- Unknown Room

De Novo Design Coupled to Synthetic Feasibility

Session I

D. F. Ortwine, *Organizer*

1:20 — Introductory Remarks.

1:30 —34. Form follows function: The de novo design of pharmaceutically active compounds. **G. Schneider**

2:05 —35. De novo design revisited: Algorithm design, validation and qualification. **J. Wang**, I. A. Watson, M. A. Bell, Y. W. Webster, R. E. Higgs Jr., M. Vieth

2:40 — Intermission.

3:00 —36. De novo design of enzyme inhibitors by growing and scoring with BOMB. **W. L. Jorgensen**

3:35 —37. SynSPROUT and SPROUT-LeadOpt: de novo ligand design and optimization guided by virtual synthesis. **A. P. Johnson**, V. Valko, A. Valko, Z. Zsoldos, K. Boda, D. Reid

4:10 —38. Fragment based docking combined with synthetic planning: De novo eHiTS. **Z. Zsoldos**, A. Simon, D. Reid

Section D

Unknown Site -- Unknown Room

Thomas Kuhn Paradigm Shift Award Competition

A. Nicholls and A. G. Skillman, *Organizers*

2:00 —39. Massive, accurate empirical datasets: New tools for drug discovery and computational chemistry. **C. N. Hodge**

2:40 —40. Bridge chemistry and biology through HTS. **S. F. Yan**, F. J. King, Y. He, J. S. Caldwell, Y. Zhou

3:20 — Intermission.

3:40 —41. ADME modeling using structural data - Structure guided elimination of PXR activity. **Y. Gao**, S. H. Olson, J. Balkovec, Y. Zhu, I. Royo, J. Yabut, R. Evers, E. Y. Tan, W. Tang, D. P. Hartley, R. T. Mosley

4:20 —42. COSMO-RS: The Novel Bridge from Quantum Chemistry to Fluid Phase Thermodynamics. **A. Klamt**

Capturing Complexity in Physical Sciences Simulation

Chemical Kinetics and Dynamics

Sponsored by PHYS, Cosponsored with COMP

Computer Assisted Drug Design: Reminiscing about the Future. A Symposium Honoring Yvonne C. Martin

Sponsored by CINF, Cosponsored with COMP, and WCC

Measures of Accuracy and Reliability in Molecular Simulation

Enzyme and Ribozyme Function

Sponsored by PHYS, Cosponsored with COMP

MONDAY MORNING

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

III

C. F. Wong, R. A. Friesner, and D. Murray, *Organizers*
N. Ben-Tal, *Presiding*

8:45 —43. Applications of Poisson-Boltzmann and generalized Born methods to protein solubility and protein folding and binding stability and kinetics. **H -X. Zhou**

9:15 —44. Calculating ion permeation through biological channel proteins. **R. D. Coalson**

9:45 —45. Challenges in calculations of electrostatic energies in macromolecules. **A. Warshel**

10:15 — Intermission.

10:30 —46. Biological macromolecules interacting with mixed fluid lipid membranes. **A. Ben-Shaul**

11:00 —47. Modeling ion transport pathways through the bacterial chloride transporter. Z. Kuang, U. Mahankali, G. Feng, **T. Beck**

11:30 —48. Continuum electrostatic models of protein-membrane interactions. **D. Murray**, A. Mulgrew-Nesbitt

Section B

Unknown Site -- Unknown Room

ACS Award for Computers in Chemistry and Pharmaceutical Research

Session II

Cosponsored with WCC
J. D. Madura, *Organizer*
A. Venkatnathan, *Presiding*

8:30 —49. Dynamics in the first hydration shell of anions. **J. T. Hynes**

9:00 —50. Efficient global optimization: From cluster structures to protein folding. **B. Hartke**

9:30 —51. Para-selective nitration of toluene in beta zeolite – a computational study. **A. Andersen**, N. Govind, L. Subramanian

10:00 —52. Minimum free energy paths and isocommittor surfaces. **G. Ciccotti**

10:30 — Intermission.

10:45 —53. Role of surface dynamics in designing ordered organic nanostructures on Si and SiC dimerized surfaces via Car-Parrinello molecular dynamics. **R. L. Hayes**, M. E. Tuckerman

11:15 —54. From first-principles to the properties of ionic materials, via transferable interaction potentials. **P. A. Madden**

11:45 —55. First principles molecular dynamics of electronically excited DNA and RNA bases. **T. J. Martinez**, H. R. Hudock, A. Virshup, S. Yang

Section C

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session II

A. E. Roitberg, *Organizer*
A. Okur, *Presiding*

8:30 —56. DFT solvation studies of carbohydrates: The effect of different hydration models on the internal coordinates and alpha/beta anomeric ratios of epimers of glucose. **U. Schnupf**, J. L. Willett, F. A. Momany

9:00 —57. Analysis of OH stretching frequencies in glucose and glucose monohydrates calculated by DFT: Rotomer and water placement effects on the calculated spectrum. **W. B. Bosma**, U. Schnupf, J. L. Willett, F. A. Momany

9:30 —58. DFT optimization studies of alpha-Maltose: Iso-energetic and internal coordinate contour maps upon rotation about the glycosidic bonds. **F. A. Momany**, J. L. Willett, W. B. Bosma, U. Schnupf

10:00 —59. Coupled-cluster property calculations of aromatic molecules. **J. R. Hammond**, K. Kowalski, W. A. deJong

10:30 — Intermission.

10:45 —60. Topological investigation of strong intramolecular hydrogen bonding systems. **J. N. Woodford**

11:15 —61. Nucleophilic substitution at silicon (SN2@Si) via a central barrier: Evidence for the steric nature of the SN2 reaction barrier. **A. P. Bento**

11:45 —62. Stability of metallic nanoclusters and negative differential resistance in organic molecules.
S. K. Pati

Broadening Participation in Undergraduate Research

Part I

Sponsored by CHED, Cosponsored with CMA, WCC, YCC, SOCED, and COMP

Capturing Complexity in Physical Sciences Simulation

Condensed Matter

Sponsored by PHYS, Cosponsored with COMP

Chemistry Applications Involving Data Analysis and Visualization

I

Sponsored by CINF, Cosponsored with COMP

Measures of Accuracy and Reliability in Molecular Simulation

Simulation Methods / Force Fields

Sponsored by PHYS, Cosponsored with COMP

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

IV

C. F. Wong, R. A. Friesner, and D. Murray, *Organizers*
F. Sheinerman, *Presiding*

1:30 —63. Implicit solvent effective potentials for simulations of protein structure and dynamics: The AGBNP effective potential with applications to protein-ligand binding, and crystallographic refinement. **R. M. Levy**, A. K. Felts, E. Gallicchio, J. Knight, Z. Zhou

2:00 —64. Computed electrostatic properties of proteins: A powerful tool for annotation in the post-genomic age. **M. J. Ondrechen**

2:30 —65. Electrostatics in ligand binding and design. **B. Tidor**

3:00 — Intermission.

