COMP

DIVISION OF COMPUTERS IN CHEMISTRY

Final Program, 230th ACS National Meeting, in Washington, DC, Aug 28-Sept 1, 2005

W. D. Cornell and J. D. Madura, *Program Chairs*

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Inorganic/Organic Applications and Methods

Cosponsored with PHYS
R. B. Ross and S. Mohanty, *Organizers*
A. McCormick, *Presiding*

8:05 — Introductory Remarks.

8:15 —1. Modeling spontaneous formation of precursor nanoparticles in clear-solution zeolite synthesis. **S. M. Auerbach**, M. Jorge, P. Monson

8:50 —2. Multiscale Modeling of the Electronic Properties and Quantum Conductance of Carbon Nanotubes Doped by Encapsulation of Organic Molecules. **B. G. Sumpter**, V. Meunier

9:25 —3. Multiscale Simulations of Polymer Modified Fullerenes in Aqueous Solution. **G. D. Smith**, D. Bedrov

10:00 — Intermission.

10:10 —4. Multiscale simulations of soft condensed systems. **S. K. Kumar**

10:45 —5. Multiscale simulation of the assembly and properties of nanostructured organic/inorganic hybrid materials. **C. McCabe**

11:20 —6. Multiscale modeling and simulation of polymer-tethered silsesquioxane assemblies. **E. R. Chan**, X. Zhang, C -Y. Lee, M. Neurock, A. Striolo, C. McCabe, P. T. Cummings, J. Kieffer, S. C. Glotzer

Section B

Unknown Site -- Unknown Room

Modeling Water in Protein-Ligand Interfaces

Force-field Based Energetics

Cosponsored with PHYS
L. A. Kuhn and M. Feig, *Organizers*

8:55 — Introductory Remarks.

9:00 —7. Water in hydrophobic confinement: structure, dynamics, and function. **G. Hummer**

9:30 —8. Effective potentials for protein folding and binding with applications using replica exchange simulations. **R. M. Levy**, M. Andrec, A. K. Felts, E. Gallicchio, Y. Z. Ohkubo

10:00 —9. Water in protein interiors and protein-ligand interfaces. **S. Rick**

10:30 — Intermission.

10:40 —10. The role of water and solvation in mediating protein-ligand interactions. **C. L. Brooks III**, O. Guvench

11:10 —11. Evaluation of continuum methods and partial charge models for estimating changes in hydration free energies associated with protein-ligand binding. **R. C. Rizzo**, T. Aynechi, D. A. Case, I. D. Kuntz

11:40 —12. Hybrid approach to explicitly consider solvent molecules in MM-PBSA binding free energy calculations. **H. Gohlke**

Section C

Unknown Site -- Unknown Room

Computers and computer algebra systems in the chemistry classroom: A tribute to Drs. Joseph Noggle and Sidney Young

Morning Session

Cosponsored with CHED
T. J. Zielinski, *Organizer*
J. D. Madura, *Organizer, Presiding*

8:30 —13. Evolution of the symmath NSDL collection: Catalysis by J. Noggle and S. Young. **T. J. Zielinski**

9:05 —14. Numeric and symbolic problem solving strategies in chemistry. **F. Rioux**

9:30 —15. Using Mathcad to teach data processing. **S. E. Van Bramer**

9:55 — Intermission.

10:05 —16. Updating the Mathcad Introduction to Statistical Thermodynamics. **H. H. Harris**

10:30 —17. Equilibrium chemistry explained through molecular partition functions. **S. K. Dunn**

10:55 —18. Applications of Computing Algebra in Teaching Undergraduate Physical Chemistry. **F. Chen**

11:20 —19. Implementation of the Numerov method for solving the one-dimensional Schrodinger equation in the undergraduate curriculum. **A. Wierzbicki**

Section D

Unknown Site -- Unknown Room

General Oral -- Quantum Chemistry

J. D. Madura, *Organizer*
T. J. Dick, *Presiding*

8:10 —20. *Ab initio* quantum chemistry calculations on the stability and geometry of dimethylcyclobutadiene. B. Saylor, **S. J. Kirkby**

8:30 —21. A theoretical study of P_4O_{10}: Vibrational analysis, infrared and Raman spectra. J. O. Jensen, A. Banerjee, D. Zeroka, C. N. Merrow, S. J. Gilliam, **S. J. Kirkby**

8:50 —22. Energy storage capacity of polymeric nitrogen. **J. Uddin**, V. Barone, G. E. Scuseria

9:10 —23. Internal rotational motions of methyl, trifluoromethyl and *tert*-butyl groups in crystalline solids. **X. Wang**, F. B. Mallory, P. A. Beckmann, M. M. Francl

9:30 — Intermission.

9:40 —24. Linear carbon chains, in their stand-alone state and as incorporated species inside carbon nanotubes. **S. Yang**, M. Kertesz, Á. Rusznyák, V. Zólyomi, J. Kürti

10:00 —25. Multicenter covalent bonding and magnetic properties of phenalenyl and spiro-biphenalenyl radical dimers: the nature of interradical interactions in the solid state. **J. Huang**, M. Kertesz

10:20 —26. Pediction of mineral structures using semiempirical methods. **J. J. P. Stewart**

10:40 —27. Pseudo JT origin of the geometry and possible pseudo rotations of molecular clusters X_4, X=Na, Mg, Al, Si, P, S. **P. García-Fernández**, J. Boggs, I. Bersuker

11:00 — Intermission.

11:20 —28. Radical cyclizations of vinyl and aryl radicals: 5-exo-dig/6-endo-dig competition and elusive 5-endo-dig pathway. **M. Mariappan**, I. V. Alabugin

11:40 —29. Superadamantane-5 ($C_{35}H_{36}$): structural, electronic, and vibrational properties of a medium-order diamondoid molecule. **S. L. Richardson**, T. Baruah, M. R. Pederson

Computational exploration of energy landscapes: challenges and solutions

Advances in coupled-cluster methods

Cosponsored with COMP

SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Inorganic Applications and Methods

Cosponsored with PHYS
R. B. Ross, *Organizer*
S. Mohanty, *Organizer, Presiding*

1:25 — Introductory Remarks.

1:30 —30. Aluminum Nanoparticles: Potentials and Dynamics. **D. G. Truhlar**, A. W. Jasper, N. E. Schultz, P. Staszewski, G. Staszewska

2:15 —31. A hybrid quantum-classical approach to the study of dislocation properties. **F. Tavazza**, A. M. Chaka, L. Levine

2:45 —32. Electronic structure of fullerene-like cages and finite nanotubes of aluminum nitride. **R. R. Zope**, B. I. Dunlap

3:15 — Intermission.

3:30 —33. Kinetic monte carlo of gelling/microstructure development in nanostructured aerosols. **A. McCormick**, M. R. Zachariah

4:15 —34. Unusually shaped multi-atom Vacancies in Diamond. **I. Laszlo**, M. Kertesz, Y. Gogotsi

Section B

Unknown Site -- Unknown Room

Modeling Water in Protein-Ligand Interfaces

Importance of Specific Interactions

Cosponsored with PHYS
L. A. Kuhn and M. Feig, *Organizers*

2:00 —35. Role of water in fragment-based drug design. **S. Vajda**, M. Silberstein, S. C. Thiel

2:30 —36. Water clusters at the dimer interface of alanine racemases: Structure and function. **J. M. Briggs**, G. Mustata

3:00 —37. A molecular dynamics study of water chain formation in cytochrome c oxidase. **R. I. Cukier**

3:30 — Intermission.