3:15 —66. Modeling membrane potentials: when does discreteness matter? B. Olsen, Y. Song, S. Lee, D. P. Tieleman, **N. A. Baker**

3:45 —67. Scaling in biomolecular hydration: A critical analysis of implicit solvents. C. Tan, **R. Luo**

4:15 —68. Membrane-mediated helix-helix interactions studied by potentials of mean force calculations in explicit and implicit membrane models. **W. Im**, J. Lee

Section B

Unknown Site -- Unknown Room

De Novo Design Coupled to Synthetic Feasibility

Session II

D. F. Ortwine, *Organizer*

2:00 —69. Practical synthetic accessibility – can we make that compound we just designed? **J. C. Baber**

2:30 —70. BIBuilder: A computational tool for receptor-based de novo design of drug-like molecules. **M. L. Teodoro**, I. A. Muegge

3:00 —71. Fragment-Based de novo Design. **C. Lemmen**, H. Claußen, M. Gastreich, J. Paern, J. Degen, M. Rarey

3:30 — Intermission.

3:45 —72. Combinatorial compound libraries: From virtual mining to synthesis. **F. Barbosa**

4:15 —73. Collaborative chemistry with rapid ligand prototyping: The MindRocket. **C. M. Ho**

4:45 —74. AllChem: Generating, searching, and manipulating 10^{20} synthetically accessible structures. **R. D. Cramer**, F. Soltanshahi, R. Jilek, B. Campbell

Section C

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics

Session I

E. X. Esposito, *Organizer*
J. A. Plumley, *Presiding*

1:00 —75. Ab initio Molecular Dynamics simulations of shock properties of water. **N. Goldman**, C. J. Mundy, I. F. W. Kuo, E. J. Reed, L. E. Fried, A. Curioni

1:30 —76. Medium effects on organic reactions featuring elimination mechanisms in pure and mixed solvents from QM/MM simulations. **O. Acevedo**

2:00 —77. Computational studies of the $[Ca_3P_2]_n$ n = 1, 2… cluster systems. **C. S. Palehepitiya Gamage**, D. S. Marynick, K. Ueno-Noto

2:30 —78. Modeling phase equilibria and transport in carbon dioxide expanded solvents. **K. Kuczera**, B. B. Laird, Y. Houndonougbo

3:00 — Intermission.

3:15 —79. Force dependence of phosphoryl transfer during DNA synthesis/repair by a high fidelity polymerase from Bacillus stearothermophilus (BF). R. Venkatramani, **R. Radhakrishnan**

3:45 —80. Long timescale dynamics of shocked nitromethane. E. J. Reed, **L. E. Fried**, M. R. Manaa, K. R. Glaesemann, J. Joannopoulos

4:15 —81. Atomistic simulation of a bound + mobile lubricant. **D. L. Irving**, D. W. Brenner

4:45 —82. Molecular dynamics simulation study of conformational and dynamic properties of self-assembled thiol monolayers on Au. **T. E. Dirama**, J. A. Johnson

Section D

Unknown Site -- Unknown Room

Rational Drug Design

Rational Drug Design I

M. R. Reddy, *Organizer*

2:00 —83. New developments in the Glide XP docking and scoring methodology. **R. Friesner**

2:30 —84. Comparative modeling and ligand binding of the dopamine transporter. **J. D. Madura**, M. Indarte, C. Surratt

3:00 —85. Accelerating Lead Discovery using Structure-based Paradigm: Genes to Leads®. **K. Ramnarayan**

3:30 —86. Progress in the development of an electron density enhanced scoring function in assessing ligand-receptor complexes. **M. D. Ryan**, M. J. Embrechts, C. M. Breneman

4:00 —87. CAESAR: a super fast conformation generation algorithm in Discovery Studio. J. Li, **K. Raghavan**, J. Sutter, A. Kulkarni

4:30 —88. Generalized knowledge-based approach to quickly generating diverse but energetically representative ensembles of ligand conformers. **R. D. Clark**, R. Dorfman, B. B. Masek

Broadening Participation in Undergraduate Research

Part II

Sponsored by CHED, Cosponsored with CMA, WCC, YCC, SOCED, and COMP

Capturing Complexity in Physical Sciences Simulation

Catalysis and Surfaces

Sponsored by PHYS, Cosponsored with COMP

Chemistry Applications Involving Data Analysis and Visualization

II

Sponsored by CINF, Cosponsored with COMP

Measures of Accuracy and Reliability in Molecular Simulation

Protein-Ligand Interactions

Sponsored by PHYS, Cosponsored with COMP

MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix

E. X. Esposito, *Organizer*

8:00 - 10:00

135, 142, 151, 153, 155, 159-161, 163-164, 167-168, 174-178, 180, 182-184, 188-189, 191, 193-194, 200-201, 203, 205-206, 208, 211-213, 216-217, 221, 225, 227, 229-230. See subsequent listings.

TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

V

C. F. Wong, R. A. Friesner, and D. Murray, *Organizers*
E. G. Alexov, *Presiding*

8:45 —89. Universal solvation models and their applications. **D. G. Truhlar**, C. P. Kelly, A. V. Marenich, A. Chamberlin, J. M. Smith, P. Jaque, N. Elmasry, C. J. Cramer

9:15 —90. Biomolecules and interfaces in solution. **B. M. Pettitt**

9:45 —91. Implicit solvent modeling of peptide-membrane interactions. **T. Lazaridis**

10:15 — Intermission.

10:30 —92. Implicit electrostatics in molecular docking. **R. Abagyan**, M. Totrov

11:00 —93. Reduction potentials of iron-sulfur proteins: From atomistic to continuum electrostatics. **T. Ichiye**

11:30 —94. Simple electrostatic models for fast protein docking. D. Kozakov, R. Brenke, **S. Vajda**

Section B

Unknown Site -- Unknown Room

ACS Award for Computers in Chemistry and Pharmaceutical Research

Session III

Cosponsored with WCC
J. D. Madura, *Organizer*
N. Govind, *Presiding*

8:30 —95. Importance of Shear in the bcc--to--hcp Transformation in Iron. **M. Ortiz**

9:00 —96. Orbital-corrected orbital-free density functional theory. **Y. A. Wang**, B. Zhou

9:30 —97. Unraveling chemistry under extreme conditions by atomistic simulations. **C. J. Wu**

10:00 —98. Multiscale simulations of complex materials for engineering and biological applications. **E. Kaxiras**

10:30 — Intermission.

10:45 —99. First-principles study of the effect of helium on the onset of dissociation in liquid hydrogen. **K. J. Caspersen**, F. Gygi, E. Schwegler

11:15 —100. Impact of local bonding interactions on condensed phase structure and reactivity. **E. A. A. Jarvis**, O. Coskuner, T. C. Allison, J. N. Crain, J. A. Stroscio, A. M. Chaka, M. D. Stiles

11:45 —101. Award presentation: synergy in computational science and engineering. **E. A. Carter**

Section C

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session III

A. E. Roitberg, *Organizer*
D. R. Roe, *Presiding*

8:30 —102. Deamidation of asparaginyl residues in peptides and proteins. **S. Catak**, G. Monard, V. Aviyente, M. F. Ruiz-López

9:00 —103. Rationalization the polymerization of acrylates. **V. Aviyente**, I. Degirmenci Jr., D. Avci Sr., V. Van Speybroeck Sr., K. K. Van Cauter Jr., M. Waroquier Sr.

9:30 —104. Angelis' Salt decomposition, a multi-scale study. **G. D. M. Seabra**, J. Torras-Costa, E. Deumens, S. Trickey, A. Roitberg

10:00 —105. Origin of high energy phosphoryl bonds. **J. D. Evanseck**, E. A. Ruben, M. S. Chapman

10:30 — Intermission.

10:45 —106. Stereoelectronic and steric factors in boron Lewis acid adducts of alpha,beta-enal compounds. **J. D. Evanseck**, J. A. Plumley

11:15 —107. Archetypal backside SN2 reactions: Effects of nucleophilicity and leaving-group ability. **A. P. Bento**, F. M. Bickelhaupt

11:45 —108. An in silico study of solvent effects on the Kolbe-Schmitt reaction kinetics. **L. E. Achenie**, I. Stanescu

TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

General Oral - Drug Discovery

Session I - Ligands: They're good for you!

I. Visiers, *Organizer*

1:30 — Introductory Remarks.

1:35 —109. Opening the 'black box': Interpreting in silico models to guide compound design. **E. J. Champness**

2:05 —110. Weighted lingos for fast similarity searching. **R. Sayle**, J. A. Haigh, J. A. Grant

2:35 —111. Active algorithm training—a key to accurate physicochemical property prediction. **G. Pearl**, K. Kassam, E. Kolovanov, S. Bhal

3:05 —112. Inverse design of quinoids-based inhibitors for redox regulation of Cdc25B. **S. Keinan**, D. N. Beratan, W. Yang, P. Wipf

3:35 — Intermission.

3:50 —113. Analysis and optimization of conformational search parameters for identifying bioactive conformations of drug-like molecules. **B. W. Sherman**, P. Dalal, J. C. Shelley

4:20 —114. Molecular grand-canonical ensemble theory and rational drug design. **O. A. von Lilienfeld**, M. E. Tuckerman

4:50 —115. Rational design of broad spectrum therapeutics using signature graph kernels. **J -L. Faulon**, S. Martin, J. Joo

Section B

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics

Session II

E. X. Esposito, *Organizer*
E. A. Ruben, *Presiding*

1:00 —116. Possible roles of mg2+ in hammerhead ribozyme catalysis from x-ray crystallography and molecular dynamics simulation. **T -S. Lee**, D. M. York

1:30 —117. Modeling G Protein-Coupled Receptors for structure-based drug discovery using low-frequency normal modes for refinement of homology models. **B. K. Rai**, G. J. Tawa, A. H. Katz, C. Humblet

2:00 —118. Characterizing the interactions between the antimicrobial peptide buforin II and nucleic acids with molecular dynamics simulations. **D. E. Elmore**, E. T. Uyterhoeven, D. Ko, C. H. Butler

2:30 —119. Dynamics of the interaction between factor Va and asymmetric mixed phospholipids. **T. Orban**, M. Kalafatis

3:00 — Intermission.

3:15 —120. Computational analysis of the searching and recognizing oxidative DNA lesion 8-oxo-guanine by formamido-pyrimidine DNA glycosylase. **K. Song**, C. De los santos, A. P. Grollman, C. Simmerling

3:45 —121. Quantitative in silico analysis of enzyme reactions: comparison of D-amino acid oxidase and monoamine oxidaze. **T. Hanai**

4:15 —122. Multiscale molecular modeling of biomembrane heterogeneities. S. V. Bennun, M. I. Hoopes, M. L. Longo, **R. Faller**

Section C

Unknown Site -- Unknown Room

Rational Drug Design

Rational Drug Design II

M. R. Reddy, *Organizer*

2:00 —123. FEP-Guided lead optimization for anti-HIV agents. **W. L. Jorgensen**

2:30 —124. Use of Computer-Assisted Drug Design in Drug Discovery: Limitations and Advantages of Available Computational Methods. **M. R. Reddy**, M. D. Erion, Q. Dang, P. D. van Poelje

3:00 —125. End-point binding free energy calculations with the LIE approach. J. Carlsson, M. Almlöf, M. Andér, **J. Aqvist**

3:30 —126. New tools for computer-aided drug-discovery. **M. K. Gilson**

4:00 —127. Accommodating receptor flexibility in structure based drug design. **R. E. Amaro**, J. A. McCammon

4:30 —128. In silico lead optimzation - results for a test set of Hsp90 ligands. **M. Brunsteiner**, P. A. Petukhov, N. Foloppe, C. Richardson