3:40 —38. Allowing for the intermittent participation of protein bound water in GOLD Dockings. **J. W. Liebeschuetz**

4:10 —39. Importance of bridging water molecules to protein-ligand binding free-energy. **S. Wang**, Y. Lu, C -Y. Yang, R. Wang

4:40 —40. Water's role in structure-based drug design. **F. P. Hollinger**, S -B. Rong, M. Clark, M. Song

Section C

Unknown Site -- Unknown Room

Computers and computer algebra systems in the chemistry classroom: A tribute to Drs. Joseph Noggle and Sidney Young

Afternoon Session

Cosponsored with CHED
J. D. Madura, *Organizer*
T. J. Zielinski, *Organizer, Presiding*

1:30 —41. Joe Noggle, the Computer, and Physical Chemistry: An Unrelenting Synergy. **C. Dybowski**

2:00 —42. MathCad: A tool for all seasons. **G. R. Van Hecke**

2:25 —43. 'The diffusion game' - Using symbolic mathematics software to play the game on a large scale. **W. T. Grubbs**

2:50 —44. Engaging students with modern applications of physical chemistry. **M. D. Ellison**

3:15 — Intermission.

3:25 —45. Nonlinear regression of a second-order kinetics using Mathcad: Ethyl acetate saponification. **E. M. Ortega**, J. L. Guinon, J. Garcia-Anton, V. Perez-Herranz

3:50 —46. Exploring thermodynamics using Mathcad and non-typical materials: Elastomers and DNA. **J. Draves**

4:15 —47. Replacing the blackboard: Using Mathematica to teach modern chemical kinetics. **M. M. Francl**

4:40 —48. The merging of physical chemistry and computer algebra systems. **J. D. Madura**, H. Metiu

Section D

Unknown Site -- Unknown Room

Translating an Academic Background Into an Industrial Career

Cosponsored with PROF
L. M. Balbes and A. Tropsha, *Organizers*

1:30 —49. Art of the scientific job search. **A. B. Richon**

1:55 —50. Skills for molecular modeling in industry: observations of a recent emigrant from theoryland to experimentistan. **D. R. McMasters**

2:20 —51. Computational chemists in pharmaceutical research. **T. R. Stouch**

2:45 —52. Tricks of the drug discovery trade. **J. M. Jansen**

3:10 — Intermission.

3:25 —53. Career opportunities in the computational chemistry software and services industry for scientists with academic background. **O. F. Güner**

3:50 —54. Preparing for a computational chemistry position in the pharmaceutical industry. **C. E. Peishoff**

4:15 —55. Academic Entrepreneur: Lessons from N=2. **G. R. Marshall**

4:40 — Discussion.

Computational exploration of energy landscapes: challenges and solutions

Multi-reference and bond-breaking methods

Cosponsored with COMP

Predictive Methods in Drug Discovery

Sponsored by Biotage

Cosponsored with COMP

Structures and properties of small clusters

Structures and properties of strongly bound clusters

Cosponsored with COMP

MONDAY MORNING

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Biological Applications and Multi-Scaling Methodologies One

Cosponsored with PHYS
S. Mohanty, *Organizer*
R. B. Ross, *Organizer, Presiding*

8:25 — Introductory Remarks.

8:30 —56. Quantum mechanical modeling of self-reproducible living PNA chip immersed in the lipid bilayer vesicle controlled by quantum computing logic gates. **A. Tamulis**, V. Tamulis, J. Tamuliene

9:00 —57. Multi-scale quantum models for RNA catalysis. **D. M. York**

9:40 —58. Coupling between protein and solvent dynamics: microscopic insights from molecular dynamics simulations. **G. A. Carri**

10:20 — Intermission.

10:30 —59. Water Diffusion Across Nano-Bio-Assemblies of Block Copolymers: A Coarse-grain Simulation Study. **G. Srinivas**, D. E. Discher, M. L. Klein

11:00 —60. Ab initio simulations of folding pathways by molecular dynamics with the united-residue model of polypeptide chains. **M. Khalili**, A. Liwo, H. A. Scheraga

Section B

Unknown Site -- Unknown Room

Structure Based Design

Predicting binding modes and affinities

Cosponsored with MEDI
S. N. Rao, *Organizer*
A. Nayeem, *Organizer, Presiding*

8:40 — Introductory Remarks.

8:45 —61. Consensus pose prediction. **M. McGann**

9:15 —62. Prediction of Binding Affinities for Structure-Based Drug Design. **S. Brown**, S. W. Muchmore

9:45 —63. Improved protein mapping for fragment based drug design. **S. Vajda**, M. Silberstein, S. C. Thiel, D. Lancia

10:15 — Intermission .

10:30 —64. Protein ensemble docking: An effective strategy for enhanced lead docking. **L. Mueller**, D. L. Cheney

11:00 —65. Accurate prediction of binding modes and binding affinities of protein-ligand complexes. **R. A. Friesner**

11:30 — Panel Discussion: Shashidhar Rao - Moderator.

Section C

Unknown Site -- Unknown Room

Chemistry in the Large -- Teraflop Computing and Beyond

Searching for chemical accuracy: terascale computing with high accuracy ab inito methods

W. A. deJong, *Organizer*
T. L. Windus, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:40 —66. Applications of electronic structure theory at the teraflop level and beyond. **D. A. Dixon**, W. A. de Jong, T. L. Windus, K. A. Peterson

9:20 —67. Quantum Monte Carlo: An ab initio molecular computational methodology for terascale computing. A. Aspuru-Guzik, R. Salomon-Ferrer, B. Austin, D. Domin, D. Skinner, R. Oliva, **W. A. Lester Jr.**

10:00 —68. Achieving sustained teraflop performance with the NWChem coupled cluster module. **W. A. deJong**, K. Kowalski

10:30 — Intermission.

10:50 —69. Scalable correlated electronic structure theory: Strategies and applications. **M. S. Gordon**

11:30 —70. Full configuration interaction (FCI) method in Teraflop computing: Implementation and application. **Z. Gan**

Section D

Unknown Site -- Unknown Room

General Oral -- Quantum Chemistry

J. D. Madura, *Organizer*

8:00 —71. Importance-sampling coupled-cluster theory. **M. Abrams**

8:20 —72. Recent developments in the linear scaling Coulomb problem for first principles DFT calculations with Gaussian functions. **L. Fusti-Molnar**, J. Kong, S. T. Brown

8:40 —73. Interpolating density values on a cartesian grid: Improving the efficiency of Lebedev based numerical integration in Kohn-Sham density functional algorithms. **S. T. Brown**, L. Füsti-Molnár, J. Kong

9:00 —74. Formulation, parametrization and performance appraisal of the analytic and variational Xα method. **R. R. Zope**, B. I. Dunlap

9:20 — Intermission.

9:30 —75. Identifying and extracting the sources of errors in the calculation of binding energies of van der Waals clusters of aromatic molecules. **I. Gonzalez**, C. A. Gonzalez, E. C. Lim

9:50 —76. Energy landscapes of bimolecular nucleophilic substitution (SN2) reactions: A comparison of density functional theory and coupled cluster methods. **M. Swart**, M. Solà, F. M. Bickelhaupt

10:10 —77. Minimal atomic multipole expansion (MAME): controlling redundancies in distributed multipole expansion of molecular fields. **E. V. Tsiper**, K. Burke

10:30 —78. Path integral thermochemistry. **K. R. Glaesemann**, L. E. Fried

10:50 — Intermission.

11:10 —79. Partial averaging theories for the path integral in curved spaces. **E. Curotto**, M. W. Aviles

11:30 —80. Quantum Monte Carlo estimation of properties of novel nanoscale compounds. J. A. W. Harkless, **F. Fayton Jr.**

11:50 —81. Quantum wavepacket ab initio molecular dynamics: An approach to perform simultaneous dynamics of electrons and nuclei in large systems. **S. Iyengar**

Advances in Data-mining and Analysis: Informatics Perspective

Cosponsored with COMP

Applied Modeling and Computations in Nuclear Science

Radiation Risk and Transport

Cosponsored with American Nuclear Society, Health Physics Society, and COMP

Computational exploration of energy landscapes: challenges and solutions

Novel approaches to electron correlation and new algorithms

Cosponsored with COMP

Structures and properties of small clusters

Structures and properties of weakly bound clusters

Cosponsored with COMP

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Biological Applications and Multi-Scaling Methodologies Two

Cosponsored with PHYS
R. B. Ross and S. Mohanty, *Organizers*
G. A. Carri, *Presiding*

1:15 — Introductory Remarks.