Capturing Complexity in Physical Sciences Simulation

Oxides and Hydrides

Sponsored by PHYS, Cosponsored with COMP

Measures of Accuracy and Reliability in Molecular Simulation

Protein Dynamics, Solvation, and Association I

Sponsored by PHYS, Cosponsored with COMP

TUESDAY EVENING

Section A

Unknown Site -- Unknown Room

Poster Session

J. D. Madura, *Organizer*

6:00 - 8:00

129. A basis set perspective on density functional performance. **B. P. Prascher**, B. Wilson, A. K. Wilson

130. Automated pharmacophore query optimization with genetic algorithms – case study of MC4R. **L. Jia**, J. Zou, H. Sun

131. Ab initio calculations on the intramolecular schmidt reaction. **J. M. Cannone**, J. L. Poutsma

132. Genetic function approximation insights into Plasmodium falciparum dihydrofolate reductase and farnesyltransferase inhibition. **P. Sivaprakasam**, A. Xie, P. N. Tosso, R. J. Doerksen

133. Hydrolysis in pure water: Car-Parrinello Metadynamics on the hydrolysis of esters at pH7. **H. Gunaydin**, K. N. Houk

134. Modified effective core potentials for the efficient modeling of metallocenes. **J. L. Lewin**, C. J. Cramer

135. Molecular dynamics simulations of R67 Dihydrofolate Reductase: Investigation into the cooperative binding. **C. Shi**, J. L. Poutsma

136. On the response of an ionic liquid to external perturbations and the calculation of shear viscosity. **Z. Hu**, C. J. Margulis

137. Optimization of ROMP poly(norbornene) as a catalyst support using molecular simulations. **A. T. Swann**, P. J. Ludovice

138. Prediction of olive oil - water partition coefficients for use in bioavailability models. **A. Chamberlin**, C. J. Cramer, D. G. Truhlar

139. Can we improve hit identification by accounting for conserved water molecules in binding sites ? **M. Brunsteiner**, R. Uddin, P. A. Petukhov

140. Probing the Energetic and Structural Role of Non-covalent Interactions in HIV protease. **S. Alla**, R. Garg, S. Kumar, N. S. Garikapati

141. Investigation of interactions between chemical weapons agents and simulants and Al_2O_3 clusters using quantum chemistry approaches. J. R. Plourde, W. P. Murdock Jr., T. J. Evans, **B. Setser**

142. Study of structure-activity relationship of steroidal alkaloids analogues as inhibitors of butyrylcholinesterase by three-dimensional quantitative modeling technique. **R. Uddin**, Z. Ul Haq

143. Comparison of basis set superposition errors for cc-pVnZ and pc-n basis sets. M. S. Marshall, **T. P. Hamilton**

144. Computational analysis of the role of key residues of formamido-pyrimidine DNA glycosylase in lesion recognition. **K. Song**, C. De los santos, A. P. Grollman, C. Simmerling

145. Computational chemistry as a dialogue: connections and components. **A. D. Walkingshaw**, T. O. H. White, P. Murray-Rust

146. Implementation of non-local electrostatic paradigm opens the door for accurate modeling of electrostatic interactions at the macromolecule-solvent interface. **A. Rubinstein**, S. Sherman

305. Orthogonal approach to mass spectral interpretation and library searching. **D. L. Sweeney**

148. Sub-Kelvin high magnetic field polarization-phase selective electronic structure studies: Challenges for quantum chemistry. **K. Rupnik**

149. Computational studies of tertiary structure of lysyl oxidase using the method of dynamic formation and breaking of disulfide bonds. **D. F. Ryvkin**, J. Bluhm

150. π-π Interactions in heterocyclic molecules. **P. Kundu**, J. F. Capitani, A. Mitra, P. J. Seaton

151. *Ab Initio* and DFT benchmark study for nucleophilic substitution at carbon (SN2@C) and silicon

(SN2@Si). **A. P. Bento**, M. Solà, F. M. Bickelhaupt

152. Database docking of protonation/tautomeric forms of selected antagonists with the Alpha-2A adrenergic receptor homology models. **W. Asher**, K. Pacheco, D. Bautista

153. A new efficient two-electron integration scheme. **Y. Feng**, X. Li

154. Discovery of electronic mechanism of concerted cycloadditions based on quantum chemical calculations. **S. Sun**

155. Ab initio method for the reactions between hydrogen chloride and protonated ^{i}propyl- and ^{t}buthyl chlorides. **P. U. Civcir**

156. Effect of cyanine-3 dye on the stability of oligonucleotide hybrid duplex on microarrays: a molecular dynamics simulation study. **Z. Wang**, N. He

157. Accelerated minimization of nudged elastic bands for determining minimum energy paths of transitions. E. Jónsson, **H. Jónsson**

158. Effect of environmental parameters on the chemical signature of TNT in soil, validation of numerical simulations. **M. Irrazabal**, V. Florian, M. E. Castro, S. P. Hernandez, J. Briano

159. Adsorption of TNT and its degradation products in soil organic matter: ab initio calculations. **M. Irrazabal**, J. Briano, A. Hernandez

160. Algorithms for fragment based drug discovery. **H. O. Villar**, J. Hodges, M. R. Hansen

161. Alpha2C QSAR studies on a database of ligands optimally protonated for physiological conditions. **K. Pacheco**, W. Asher, D. Bautista

162. Electronic organizing elements of boron Lewis acid adducts of α,β-enal compounds. **J. A. Plumley**, J. D. Evanseck

163. An improved REMD sampling method: Temperature intervals with global energy reassignment (TIGER). **X. Li**, G. Collier, C. O'Brien, F. Wang, N. Vellore, D. A. Bruce, B. Dominy, S. J. Stuart, R. A. Latour Jr.

164. Analysis of charge distribution in excited states of substituted benzenes. **S. Cooks**, T. P. Hamilton

165. Estimation of normal frequencies and vibrational entropies from quasi-Newton Hessian optimization. **S. Wlodek**, A. G. Skillman, A. Nicholls

166. Examining the effects of the nucleophile and leaving group in the cleavage of phosphonate ester derivatives. **L. A. Kopff**, E. R. Kuechler, E. V. Patterson

167. Aromatic substituent effects on arene-arene binding energies. **S. Beg**, M. Lewis

168. Atomistic simulation of nanostructure of solvated polymer electrolyte membrane and small molecule transport. **A. Venkatnathan**, R. Devanathan, M. Dupuis

169. Automate setup for molecular dynamics simulations of protein/membrane complexes. **R. Kumar**,

S. Jo, V. G. Iyer, W. Im

170. Calculations on hexafluorocyclopropane and Its "bond-stretched invertomer". **H. Wei**, D. A. Hrovat, W. T. Borden

171. Fragment linking using molecular shape. **G. Skillman**, A. Nicholls

172. CHARMM-GUI: A graphical user interface for the CHARMM users. **R. Kumar**, **V. G. Iyer**, W. Im

173. Cheminformatics: Chelation vs. toxicity. **A. C. Lee**, G. M. Crippen

174. Comparing field-based and atom type-based electrostatic similarity. **R. Tolbert**, G. Skillman, P. Hawkins, A. Nicholls