1:20 —82. Symmetry, form and shape: Guiding principles for robustness in macromolecular machines. **C. L. Brooks III**, F. Tama

2:00 —83. Mixed level coarse-graining of protein structures for dynamics. **R. L. Jernigan**, P. Doruker

2:40 —84. The multi-scale simulation of biomolecular assemblies. **G. A. Voth**

3:20 — Intermission.

3:30 —85. Simulating, Modeling and Refining Supramolecular Complexes at Multi-resolution and Multi-length Scales. **J. Ma**

4:10 —86. Coarse grained to atomistic mapping algorithm: a tool for multiscale simulations. **S. O. Nielsen**, M. L. Klein

Section B

Unknown Site -- Unknown Room

Structure Based Design

Applications to specific targets

Cosponsored with MEDI
S. N. Rao, *Organizer*
A. Nayeem, *Organizer, Presiding*

1:30 —87. Computational modeling for kinase inhibitor discovery. **Y. Zhu**

2:00 —88. Docking Studies on inhibitors of GSK-3Beta Kinase. **V. N. Balaji**, P. M. Dattatreya, S. Phukan, P. K. Gadakar

2:30 —89. Structure-based design of acylguanidine BACE1 inhibitors. **E. S. Manas**, R. Chopra, D. C. Cole, J. R. Stock, L. D. Jennings, F. E. Lovering, J. S. Condon, P. Zhou, W. R. Solvibile, A. Aulabaugh, M -C. Lo, R. Cowling, G. Jin, M. J. Turner, Y. Hu, E. Wagner, K. Y. Fan, J. C. Alvarez, M. S. Malamas, J. Bard

3:00 — Intermission.

3:15 —90. Structure-based Drug Design for Nuclear Hormone Receptors. **S. Krystek Jr.**, L. G. Hamann, M. E. Salvati, A. Balog, J. Hunt, J. Li, M. Manfredi, R. Martinez, A. Nayeem, A. Nirschl, D. Pickering, D. Schnur, W. Shan, C. Sun, D. Wei, H. Zhu

3:45 —91. Structure-based prediction of drug binding to human serum albumin. **J. Li**, B. A. Tounge, C. H. Reynolds

4:15 — Panel Discussion: Richard Friesner - Moderator.

Section C

Unknown Site -- Unknown Room

Chemistry in the Large -- Teraflop Computing and Beyond

Simulating biological processes on thousands of processors

T. L. Windus and W. A. deJong, *Organizers*
T. H. Dunning Jr., *Presiding*

1:30 —92. Folding@Home: Using desktop grid computing to overcome fundamental barriers in biomolecular simulation. **V. S. Pande**

2:10 —93. Molecular Modeling of Complex Biological Systems: Microbial Membranes. **T. P. Straatsma**

2:50 —94. Distributed computations for biomolecular structure, dynamics and folding. **A. E. Roitberg**

3:20 — Intermission.

3:40 —95. Fast Multipole Communications Scaling. **B. M. Pettitt**, J. Kurzak

4:20 —96. Scalable molecular dynamics simulation of cellular processes. **E. Tajkhorshid**

5:00 —97. Use of NASA's Columbia teraflop supercomputer to study DNA damage by charged particles. **G. M. Chaban**, W. M. Huo, D. Wang, C. E. Dateo

Section D

Unknown Site -- Unknown Room

General Oral -- Quantum Chemistry

J. D. Madura, *Organizer*

1:10 —98. Calculations to determine the experimental conformation of a cyclic insect pheromone using a novel multi-faceted ab initio approach. **F. A. Momany**, R. J. Bartelt, W. B. Bosma

1:30 —99. Investigations of Light Harvesting Complexes. **I. R. Gould**

1:50 —100. Substituent effects on hydrogen bonding in Watson-Crick base pairs. **F. M. Bickelhaupt**

2:10 —101. Coupled cluster methods including non-iterative approximate quadruple excitation corrections . A new alternative for thermochemistry. **Y. J. Bomble**, J. F. Stanton, M. Kállay, J. Gauss

2:30 — Intermission.

2:40 —102. Efficient SCF method for large systems of weakly interacting components. **R. Z. Khaliullin**, A. T. Bell, M. Head-Gordon

3:00 —103. Electronic structure of "difficult" systems: Quantum Monte Carlo estimates of transition metal IP and EA. **J. A. W. Harkless**, A. A. Gibson, G. Taylor

3:20 —104. Charge-transfer effects and counterions in electroactive polymers. **N. E. Miller**, D. Scherlis, N. Marzari

3:40 —105. Hydronium on Pt (111) surface and their roles in O_2 reduction. L. Qi, J. Fujiwara, **J. Li**

4:00 — Intermission.

4:20 —106. Mechanism of the Rh(I)-catalyzed asymmetric hydrogenation of unprotected enamines: A density functional theory study. **Y -L. Zhao**, K. N. Houk, T. Rosner

4:40 —107. Mechanistic explorations of the vinylcyclobutane-cyclohexene and sceptrin-ageliferin rearrangements using density functional theory. **B. H. Northrop**, K. N. Houk

5:00 —108. Rational design of organocatalysts using quantum mechanical calculations - towards new catalytic proline derivatives for the diastereoselective intermolecular aldol and Mannich reactions. **P. H -Y. Cheong**, K. N. Houk, C. F. Barbas III, R. Thayumanavan

Advances in Data-mining and Analysis: Informatics Perspective

Pharmaceutical Applications

Cosponsored with COMP

Applied Modeling and Computations in Nuclear Science

Radiation Transport and Dosimetry

Cosponsored with American Nuclear Society, Health Physics Society, and COMP

Computational exploration of energy landscapes: challenges and solutions

Spectroscopy from potential energy surfaces

Cosponsored with COMP

MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix

W. D. Cornell, *Presiding*

8:00 - 10:00

155, 157, 161, 165, 170, 175, 178, 184-185, 195-196, 205, 209, 218, 223, 225, 229, 232, 237. See subsequent listings.

TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Water and Organic Applications and Methods

Cosponsored with PHYS
R. B. Ross and S. Mohanty, *Organizers*
M. P. Makowski, *Presiding*

8:25 — Introductory Remarks.

8:30 —109. Simulations of Liquid/Vapor Interface for Water and Methnol From First Principles. **I -F. W. Kuo**, C. J. Mundy, M. J. McGrath, J. I. Siepmann

9:00 —110. Large-scale Monte Carlo simulations for aggregation, self-assembly, and phase equilibria. **J. I. Siepmann**, J. M. Stubbs, L. Zhang, M. J. McGrath, N. Rai, C. D. Wick

9:40 —111. Spanning scaling regimes with the SPEAD model. **J. Elliott**, Z. Gerek, N. H. Gray

10:20 — Intermission.

10:30 —112. Strategies for Monte Carlo simulations using quantum chemical energetics. **K. D. Jordan**, R. A. Christie, J. Cui

11:10 —113. Watching crystals grow: Determining microscopic behaviour from nanoscale simulation. **J. D. Gale**, S. Piana

Section B

Unknown Site -- Unknown Room

Structure Based Design

Virtual screening and lead optimization

Cosponsored with MEDI
A. Nayeem, *Organizer*
S. N. Rao, *Organizer, Presiding*

8:40 — Introductory Remarks.

8:45 —114. Current challenges in molecular docking and virtual screening. **R. D. Taylor**

9:15 —115. Lead optimization via high-throughput molecular docking. **D. Joseph-McCarthy**

9:45 —116. Structure based lead optimization of isosteric analogues. **R. Sayle**, R. Tolbert, A. Nicholls, A. G. Skillman

10:15 — Intermission.

10:30 —117. Structure-based design of focused drug-like combinatorial libraries. **P. S. Shenkin**, L. L. Frye, R. B. Murphy, M. P. Repasky, D. T. Mainz, M. Reboul, R. A. Friesner

11:00 —118. Novel scoring functions for *in silico* database screening: Binding response and pose-based scaling. **S. Zhong**, A. D. MacKerell Jr.

11:30 — Panel Discussion: Deborah Loughney - Moderator.

Section C

Unknown Site -- Unknown Room

Chemistry in the Large -- Teraflop Computing and Beyond

Challenges in computational chemistry: science on teraflop computing platforms and beyond

T. L. Windus, *Organizer*
W. A. deJong, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:35 —119. Realizing teraflops computing, striving for petaflops computing. **T. H. Dunning Jr.**

9:15 —120. Parallel DFT calculations with ADF: A software vendor's perspective on code optimization. **S. J. A. van Gisbergen**

9:45 —121. High performance computational chemistry in the 21st century. **T. L. Windus**

10:15 — Intermission.

10:35 —122. Leadership computing and chemistry. **R. J. Harrison**

11:15 —123. Large scale computing with GAMESS-UK. **J. H. Van Lenthe**, M. F. Guest, H. J. J. van Dam, I. J. Bush, P. Sherwood, J. M. H. Thomas, R. W. A. Havenith, J. N. J. van Lingen, M. de Jonge

11:45 —124. What can we use a Teraflop computer for? **E. Aprà**

Section D

Unknown Site -- Unknown Room

Advances in Data Mining and Analysis: Computational Perspective

Cosponsored with CINF
A. Tropsha, *Organizer*
O. F. Güner, *Organizer, Presiding*

8:50 —125. BioSimGrid: A distributed environment for archiving and the analysis of biomolecular simulations. **S. E. Murdock**, K. Tai, M. H. Ng, S. Johnston, B. Wu, H. Fangohr, J. W. Essex, P. Jeffreys, S. Cox, M. S. P. Sansom

9:20 —126. Automated QSPR by competitive workflow. **D. E. Leahy**, J. Cartmell, S. Enoch, D. Krstajic, J. Bowen

9:50 —127. Building predictive models using fuzzy biological data: Data mining of the docking results

of GSK-3 inhibitors using artificial intelligence approaches. **P. A. Petukhov**, A. N. Pae

10:20 — Intermission.

10:30 —128. Modeling Polymer Sorption. **M. Charton**

11:00 —129. Computational Chemistry Robots. **J. A. Townsend**, P. Murray-Rust, S. M. Tyrrell, Y. Zhang

11:30 —130. Assessment of model protein structures using an entropic metric of dihedral-angle correlation. **S. Zhong**, S. Quirk, R. Hernandez

Applied Modeling and Computations in Nuclear Science

Radiation Detection

Cosponsored with American Nuclear Society, Health Physics Society, and COMP

Structures and properties of small clusters

Cluster Dynamics

Cosponsored with COMP

TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Polymer Applications and Methods

Cosponsored with PHYS
R. B. Ross, *Organizer*
S. Mohanty, *Organizer, Presiding*

1:25 — Introductory Remarks.

1:30 —131. Modelling the thermal decomposition of large molecules and nanostructures. **M. R. Nyden**, S. I. Stoliarov, P. R. Westmoreland

2:10 —132. Multiscale simulation of ultraviolet absorber function in polymers. **M. L. Greenfield**

2:50 —133. Using Nanoconfinment to Tailor Semiconducting Polymers. **M. L. Drummond**, B. G. Sumpter, M. D. Barnes, W. A. Shelton, R. J. Harrison

3:20 — Intermission.

3:30 —134. Mean-field prediction of block copolymer phase behavior and structure in selective solvent. **P. Alexandridis**

4:10 —135. Computer simulation studies on mechanisms of poration for hydrolytically degradable diblock copolymer membranes. **V. Ortiz**, S. O. Nielsen, M. L. Klein, D. E. Discher

Section B

Unknown Site -- Unknown Room

Structure Based Design

Emerging methods

Cosponsored with MEDI
A. Nayeem, *Organizer*
S. N. Rao, *Organizer, Presiding*

1:30 —136. Development of small molecules designed to modulate protein-protein interactions. **Y. Che**, B. R. Brooks, G. R. Marshall

2:00 —137. Decoupling torsional and Cartesian alignment: Applications to pharmacophore alignment problems. **R. D. Clark**, E. Abrahamian, A. Strizhev, P. R. N. Wolohan, C. Abrams

2:30 —138. Induced-fit docking to account for receptor flexibility. **B. W. Sherman**, T. Day, M. P. Jacobson, R. A. Friesner, R. Farid

3:00 — Intermission.

3:15 —139. Physics-based methods in virtual screening: Factors impacting practical application. **D. Singh**, N -J. Deng

3:45 —140. Direct calculation of absolute free energies of ligand binding without knowledge of the bound state. **M. R. Shirts**, G. Jayachandran, H. Fujitani, C. D. Snow, V. S. Pande

4:15 — Panel Discussion: Akbar Nayeem - Moderator.

Section C

Unknown Site -- Unknown Room

Chemistry in the Large -- Teraflop Computing and Beyond

Teraflop computing in geochemistry, nanoscience and catalysis

T. L. Windus and W. A. deJong, *Organizers*
E. Aprà, *Presiding*

1:30 —141. Large scale first principles simulations for problems in earth and planetary science (ion hydration) and biochemistry (phosphoryl transfer signaling reactions). E. J. Bylaska, M. Valiev, S. Bogatko, **J. H. Weare**

2:10 —142. Million-to-Billion Atom Simulation of Chemical and Mechanical Processes. **R. Kalia**, A. Nakano, K -I. Nomura, A. Sharma, P. Vashishta

2:50 —143. Al nanoparticles: Accurate energetics and structures. **N. E. Schultz**, A. W. Jasper, D. G. Truhlar

3:20 — Intermission.

3:40 —144. Recent progress in large-scale first-principles molecular dynamics simulations. **F. Gygi**

4:20 —145. Computational Chemistry at the Terascale. **W. A. Shelton**, B. G. Sumpter, V. Meunier, R. J. Harrison

5:00 —146. Implementation Of Self Interaction Corrected DFT And Hybrid Functionals For Pseudopotential Plane-Wave Programs. **E. J. Bylaska**, K. Tsemekhman, J. H. Weare, H. Jonsson

5:30 — Concluding Remarks.

Section D

Unknown Site -- Unknown Room

Advances in Data Mining and Analysis: Computational Perspective

Applications

Cosponsored with CINF
A. Tropsha, *Organizer*
O. F. Güner, *Organizer, Presiding*

1:30 —147. Building and using an in-house platform for data mining and analysis integrating open source and proprietary software: II. Model building and library analysis. **H. E. Purkey**, E. Evensen, K. E. Lind, E. K. Bradley

2:00 —148. Use of structural keys to classify cytochrome P450 substrates. **J. H. Block**, D. R. Henry

2:30 —149. Use of multiple-category Bayesian modeling to predict side effects. **R. D. Brown**, D. Rogers, T. Van Daelen

3:00 —150. Property matching of reference datasets for classification models. **N. Blomberg**, S. Muresan

3:30 — Panel Discussion.