175. Mechanism of the Schmidt reaction. **D. G. English**, J. L. Poutsma

176. Computational approach for predicting biodegradation rates of alkylnaphthalenes. **V. Librando**, **A. Alparone**

177. Computational modeling and Brownian dynamics simulation of C. reinhardtii hydrogenase - ferredoxin docking complexes. **H. Long**, C. H. Chang, P. King, M. L. Ghirardi, K. Kim

178. Computational studies of metalloporphyrin-oxygen systems. **J. Lennartz**, J. M. Galbraith

179. Computational studies on RPE65. **H. Guo**, C. Zheng, E. R. Gaillard

180. Effects of binding and wave difusion during controlled rate drug delivery. **K. R. Sharma**

181. On the separation of styrene from ethylbenzene using a Z step-wise cross-current extraction procedure. **K. R. Sharma**

182. Computational studies on the nucleophilic destruction of nerve agent VX. **K. A. Daniel**, L. A. Kopff, E. V. Patterson

183. Computational study of IdeS inhibitors. **R. A. Grimminger**, J. P. Wolbach

184. Computer modeling study of small molecular inhibitors of ubiquitin-activating enzyme (E1). **Z. Hu**, Y. Yang, W. M. Southerland

185. Performance of density functional theory for transition metal-containing complexes using correlation consistent basis sets. **S. M. Tekarli**, T. R. Cundari, A. K. Wilson

186. R67 Dihydrofolate Reductase: Full ligand binding modes and effects on binding cooperativity. **J. L. Bass**, **J. L. Poutsma**

187. Computer simulation of Escherichia coli peptide déformylase. **A. Chikhi**

188. Conformational interconversion mechanisms of tetraoxacyclohexanes (Tetraoxanes): A theoretical study. **F. Freeman**, C. Cha, E. Derek, C. Do, J. H. Hwang, L. Phung, Q. T. Phung, T. Picorelli, T. Wang

189. Density functional computations of substituent effects on energetics of ethylene polymerization mediated by zirconocene catalysts. **P. Das**, D. C. Becker, D. G. McGuire

190. Relative stability of intermediates in the lipid peroxidation of arachidonic acid. **C. E. Tornow**, M. C. Milletti

191. Development of docking protocols and scoring functions using frequent geometric and chemical patterns of inter-atomic interactions at the interface of protein-ligand complexes. **R. Khashan**, W. Zheng, A. Tropsha

192. Effect of modifications on the dihedral angles of peptide nucleic acids. **A. K. Manukyan**, J. Radkiewicz-Poutsma

193. Electron attachment to the microsolvated Watson-Crick guanine cytosine base pair. **J. D. Zhang**, H. F. Schaefer III

194. Estimation of Vitamin-D Receptor Ligand Binding Affinity using a New Multi-Step Computer-Aided Approach. **S. Dakshanamurthy**, M. N. Islam, S. shah, S. Byers

195. Evaluation of descriptors that discriminate between CYP metabolized substrates. **J. H. Block**, D. Henry

196. Exploring folding landscapes with a flavored Go model. **R. D. Hills Jr.**, S. Kathuria, R. C. Matthews, C. L. Brooks III

197. Tautomerization mechanisms in 2-pyrimidinethiols: A theoretical study. **F. Freeman**, H. N. Po

198. Factors that shift Lewis acid catalyzed aza-Diels-Alder reactions to a stepwise mechanism. **A. J. Ross**, J. D. Evanseck

199. Valence bond interpretation of 4 electron, 3 center g systems. **A. DeBlase**, J. M. Galbraith

200. FLIPDock: Docking flexible ligands into flexible receptors. **Y. Zhao**, M. F. Sanner

201. High-speed pseudo-orthogonalization for the Car-Parrinello method. **U. Nagashima**, T. Aoyama

202. Implemention of the fast multipole method in molecular dynamics. **R. G. Ormseth**, R. Pachter

203. Implicit solvation modeling drug permeability of Caco-2 membranes. **N. Elmasry**, C. P. Kelly, C. J. Cramer, D. G. Truhlar

204. Improvement of nonbonded QM/MM interaction energies. **T. J. Giese**, D. M. York

205. Inhibitors of pantothenate synthetase: Initiating a quest for new tuberculosis drugs. **P. A. Petukhov**, M. Brunsteiner, R. Uddin

206. Intersystem crossing dynamics in acetylene. **B. M. Wong**, R. L. Thom, R. W. Field

207. Investigating M20 loop conformers of dihydrofolate reductase. J. Poutsma, **J. A. Tibbitt**

208. Investigation of interactions between chemical weapons agents and simulants and SiO_2 clusters

using quantum chemistry approaches. J. R. Plourde, W. P. Murdock Jr., T. J. Evans, **K. McConkey**

209. Kinetic isotope effects and free energy barriers of methyl triphosphate hydrolysis. Y. Liu, **D. M. York**

210. Modeling of human glutathione synthetase. An ATP-Grasp enzyme. **M. E. Anderson**, T. R. Cundari, A. Dinescu, M. Carter, S. Hernandez

211. Molecular dynamics simulations of oligonucleotide hybrid duplexes containing different length of poly-thymidine spacer sequence with one end tethered: free energy comparison and stability analysis. **Z. Wang**, **S. Li**, **N. He**

212. Molecular dynamics study of inhibitor binding to bacterial ribosome. **X. GE**, B. Roux

213. Molecular orbital of fragment molecular orbital method with Sakurai-Sugiura method on grid computing environment. **U. Nagashima**, T. Watanabe, Y. Inadomi, H. Umeda, T. Ishimoto, T. Sakurai

214. MRPT investigations of the ground state of NiO_2. **J. Song**, G. Schoendorff, Y. G. Khait, M. R. Hoffmann

215. Olefin coordination effects upon aza-bis(oxazoline) copper(I) catalyzed cyclopropanation. **L. M. Matosziuk**, J. D. Evanseck

216. P450 inhibition: some insights from data mining, docking and crystal structural studies. **H. Wang**, P. Orth

217. Predicting and validating the binding site of Telmisartan: Molecular dynamics simulation of the G-protein-coupled Angiotensin II receptor. **A. Patny**, P. V. Desai, M. A. Avery

218. Pressure annealing as a complement to simulated annealing for conformational sampling of long-chain oligomers. **R. A. Wheeler**, C. A. Hixson

219. Protein Interaction Score (PI-Score): The derivation and validation of a novel empirical free energy function that explains and predicts protein-protein binding affinities. **J. Audie**

220. PI-Score and accurate protonation state assignment can be used to rationalize the binding thermodynamics of the OppA peptide binding protein. J. Audie, **C. Bleaken**, M. M. Cheng

221. Secondary structure bias in generalized Born solvent models: Comparison of conformational ensembles and free energy of solvent polarization from explicit and implicit solvation. **D. R. Roe**, V. Hornak, C. L. Simmerling

222. Side-chain and backbone ordering in homopolymers. **Y. Wei**, W. Nadler, U. H. Hansmann

223. Stability and structure of oligomers of the Alzheimer peptide from computer simulations. **J. Zheng**, B. Ma, H. Jang, R. Nussinov

224. Steered molecular dynamics (SMD) simulation of anthrax edema factor translocation through a protective antigen pore. **M. R. Lacina**, A. Loccisano, J. D. Evanseck

225. Stereoelectronic effects in phosphates. **E. A. Ruben**, J. D. Evanseck, M. S. Chapman

226. Structure determination of water clusters of serotonin and its protonated form using computational method. **Y. S. Lee**, H. J. Lee, S. Jang, S. H. Lee, S. I. Jin, J. Y. Lee, C. R. Park

227. Substrate binding and kinetic aspects of the oxygenation reaction mechanism in COX-1. **M. A. Lukowski**, M. C. Milletti

228. The structural origin of melting temperatures in DNA dumbbell conjugates as determined by molecular dynamics. **M. McCullagh**, G. C. Schatz, F. D. Lewis

229. The structure and organization of fatty alcohols at the water/vapor interface: A molecular dynamics study. **T -M. Chang**, M. M. Dolnik

230. The theory study on the absorption chromatograph of Cd(II) complex with 2,2'-bipyridine and terephthalate. **L. Chen**

231. Using ensembles of protein conformations in structure-based drug discovery. **K. L. Damm**, K. L. Meagher, H. A. Carlson

Section B

Unknown Site -- Unknown Room

Chemical Computing Group Graduate Student Excellence Award

A. C. Good, *Organizer*

6:00 - 8:00

232. Neural network and ab initio studies of metal hydride nanoparticles. **W. O. Griffin**, J. A. Darsey

233. Externally Corrected Coupled-Cluster Methods Employing Method of Moments of Coupled-Cluster Equations and Multi-Reference Perturbation Theory. **M. D. Lodriguito**, P. Piecuch

234. Molecular Dynamic Simulations help capture TB-drug-design's most wanted: Mechanism of active site loop ordering. **S. B. Rafi**, K. Song, T. J. Sullivan, C. Kisker, P. J. Tonge, C. Simmerling

235. Electron-Phonon Coupling in Organic Semiconductors: A DFT-based Approach. **R. S. Sánchez-Carrera**, V. Coropceanu, P. Paramonov, J -L. Brédas

236. Monte Carlo investigations of fundamental properties of organic molecules in the gas and liquid phases. **L. L. Thomas**, T. J. Christakis, W. L. Jorgensen

WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

VI

C. F. Wong, R. A. Friesner, and D. Murray, *Organizers*
M. K. Gilson, *Presiding*

8:45 —237. Development and application of a Poisson-Boltzmann/semiempirical quantum mechanical method to problems in protein structure and function. **K. M. Merz Jr.**

9:15 —238. Excitation energy transfers in condensed phases: a quantum mechanical solvation model. **B. Mennucci**

9:45 —239. Electrostatics and boundary condition for QM/MM simulations. **Q. Cui**

10:15 — Intermission.

10:30 —240. Methods for treatment of the solvated macromolecular environment in simulations of phosphoryl transfer reactions in solution and in ribozymes. **D. M. York**

11:00 —241. Implicit solvation in QM/MM and QM calculations on proteins. **J. H. Jensen**, H. Li, D. Fedorov, K. Kitaura, M. S. Gordon

11:30 —242. A quantum method for calculation of protein solvation energy. **J. Z. Zhang**, Y. Mei, C. G. Ji

Section B

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session IV

A. E. Roitberg, *Organizer*
K. Song, *Presiding*

8:30 —243. Molecular conductance from density functional theory calculations. **D. Kosov**, Z. Li

9:00 —244. Alcohol-water mixing from first principles. **L. V. Slipchenko**, J. M. Mullin, M. S. Gordon

9:30 —245. DFT and AIM studies of strong intramolecular hydrogen bonding. **J. N. Woodford**, K. W. Elliott, D. W. Brown, M. Lewis, R. Hansen, W. Richards

10:00 —246. Neutral vanadium oxide clusters and their reactions with sulfur dioxide: Interaction of theory and experiment. **E. Jakubikova**, S -G. He, Y. Xie, Y. Matsuda, E. R. Bernstein

10:30 — Intermission.

10:45 —247. Computational investigation of Bi containing pyrochlores. **B. B. Hinojosa**, A. Asthagiri

11:15 —248. First-principles studies of sila-diamondoids. **S. L. Richardson**, R. R. Zope, T. Baruah, M. R. Pederson

11:45 —249. Calculation of crystal structures using semiempirical methods. **J. J. P. Stewart**

Section C

Unknown Site -- Unknown Room

Rational Drug Design

Rational Drug Design III

M. R. Reddy, *Organizer*
K. Raghavan, *Presiding*

9:00 —250. Assessing, improving and using grid-based docking algorithms in CHARMM. **C. Brooks III**

9:30 —251. Cheminformatics approaches to ligand docking and scoring. **A. Tropsha**

10:00 —252. FLIPDock: Docking Flexible Ligands into Flexible Receptors. **Y. Zhao**, M. F. Sanner

10:30 —253. Simultaneous docking and virtual screening against multiple targets: Application to protein kinase inhibitors. S -Y. Huang, **X. Zou**

11:00 —254. Identification and characterization of hot spot regions in druggable protein binding sites by computational solvent mapping. **M. R. Landon**, D. Lancia, S. C. Thiel, S. Vajda

11:30 —255. Insights into the metal chelating mechanism in urease inhibitors using molecular docking simulation and 3D-QSAR analysis. **Z. Ul Haq**, M. A. Lodhi, M. I. Choudhary

Advanced mining and use of life science information

Sponsored by CINF, Cosponsored with CSA Trust, BIOT, COMP, BTEC, and MEDI

Measures of Accuracy and Reliability in Molecular Simulation

Protein Dynamics, Solvation, and Association II

Sponsored by PHYS, Cosponsored with COMP

WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

General Oral - Drug Discovery

Session II - Proteins: Got binding?