Applied Modeling and Computations in Nuclear Science

Nuclear Data Analysis 1

Cosponsored with American Nuclear Society, Health Physics Society, and COMP

Computational exploration of energy landscapes: challenges and solutions

Dynamic exploration of potential energy surfaces

Cosponsored with COMP

Structures and properties of small clusters

Cluster Reactivity

Cosponsored with COMP

TUESDAY EVENING

Section A

Unknown Site -- Unknown Room

Poster Session -- Sponsored by Novartis Institutes for BioMedical Research

W. D. Cornell, *Organizer*

6:00 - 8:00

151. Electron paramagnetic resonance and equilibrium atomic configurations studies of binuclear niobium molecules in Li-Nb phosphate glass dielectrics. **S. A. Arrington-Peet**, R. R. Rakhimov, V. I. Gavrilenko

152. Novel docking and scoring approach to rank-ordering compounds by potency. **X. Hong**, S. Kahn, C. M. Venkatachalam, C. Duraiswami, C. E. Peishoff, M. S. Head

153. Quantum Mechanical Modeling of self-reproducible living PNA chip immersed in the lipid bilayer vesicle controlled by quantum computing logic gates. **A. Tamulis**, V. Tamulis, J. Tamuliene

154. Application of Swarm algorithm for efficient in silico screening of chemical database. **L. Wang**, J. Graham, J. O. Trent

155. Dynamics of single-substrate continuous cultures: An integrated model of bacterial cell. **S. Gupta**, S. S. Pilyugin, A. Narang

156. On the use of suffix trees in multiple sequence alignment. **K. R. Sharma**

157. Parallel computing in the undergraduate chemistry curriculum. **K. Siam**

158. Q-Chem 3.0: More chemistry, faster. **J. Kong**

159. QSPR analysis of solvent effect on selectivity of 18-crown-6 between Nd^{3+} and Eu^{3+} ions: A Monte Carlo simulation study. **H. S. Kim**

160. QSPR analysis on selectivity of between K^+ and Na^+ ions to 12-Crown-4: A Monte Carlo simulation study. **H. S. Kim**

161. Solid state DFT methods and the property prediction of energetic materials. **J. A. Ciezak**, S. F. Trevino

162. Theoretical study of hydrogen-bonded complexes of bromophenols with ammonia: Correlations and predictions of pKa values. **J. Han**, F -M. Tao

163. Toward the development of an accurate virtual screening protocol: Recent improvements in protein ensemble docking. **L. Mueller**, D. L. Cheney

164. Computational analysis of the folding pathway of a mutant cold shock protein. **S. Urahata**, A. Clarke, A. E. Cardenas

165. MM/PBSA studies on conformational changes of Yersinia Protein Tyrosine Phosphatase and use in structure-based inhibitor design. **X. Hu**, C. E. Stebbins

166. Molecular dynamics simulations of R67 DHFR: Investigation of the cooperative binding. C. Shi, **J. L. Radkiewicz**

167. New Krypton bonded molecules: A theoretical study. **S. Yockel**, A. K. Wilson

168. Binary QSAR-based library design. **H. Gao**

169. Revisiting the estimation of relative free energies from a single ensemble. **D. J. Price**, C. L. Brooks III

170. RMSD: Routine measure stirs doubts. **J. J. Yang**

171. A novel MD/BD model for the simulation of multi-scale. **P. E. Krouskop**, J. D. Madura

172. Active site structure and reaction mechanism of DNA polymerase β studied by molecular dynamics simulation and QM/MM method. **P. Lin**, L. G. Pedersen

173. Classical and ab initio molecular dynamics of quartz surfaces. A. D. MacKerell Jr., **P. E. M. Lopes**

174. Conformationally sampled pharmacophore for δ opioid ligands. **D. Bernard**, A. Coop, A. D. MacKerell Jr.

175. Controllable water channel gating of nanometer dimensions. **R. Wan**, J. Li, H. Lu, H. Fang

176. Development and parametrization of MMFF/NQEq. **N. Nakayama**, S. Obata, H. Goto

177. Development of fragment-based chemical descriptors using novel frequent common subgraph mining approach and their application in QSAR modeling. **R. Khashan**, W. Zheng, J. Huan, W. Wang, A. Tropsha

178. Developpement and aplication of a novel software for asymmetric catalyst design. **C. R. Corbeil**, N. Moitessier

179. Electron paramagnetic resonance and equilibrium atomic configurations studies of binuclear niobium molecules in Li-Nb phosphate glass dielectrics. **S. A. Arrington-Peet**, R. R. Rakhimov, V. I. Gavrilenko

180. Folding Trp-cage to atomic resolution: Searching parameter space for a free-energy minimum. **O. Guvench**, C. L. Brooks III

181. Hydration and dewetting near graphite-CH3 and graphite-COOH Plates. **J. Li**, T. Liu, X. Li, L. Ye, H. Chen, H. Fang, Z. Wu, R. Zhou

182. Inhibition of protein-protein interactions in the extracellular signal-regulated kinase (ERK). **A. T. Macias**, C. N. Hancock, E. K. Lee, S. Y. Yu, A. D. MacKerell Jr., P. Shapiro

183. Investigating the effects of methanol and n-octane entrainers on solubility and microscopic structure in supercritical carbon dioxide. **K. E. Anderson**, J. I. Siepmann

184. Learning chemistry from available compounds. **G. Skillman**, R. Sayle

185. Library design based on privileged structures through docking and direct design in the protein binding pocket. **C. Gerlach**, H. F. Velec, M. Smolinski, D. G. Hangauer, A. Heine, G. Klebe

186. Ligand refinement with combined force field and shape potential. **S. Wlodek**, G. Skillman, A. Nicholls

187. Mapping protein-ligand binding free energy contributions solely onto the ligand atoms. S. Bhat, E. O. Purisima, **T. Sulea**

188. Modeling of interfaces: Adsorption of 2-methyl-4-nitroaniline on hydrogen-terminated Si(100) 2x1 surface. S. M. Black, **S. Inge**

189. Molecular docking and analysis of conformation adopted by tetrapeptide inhibitors into active site of thrombin. **C. C. Clement**, M. Philipp

190. Molecular dynamics of helical m-phenylene ethynylene foldamer with PEG side chains. **O -S. Lee**, J. G. Saven

191. Molecular modeling study of binding between DNA and CC-1065 analogue. **G. Sun**, M. C. Nicklaus, D. P. Simmons, J -Y. Lai

192. New estimate of beta-sheet folding cooperativity based on molecular dynamics simulations of a three-stranded beta-sheet. **D. R. Roe**, V. Hornak, C. Simmerling

193. Predictive tools for structure-based drug design: A comparative study of force field-based scoring functions. **P. Englebienne**, N. Moitessier

194. Probing inherent helical preferences in Pt-beanpole complexes using molecular mechanics. P. O. Norrby, J. A. Gladysz, **F. A. Zhuravlev**

195. Schering-Plough 3D – A web-based application to share three-dimensional project information. **J. H. Voigt**, R. Radhakrishnan, C. Strickland

196. Standard reference simulations for docking and scoring: enabling robust computational screening for drug design. **A. J. Oliver-Kapur**, A. M. Chaka, M. K. Gilson, F. P. Schwarz

197. Stereoselectivity of hydroxyethyl azide reactions. **D. G. Withrow**, J. L. Poutsma

198. Studies on different interactions of beta-cyclodextrin with ferrocene derivatives and adamantane derivatives. **M. Ning**, R. E. Brown

199. Techniques for efficiently studying reactive events with electronic structure based biasing and transition path sampling. **C. N. Rowley**, N. J. Mosey, T. K. Woo

200. Theoretical study of the optical properties of Rhodamine 6G in Ag-ethanol suspension. **A. C. Sykes**, S. M. Black

201. Two mechanisms served by a single transition state: The branching ratio for $CH2O•^-$ + CH3Cl on improved potential energy surfaces. **J. Li**, X. Li, S. Shaik, H. B. Schlegel

202. Unraveling the role of (6-4) Photolyase in DNA repair through homology modeling, consensus docking, and MD simulations. **C. Harrison**, O. Wiest

203. Virtual screening of chemical libraries based on predictive QSAR methods. **M. Wang**, S. Zhang, S. Oloff, A. Golbraikh, H. Kohn, A. Tropsha

204. Visualization and interpretation of computational models. **K. Schmidt**, B. Kelley, J. Corkery, J. Christopher, R. Tolbert

205. Wavelet transforms for calculating time-dependent vibrational frequencies from dynamics simulations. **R. A. Wheeler**, A. Rahaman

206. A simulation study of the binding modes of formamido-pyrimidine bound to DNA containing 8-oxo guanine. **K. Song**, A. P. Grollman, C. D. L. Santos, C. Simmerling

207. Ab initio studies of a 1,2,3,5-tetrazocine. **S. A. Kebbell**, D. F. Brougham

208. Ab-initio calculations on the energetics of H_2 oxidation by FeO^+ using GGA+U. **H. J. Kulik**, D. Scherlis, N. Marzari

209. Accurate calculations of interaction energies of H-bonded clusters. **J. Cui**, V. N. McCarthy, R. A. Christie, K. D. Jordan

210. AEI: Exploring solvent effects and mechanisms for organic reactions using computational methods. **O. Acevedo**, W. L. Jorgensen

211. Atomic-scale mechanism of *met* repressor function. **J. Zheng**, I. Balabin, D. N. Beratan

212. Calculation of absorption line shape based on reduced density matrix approach. **M. Yang**

213. CHARMM Drude polarizable force field parameter development for model compounds representative of biological systems. I. V. Vorobyov, **V. M. Anisimov**, A. D. MacKerell Jr.