I. Visiers, *Organizer*
E. X. Esposito, *Presiding*

1:30 —256. Binding of anti-fusion peptides with HIVgp41 from molecular dynamics simulations. **R. C. Rizzo**, B. Strockbine

2:00 —257. An efficient method for docking flexible peptides to rigid receptors. **J. Audie**, K. Hannigan, K. Naik

2:30 —258. Blind evaluation of absolute binding free energies of eight ligands to CHK1 kinase. **H. Fujitani**, A. Matsuura, A. Tomonaga, M. S. Head

3:00 —259. Analyzing binding sites of ATP-binding proteins to aid in designing inhibitors specific to class II aminoacyl tRNA synthetase. **S. C. K. Sukuru**, L. A. Kuhn

3:30 — Intermission.

3:45 —260. Docking of selected compounds with alpha1A adreneroceptor. **D. Bautista**, W. Asher, S. Hoskins

4:15 —261. Development of docking protocols and scoring functions using frequent geometric and chemical patterns of inter-atomic interactions at the interface of protein-ligand complexes. **R. Khashan**, W. Zheng, A. Tropsha

4:45 —262. High throughput binding free energy calculations with different solvent models. **D. Risal**

5:15 —263. Improving binding affinity prediction through docking into X-Ray and computationally derived receptor ensembles. **S. N. Rao**, B. W. Sherman, P. Sanschagrin, J. R. Greenwood, R. Farid

Section B

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics

Session III

E. X. Esposito, *Organizer*

J. A. Plumley, *Presiding*

1:00 —264. A dynamically equilibrated solutional structural model for human factor VIIIa: A Homology modeling and MD refinement Study. **D. Venkateswarlu**

1:30 —265. Exploration of conformational transitions and enhanced sampling in simulations of HIV protease. **I. pflaum**, C. L. Simmerling

2:00 —266. Unfolding of AAAAA(AAARA)$_3$A: A molecular dynamics study. **E. Asciutto**, J. D. Madura, S. Asher

2:30 —267. Improving Convergence of Replica Exchange Simulations through Coupling to a High Temperature Structure Reservoir. **A. Okur**, D. R. Roe, G. Cui, V. Hornak, A. E. Roitberg, C. Simmerling

3:00 — Intermission.

3:15 —268. Functional Role of Asp160 in the Ammonia/Ammonium Transporter Proteins: A Molecular Dynamics Simulation Study. **Y. Lin**, Y. Mo

3:45 —269. Secondary structure bias in generalized Born solvent models: Comparison of conformational ensembles and free energy of solvent polarization from explicit and implicit solvation. **D. R. Roe**, V. Hornak, C. L. Simmerling

4:15 —270. Hydrophobic cooperativity as a mechanism for amyloid nucleation. **R. D. Hills Jr.**, C. L. Brooks III

Section C

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session VI

A. E. Roitberg, *Organizer*
A. Okur, *Presiding*

1:30 —271. Diameter and electronic structure dependence of noncovalent interactions between cytosine and SWCNT: QM/MM study. **Y. Wang**

2:00 —272. Remarkable group additivity properties from DFT calculations: total energy and frontier orbital energies and shapes. **M. E. Zandler**, L. Opara, F. D'Souza

2:30 —273. Static DFT and Car-Parinello molecular dynamics dimulation of ethanol electro-oxidation on bimetallic nano-particles. **Y. Wang**

3:00 —274. Thermodynamic considerations in hydrogen containing materials using abintio DFT calculations. **A. J. Ramirez-Cuesta**

3:30 — Intermission.

3:45 —275. Transition metals catalyzed $NaAlH_4$(001) surface for hydrogen storage. **J. Liu**, Q. Ge

4:15 —276. Density functional theory study of the growth of InN on the Si(001) surface. **J. M. Hawkins**, A. Asthagiri

4:45 —277. First-principles study of ethanol adsorption on Si (111) surfaces. **A. V. Gavrilenko**, C. E. Bonner Jr., V. I. Gavrilenko

Broadening Participation in Undergraduate Research

Part III

Sponsored by CHED, Cosponsored with CMA, WCC, YCC, SOCED, and COMP

Capturing Complexity in Physical Sciences Simulation

Nanotechnology

Sponsored by PHYS, Cosponsored with COMP

Measures of Accuracy and Reliability in Molecular Simulation

Force Fields / Simulation Methods

Sponsored by PHYS, Cosponsored with COMP

THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models

VII

R. A. Friesner and D. Murray, *Organizers*
C. F. Wong, *Organizer, Presiding*

8:45 —278. Hybrid supermolecule-continuum approach to first-principles electronic structure calculations of absolute solvation free energies of ions and activation free energies of chemical reactions. **C -G. Zhan**

9:15 —279. The SCP-ISM and long-time simulations for studying protein and peptide self-oligomerization. **E. L. Mehler**

9:45 —280. Variable probe molecular surface (VPMS): Implications for continuum solvent calculations. **E. O. Purisima**, S. Bhat

10:15 —281. Computing pKa shifts of turkey ovomuvoid third domain (OMTKY3) residues with a polarizable force field. **G. A. Kaminski**, C. M. MacDermaid

10:45 — Intermission.

11:00 —282. AMBER Score in DOCK6: Application of molecular dynamics simulations and implicit solvent model (GB/SA) in protein-ligand docking. **D. M. Shivakumar**, D. A. Case

11:30 —283. Effect of implicit versus explicit solvation models on saccharide conformations: a free energy study. **M. M. Kuttel**

Section B

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session V

A. E. Roitberg, *Organizer*
G. D. M. Seabra, *Presiding*

8:30 —284. Spin-orbit hybrid DFT studies of actinide oxidation states. **P. J. Nichols**, E. J. Bylaska, W. A. de Jong

9:00 —285. Quantum Molecular Dynamics and Computational Fluid Dynamics Study on Phase Change Behavior of Water under Laser Irradiation. **H. Takaba**, A. Nomura, Y. Sasaki, K. Chiba, H. Hata, H. Tsuboi, M. Koyama, N. Hatakeyama, A. Endou, M. Kubo, C. A. Del Carpio, M. Kitada, S. Muroga, A. Miyamoto

9:30 —286. Beyond exciton theory: A time-dependent DFT and Franck-Condon study of perylene diimide and its chromophoric dimer. **A. Clark**

10:00 —287. Quantum Chemical Molecular Dynamics Study on the Bond Dissociation of Excited Water Molecules. **A. Endou**, A. Nomura, Y. Sasaki, K. Chiba, H. Hata, H. Tsuboi, M. Koyama, N. Hatakeyama, H. Takaba, M. Kubo, C. A. Del Carpio, M. Kitada, S. Muroga, A. Miyamoto

10:30 — Intermission.