214. Collaborative filtering on a family of biological targets. D. Erhan, **P -J. L'Heureux**, Y. Bengio, S. Y. Yue

215. Comparison of methods of density functional theory modeling of the specific rotation of amino acid solutions. **M. D. Kundrat**, J. Autschbach

216. Comparisons of potential energy landscapes and conformations of polyalanine with different force fields by new molecular dynamics simulation protocols. **Z. Huang**, R. A. Wheeler

217. Computation of quartic potential energy surfaces and excited vibrational levels of H2O. **N. R. Brinkmann**, J. L. Davisson, M. H. Cortez, W. F. Polik

218. Computational analysis and prediction of bioisosteres. J. Ban, R. Tolbert, A. Nicholls, **G. Skillman**

219. Computational study on the vanadium-catalyzed asymmetric oxidation of sulfides. **D. Balcells**, F. Maseras, G. Ujaque

220. Cycloreversion of the (6-4) photolesion: DFT studies of the DNA repair mechanism. **C. Harrison**, O. Wiest

221. Digging the past for a clue: A novel in-silico approach for new leads on 4-OH-pyran-2-ones HIV Protease Inhibitors. **B. Bhhatarai**, R. Garg

222. Dissociation energy estimation of insulins using all-electron density functional calculation. **T. Inaba**, F. Sato

223. Do similar ligands bind in a similar fashion? J. Boström, A. Hogner, **S. Schmitt**

224. Drying and hydrophobic collapse in the multi-domain protein and protein oligomers. **X. Huang**, R. Zhou, P. Liu, C. J. Margulis, B. J. Berne

225. Dynamic equilibrium between fast and slow forms of thrombin: A structural investigation of thrombin paradox. **D. Venkateswarlu**, L. G. Pedersen

226. Effect of solvent on the stereoselectivity of reactions between hydroxyalkyl azides and ketones. A. K. Manukyan, **J. Radkiewicz-Poutsma**

227. Exhaustive computational analysis of peptides for the fragmentation in low-energy dissociation mass spectrometry. **K. Fukui**, Y. Akiyama

228. Forward-Backward Semiclassical Dynamics. **N. J. Wright**, N. Makri

229. Homology modeling, docking and molecular dynamics simulation of class I HDACs. **D -F. Wang**, O. G. Wiest, P. Helquist

230. Impact of multiple conformations on fingerprint descriptors uses in QSAR. P -J. L'Heureux, **B. Cromp**, S. Y. Yue, Y. Bengio

231. Mechanisms for induced diamagnetic and paramagnetic fields. **K. W. Wiitala**

232. Modeling gene regulatory networks. **P. Zhang**, M. Ouyang, W. J. Welsh

233. Molecular dynamics simulations of a DNA strand containing two thymine dimers. L. L. O'Neil, **O. Wiest**

234. Monte Carlo simulation study for QSPR of solvent effect on the selectivity of 18-Crown-6 between Gd^{3+} and Yb^{+3} ions. **H. S. Kim**

235. Origins of the high affinity binding of the biotin-(strept)avidin complex. **J. DeChancie**, K. N. Houk

236. Reduction of computational requirements and trends for high accuracy description of molecular properties. **B. Mintz**, A. K. Wilson

237. Simulation of water soluble potassium channel. **O -S. Lee**, J. Bronson, J. G. Saven

238. Solvent effect on relative Gibbs free energy and structural property of Eu^{3+} to Yb^{3+} ion mutation: A Monte Carlo simulation study. **H. S. Kim**

239. Structural and thermodynamic properties of ammonium chloride clusters. **R. Q. Topper**

240. Study on fiber bonding strength in modeling of paper tensile strength with fiber characteristics. **T. J S**, Y. D B, L. H B, X. Y G, K. S L, G. H k

241. Computational prediction of adenosine receptor homodimerization. **S -K. Kim**, K. A. Jacobson

242. New tool for the interrogation of macromolecular structure. **F. Torrens**

WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Methods Development and Electronic Applications

Cosponsored with PHYS
R. B. Ross and S. Mohanty, *Organizers*
S. O. Nielsen, *Presiding*

8:25 — Introductory Remarks.

8:30 —243. Computer simulations of physical adsorption. **Z. Ying**, Y. Zifeng Sr.

9:00 —244. Thermodynamically accurate particle-based mesodynamics. **A. Strachan**

9:40 —245. Interactions between nanoparticles in supercritical fluids: From repulsions to attractions. **S. Egorov**

10:10 — Intermission.

10:20 —246. Encoding and transport of information in molecular and biomolecular systems. **J. M. Seminario**, L. Yan, Y. Ma

10:50 —247. Coupling classical molecular dynamics simulations to continuum current and heat flow equations: Application to Joule heating, friction, and magnetic lift-off of nanoscale metal contacts. **C. W. Padgett**, D. W. Brenner

Section B

Unknown Site -- Unknown Room

Visualization and Interpretation of Computational Models

Cosponsored with MEDI
A. Smellie, A. Filikov, and R. Palma, *Organizers*
A. Smellie, *Presiding*
A. Filikov, *Facilitator*

8:10 — Introductory Remarks.

8:20 —248. Visualizing structure-activity relationships in ABCD. **D. K. Agrafiotis**

8:50 —249. Molecular Property eXplorer - A Novel Approach to Visualizing SAR. **C. Kibbey**

9:20 —250. SAESAR: software workbench for the interpretation and visualization of shape, electrostatics and structure activity relationships. **N. E. MacCuish**, A. Nicholls, J. D. MacCuish, M. Chapman

9:50 — Intermission.

10:05 —251. Sherloque: A general purpose SAR and property viewer. **A. Smellie**

10:35 —252. Cassandra - A Web Interactive Molecular Modelling and Cheminformatics Visualisation Interface. **L. Whitehead**, P. Gedeck, W. D. Cornell, P. Finan

11:05 —253. Use of Spotfire™ profile charts to display dose-response curves for comparison of compounds' in vitro transcriptional activities. **D. R. McMasters**, J. C. Culberson

11:35 —254. PyMOL: A communications tool for computational models. **W. L. DeLano**, J. W. Lam

Section C

Unknown Site -- Unknown Room

Emerging Technologies in Computational Chemistry

Emerging Technologies in Computational Chemistry - Finalist Presentations

C. M. Breneman, *Organizer*

9:00 — Introductory Remarks.

9:10 —255. Quantum computation for quantum chemistry. **A. Aspuru-Guzik**, A. D. Dutoi, M. Head-Gordon

9:30 —256. Accurate computation and interpretation of spin-dependent properties in metalloproteins and bioinorganic complexes. **J. H. Rodriguez**

9:50 —257. First-principles electronic structure approach for molecular structures, properties, and reactivity in solution: Towards chemical accuracy. **C -G. Zhan**

10:10 —258. Complete coverage of the shape space of drug-like molecules. **A. Nicholls**, J. A. Grant, J. Haigh

10:30 — Intermission.

10:45 —259. Surrogate docking: Structure-based virtual screening at high throughput speed. S. Yoon, A. Smellie, D. S. Hartsough, **A. Filikov**

11:05 —260. Multi-timescale events simulation: From tensioned dynamics to chemo-coupled dynamics. **W. Yang**, M. Karplus

11:25 —261. New methods for calculating the absolute entropy and free energy from a Monte Carlo or molecular dynamics trajectory. **H. Meirovitch**, R. P. White, S. Cheluvaraja

11:45 — Award Presentation.

Applied Modeling and Computations in Nuclear Science

Nuclear Data Analysis 2

Cosponsored with American Nuclear Society, Health Physics Society, and COMP

Computational exploration of energy landscapes: challenges and solutions

Nonadiabatic and non-Born-Oppenheimer approaches

Cosponsored with COMP

Structures and properties of small clusters

Electronic structure theory of soft clusters

Cosponsored with COMP

WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap

Industrial Applications and Methods

Cosponsored with PHYS
S. Mohanty, *Organizer*
R. B. Ross, *Organizer, Presiding*

1:15 — Introductory Remarks.

1:20 —262. Dissipative particle dynamics simulations on powder clearcoat melts, aqueous nanogels and core-shell lattices. **M. P. Makowski**, L. I. Kioupis, K. Ragunathan

2:00 —263. Predicting dynamic mesoscale structure of soft or fluid consumer products. **F. H. Case**, J. G. E. M. (. Fraaije, S. K. Nath

2:40 —264. Application of atomistic simulation to materials design of lubricants and high strength steels. **P. A. Gordon**, M. J. Luton, C. A. Halsey

3:20 — Intermission.

3:30 —265. Multiscale modeling for self-assembled materials and composites in industrial nanotechnology. **S. Mohanty**, R. B. Ross, G. Caldwell, M. Jain

4:10 —266. From molecular simulations to Computer-Aided Nanodesign™ (CAN). **G. Goldbeck-Wood**

Section B

Unknown Site -- Unknown Room

Visualization and Interpretation of Computational Models

Cosponsored with MEDI
A. Smellie, A. Filikov, and R. Palma, *Organizers*
A. Smellie, *Presiding*
R. Palma, *Facilitator*

1:30 — Introductory Remarks.

1:35 —267. Visualization of model domain, modeling parameters and applicability domain. **G. J. Myatt**, P. E. Blower, K. P. Cross, C. Yang

2:05 —268. Using interactive visualization tools to support discovery, optimization, and library design. **J. F. Lowrie**, D. J. Diller, R. K. Delisle

2:35 —269. Novel interpretation method for the contribution of structure-information representation

indices and predicted physical properties in models of ADME/tox behavior. ANN case studies: Human oral absorption and plasma protein binding. **L. H. Hall II**, L. M. Hall, M. E. Parham, J. Votano, L. B. Kier

3:05 — Intermission.

3:20 —270. Computational methods for evaluating ideas for kinase targeted libraries. **M. S. Lawless**, J. Swanson, R. Foster, C. Harding, R. Clark

3:50 —271. Visualization of domain applicability of in vitro Chromosome Aberration QSAR models. **D. Morrall**, C. Yang, G. J. Myatt, K. Cross, P. E. Blower

4:20 —272. Link3D software: Remote interactive molecular visualization thru Internet. **F. Sanz**, J. A. Naranjo, M. Pastor

4:50 —273. Interpretation techniques for promolecular electron density distribution functions. **L. Leherte**, D. P. Vercauteren

Section C

Unknown Site -- Unknown Room

General Oral -- Molecular Mechanics and Simulation

J. D. Madura, *Organizer*

1:20 —274. Diameter and chiral dependence of the radial breathing mode in single-walled carbon nanotubes. **H. M. Lawler**, J. W. Mintmire, D. Areshkin, C. T. White

1:40 —275. Quantum mechanical reaction rate constants by vibrational configuration interaction. **A. Chakraborty**, D. G. Truhlar

2:00 —276. Atomistic simulations of shocks in HMX crystals. **E. Jaramillo**, A. Strachan, T. D. Sewell

2:20 —277. Osmolyte (TMAO) effects on the strength of hydrophobic interactions: Origin of osmolyte compatibility. **M. V. Athawale**, J. S. Dordick, S. Garde

2:40 — Intermission.

2:50 —278. Dewetting transition and hydrophobic collapse in protein aggregates. **R. Zhou**

3:10 —279. Folding mechanisms of cold shock proteins. **A. E. Cardenas**, S. Urahata, A. Clarke

3:30 —280. Molecular dynamics simulation of folding of a short helical peptide with two disulfide bonds. **Y -C. Sun**, Y -L. Tsai

3:50 —281. Simulations of polymer nanocomposites. **T. C. Clancy**

4:10 — Intermission.

4:20 —282. Simulations of monolayer lubricants on solid surfaces. **D. L. Irving**, D. W. Brenner

4:40 —283. A phenomenological model for surface diffusion: Diffusive dynamics across stochastic potentials. **J. M. Moix**, R. Hernandez

5:00 —284. Multiscale simulations of sulfonated SIBS triblock copolymers. **J. Andzelm**, J. M. Sloan, E. Napadensky, S. H. McKnight, D. Rigby, J. Baker

Computational exploration of energy landscapes: challenges and solutions

Potential energy functions for biologically relevant systems

Cosponsored with COMP

Structures and properties of small clusters

Electronic structure theory of hard clusters

Cosponsored with COMP

THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Chemistry in the Discovery and Development of New Anti-Infective Agents

first session

Cosponsored with MEDI
G. S. Weston, *Organizer*

8:30 —285. Structure-Based Inhibitor Design vs. Beta-Lactamase. **B. Shoichet**, D. Tondi, F. Morandi, K. Babaoglu

9:00 —286. Structure guided design, synthesis and characterization of novel inhibitors of bacterial Enoyl ACP Reductase. **H. W. Pauls**, D. D. Manning, D. Xie, T. N. Duong, H. Y. Decornez, D. Kitchen, T. Clarke, M. Dorsey, D. E. Awrey, N. Kaplan, E. Bardouniotis, R. Thalakada, F. Martin, J. Berman

9:30 —287. Modeling of enoyl reductase inhibition by triclosan analogs. **J. P. Wolbach**, R. R. Hark, J. G. Longenecker, P. D. Schettler Jr., J. Strobl

10:00 —288. Back to the future: A computational, chemical and structural study of Dihydropteroate Synthase as a target for the discovery of new antimicrobial agents. **R. E. Lee**, S. W. White, K. Babaoglu, K. Hevener, K. Virga, J. Qi, I. Kerr, S. Mehra

10:30 — Intermission.

10:40 —289. Design of antibiotics targeting ribosomal decoding-site RNA. **T. Hermann**

11:10 —290. Stereochemical distinction using computed nuclear shieldings. **K. W. Wiitala**, C. J. Cramer, T. R. Hoye

11:40 —291. Role of conformational relaxation and entropy in the computation of binding affinities of flexible peptides with their protein targets. **L. Carlacci**, M. S. Lee, M. Olson

Section B

Unknown Site -- Unknown Room

General Oral -- Molecular Mechanics and Simulation

J. D. Madura, *Organizer*
F. H. Case, *Presiding*

8:00 —292. Ion partitioning at the air-water interface. **B. L. Eggimann**, J. I. Siepmann

8:20 —293. Ionic activities in brine solution from computer simulation. **P. E. Krouskop**, J. D. Madura, T. J. Dick

8:40 —294. Carbon dioxide sequestration: MM CO_2/ brine simulations. **T. J. Dick**, J. D. Madura

9:00 —295. Molecular simulation at constant pH: Direct approach from a semigrand partition function. **H. A. Stern**

9:20 — Intermission.

9:30 —296. Refining the structure of lipid bilayers with insight from molecular dynamics simulations. **J. B. Klauda**, R. W. Pastor, N. Kucerka, B. R. Brooks, J. F. Nagle

9:50 —297. Comparison of the CHARMM27, AMBER4.1 and BMS nucleic acid force fields via free energy calculations of base flipping. **U. D. Priyakumar**, A. D. MacKerell Jr.

10:10 —298. Complete structural and dynamical solution equilibrated model for Tissue Factor/Factor VIIa. **C. M. Colina**, D. Venkateswarlu, R. E. Duke, L. Perera, T. Darden, L. G. Pedersen

10:30 —299. Molecular basis for the Cu^{2+} binding induced destabilization of beta2-Microglobulin revealed by MD simulation. **N -J. Deng**, L. Yan, D. Singh, P. Cieplak

10:50 — Intermission.