10:45 —288. Optimized Configuration Interaction Method for Electronic Excitations in Nanostructures.

A. Franceschetti, C. Troparevsky

11:15 —289. Exciton scattering and localization in branched dendrimeric structures. C. Wu, **S. Tretiak**, V. Chernyak

11:45 —290. Hybrid molecular dynamics-quantum mechanics simulations of solute spectral properties in the condensed phase: Evaluation of simulation parameters. M. C. Zwier, J. M. Shorb, **B. P. Krueger**

Section C

Unknown Site -- Unknown Room

Rational Drug Design

Rational Drug Design IV

M. R. Reddy, *Organizer*
K. Raghavan, *Presiding*

9:00 —291. Combining ligand and structure-based design. **M. McGann**, G. Skillman

9:25 —292. Cell-based pharmaceutical design of cell permeant-nontoxic, extracellular targeting molecules. **G. R. Rosania**

9:50 —293. Targeting protein–protein interactions in the Wnt signaling pathway: Discovery and development of small molecules for the treatment of cancer, osteoporosis, and other Wnt related diseases using structure-based drug design techniques. **J. Shan**, Y. Zhang, X. Li, P. Liu, D -L. Shi, J. Wang, D. Liu, D. Wu, J. Zheng

10:15 —294. Analysis of Multiple SAR Models from Regression and Classification Methods. **R. R. Gupta**, E. A. Jamois, K. Subramanian

10:40 —295. Using shape and electrostatics to predict bioisosteric pairs. **G. Skillman**, P. Hawkins, A. Nicholls

11:05 —296. Rational design of an enzyme mutant for anti-cocaine therapeutics. D. Gao, W. Yang, H. Cho, Y. Pan, H -H. Tai, **C -G. Zhan**

11:30 —297. An iterative knowledge-based scoring function to predict protein-ligand interactions. S -Y. Huang, **X. Zou**

11:55 —298. Virtual Screening of Cathepsin K inhibitors using Docking and Pharmacophore Models. **M. Sumakanth**, R. Muttineni

Capturing Complexity in Physical Sciences Simulation

Electronic Structure Methods

Sponsored by PHYS, Cosponsored with COMP

Measures of Accuracy and Reliability in Molecular Simulation

Ion Channels / Membranes

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THURSDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

General Oral - Drug Discovery

Session III - Data Mining: Finding what's important!

I. Visiers, *Organizer*

1:30 —299. Development of DARS (Decoys As the Reference State) potentials for docking and scoring. D. Kozakov, R. Brenke, M. R. Landon, S. R. Comeau, **S. Vajda**

2:00 —300. eHiTS and the Sun Grid Compute Utility: using massively parallel computation for docking. **D. Reid**, A. Simon, Z. Zsoldos, B. Sadjad, M. Duey, B. Foley

2:30 —301. Mobius: a Molecular and Biological Information Utilization System to drive Discovery. **M. S. Lajiness**

3:00 —302. Reverse fingerprinting and mutual information-based activity labeling and scoring (MIBALS). **S. Schreyer**, C. Williams

3:30 — Intermission.

3:45 —303. Combining ligand- and structure-based approaches: Database screening with pharmacophores derived from fragment docking. **B. W. Sherman**, R. Farid

4:15 —304. Nature of binding between glycopeptide antibiotics and bacterial cell walls. **J -G. Lee**, C. Sagui, C. Roland

4:45 —305. Orthogonal approach to mass spectral interpretation and library searching. **D. L. Sweeney**

Section B

Unknown Site -- Unknown Room

General Oral - Molecular Mechanics

Session IV

E. X. Esposito, *Organizer*
E. A. Ruben, *Presiding*

1:00 —306. Custom-Designed Nesting Sites for Biological Molecules on Material Surfaces. **P. Kral**, B. Wang

1:30 —307. Denaturation of hen egg white lysozyme in electromagnetic fields: a molecular dynamics study. **N. J. English**

2:00 —308. Flexible boundary hybrid solvation model for biomolecular simulations. **G. Krilov**

2:30 — Intermission.

2:45 —309. Replica exchange with dynamical scaling: a new approach for large systems. **S. Rick**

3:15 —310. Hybrid monte carlo and molecular dynamics simulation of mixed lipid bilayer systems: Methods and applications. **Y. Jiang**, J. D. Joannis, K. Khanna, J. T. Kindt

3:45 —311. Dielectric effect dissected and reassembled. **E. G. Zoebisch**

Section C

Unknown Site -- Unknown Room

General Oral - Quantum Chemistry

Session VII

A. E. Roitberg, *Organizer*
D. R. Roe, *Presiding*

1:30 —312. Impact of correlation consistent basis sets on transition metal species. **T. G. Williams**, A. K. Wilson

2:00 —313. Beyond BMK: adventures in hemi-semiempirical density functionals. **J. M. Martin**, A. Tarnopolsky, A. Karton, A. D. Boese

2:30 —314. Molecular symmetry and variational perturbation theory in analytic density functional theory. **B. I. Dunlap**

3:00 —315. Molecular grand-canonical ensemble density functional theory. **O. A. von Lilienfeld**, M. E. Tuckerman

3:30 — Intermission.

3:45 —316. Accurate self-interaction correction to semilocal density functionals. **H. Jónsson**, K.

Tsemekhman, E. J. Bylaska

4:15 —317. Restricted-open-shell complete basis set (ROCBS-QB3) model chemistry. G. P. F. Wood, L. Radom, G. A. Petersson, **E. C. Barnes**, M. J. Frisch, J. A. Montgomery Jr.

4:45 —318. Variational approaches for optimizing electron distribution functions. **P. W. Ayers**

Capturing Complexity in Physical Sciences Simulation

Liquids and Interfaces

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