11:00 —300. Molecular modeling of Lysl_tRNA synthetase: simulation meets experiment. **I. R. Gould**

11:20 —301. Simulating E-selectin complex with calcium ion and sialyl LewisX with a polarizable force field. **G. A. Kaminski**

11:40 —302. Refining the computational procedures for predicting complex hydrogen bonding patterns

in crystals. P. H. Young, **H. Y. Ando**

Section C

Unknown Site -- Unknown Room

General Oral -- Drug Discovery

W. D. Cornell, *Organizer*
C. Duraiswami, *Presiding*

8:30 —303. In search for active conformations and meaningful alignments for 3D-QSAR. **P. A. Petukhov**, H. Yuan

8:50 —304. 3D similarity searching and docking of flexible molecules using fuzzy molecular representations. **M. Glick**, J. L. Jenkins, W. G. Richards, J. W. Davies

9:10 —305. Using atomic property values for the selection of small molecule superposition. **S. A. Wildman**, R. V. Stanton

9:30 —306. A novel approach to QSAR model validation based on training and test set resampling. **A. Golbraikh**, A. Tropsha

9:50 —307. Application of SCOPE (Statistical Conformational Occupancy analysis and Pharmacophore Elucidation) to a set of DHFR and CDK2 inhibitors. **C. Duraiswami**, C. Williams

10:10 — Intermission.

10:20 —308. Applications by scripting: Creation and use of a chemically-aware Python toolkit. **J. M. Leonard**, R. Camarra, R. W. Dixon

10:40 —309. Development and application of methods based on a one-dimensional molecular representation. **D. J. Diller**, N. Wang

11:00 —310. Ab initio quantum chemical calculations of the preferred tautomeric forms and binding affinities to CDK2 of substituted pyrazolopyridines. **J. Duca**

11:20 —311. Structure-based identification of the binding site for the hemiasterlin analog HTI-286 on tubulin. **M. Ravi**, A. Zask, T. S. Rush

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Methodology

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THURSDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Chemistry in the Discovery and Development of New Anti-Infective Agents

second session

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G. S. Weston, *Organizer*

1:00 —312. Understanding the mode of action and drug resistance of anti-HIV nucleosides by molecular modeling. **C. K. Chu**, V. Yadav, Y. Chong

1:30 —313. BARACLUDE^{tm} (Entecavir), a potent and selective inhibitor of HBV-RT: Molecular mechanism(s) of resistance in viruses with pre-existing lamivudine resistance substitutions. **D. Langley**, A. J. Oliver Kapur, D. J. Tenney, B. E. Rose, S. M. Levine, K. A. Pokornowski, M. J. Plym, C. Yu, C. J. Baldick, S. Zhang, A. W. Walsh, L. Discotto, C. Mazzucco, J. Fang, R. J. Colonno

2:00 —314. Molecular modeling of covalent complexes and structural-based design of irreversible inhibitors of Rhinovirus 3C protease. **X. Hou**, B. J. Burke, D. A. Matthews, P. S. Dragovich

2:30 —315. Computational Studies towards the design of a potent HCV NS3•4A protease inhibitor: VX-950. **B. G. Rao**

3:00 — Intermission.

3:10 —316. Computer modeling analysis of the K65R mutation in HIV-1 reverse transcriptase and its effects on nucleotide binding. **J. M. Chen**, K. L. White, J. Feng, N. A. Margot, J. Ly, A. S. Ray, H. L.

MacArthur, M. McDermott, M. D. Miller, S. Swaminathan

3:40 —317. Computational studies and biological evaluation of geminal disulfones as HIV-1 integrase inhibitors. **J. Gervay-Hague**, D. J. Tantillo, D. C. Meadows

4:10 —318. Computational titration analysis of the pH dependence of human parainfluenza virus hemagglutinin-neuraminidase. **M. Fornabaio**, M. Porotto, A. Moscona, G. E. Kellogg

4:40 —319. Automatic short-list generation using sum-rank. **J. I. Manchester**, L. MacPherson

Section B

Unknown Site -- Unknown Room

General Oral -- Molecular Mechanics and Simulation

J. D. Madura, *Organizer*
P. E. Krouskop, *Presiding*

1:00 —320. A QM/MM calculation of the reduction potential of flavin adenine dinuclotide in medium chain Acyl-CoA dehydrogenase using SCC-DGTB-GHO method. **S. Bhattacharyay**, M. T. Stankovich, J. Gao

1:20 —321. QM/MM study of the 1H NMR and 205Tl NMR spectra of Thallium bound G-quadruplex from Oxytricha Nova. **C. M. Ragain**, J. A. Gascon, M. L. Gill, S. A. Strobel, J. P. Loria, V. S. Batista

1:40 —322. A self-consistent QM/MM protocol for the description of protein polarization. **J. A. Gascon**, S. Leung, E. R. Batista, V. Batista

2:00 —323. The Effective Fragment Potential method for solvation: Modeling bulk behavior with molecular dynamics. **H. M. Netzloff**, M. S. Gordon

2:20 — Intermission.

2:30 —324. Calculating absolute free energies using a "smart" reference system. **F. M. Ytreberg**, D. M. Zuckerman

2:50 —325. Advances in conformational sampling and free energy calculations via adiabatic dynamics. **J. B. Abrams**, L. Rosso, M. E. Tuckerman

3:10 —326. Relaxation simulations of a multiple-copy region in locally enhanced sampling indicates the large change in free energy surface through mean-field approximation. **Z. Huang**, C. A. Hixson, R. A. Wheeler

3:30 —327. Direct calculation of binding free energy of biological ligands using Fujitsu BioServer. **H. Fujitani**, Y. Tanida, M. Ito, M. R. Shirts, G. Jayachandran, E. J. Sorin, V. S. Pande

3:50 — Intermission.

4:00 —328. Flexligdock: a flexible ligand-protein docking algorithm. **P. R. Oledzki**, R. M. Jackson, P. C. Lyon

4:20 —329. Standard binding free energy: aromatic molecules bind T4 lysozyme mutant. **Y. Deng**, B. Roux

4:40 —330. Calculation of local pressure tensors in systems with many-body interactions. **H. Heinz**, W. Paul, K. Binder

Section C

Unknown Site -- Unknown Room

General Oral -- Drug Discovery

W. D. Cornell, *Organizer*
L. Whitehead, *Presiding*

1:20 —331. Fragment based data mining of P450 inhibition data – Deriving knowledge for drug design. **X. Q. Lewell**, S. Modi

1:40 —332. Development of in-silico models for metabolic stability of drugs in human hepatocyte. **H. Zhang**, P. H. Lee, H. Cai, E. M. Gifford

2:00 —333. An Accurate and Interpretable Bayesian Classification Model for Prediction of HERG Liability. **H. Sun**

2:20 —334. Maximising the coverage and flexibility of a diverse representative subset for screening variable number of compounds to suit target knowledge. **S. K. Yeap**, R. J. Walley, J. S. Mason

2:40 —335. Need to select lead candidates? ROC curves can help. **N. Triballeau**, F. Acher, J -P. Pin, H -O. Bertrand

3:00 — Intermission.

3:10 —336. Opening up binding sites of homology models via a balloon potential: A molecular dynamics refinement approach. S. R. Kimura, **R. Rajamani**, D. Langley

3:30 —337. Development of fragment-based chemical descriptors using novel frequent common subgraph mining approach and their application in QSAR modeling. **R. Khashan**, W. Zheng, J. Huan, W. Wang, A. Tropsha

3:50 —338. Identification of novel anticonvulsant agents by virtual screening of chemical databases with validated QSAR models. **M. Wang**, S. Zhang, S. Oloff, A. Golbraikh, H. Kohn, A. Tropsha

4:10 —339. Consideration of binding site characteristics for structure-based design. **M. Kontoyianni**, M. Lim-Wilby

Computational exploration of energy landscapes: challenges and solutions

Advances in methodology

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