COMP

DIVISION OF COMPUTERS IN CHEMISTRY

Program Not Yet Complete -- Run Data Integrity Report to Identify Errors

Times, days, and paper numbers may not be final.

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

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

General

E. A. Carter and M. S. Gordon, Organizers, Presiding

9:00 — 1. First principles approaches to design of materials with applications to catalysis, nanoelectronics, fuel cells, and pharma. W. A. Goddard III

9:35 — 2. Chemical bonding in very tight places. R. Hoffmann

10:10 — 3. Electron tunneling through proteins. H. Gray, J. R. Winkler

10:45 — Intermission.

11:00 — 4. Photoelectron spectroscopy of organic anions. W. C. Lineberger, G. B. Ellison


Section B

Unknown Site -- Unknown Room

Molecular Mechanics

Advancing Methodology

E. X. Esposito, Organizer
N. Vaidehi, Presiding

8:30 — 6. Application of Ewald summations to long-range dispersion forces. P. J. In 't Veld, A. E. Ismail, G. S. Grest

8:55 — 7. Microscopic analysis of the dielectric effect. E. G. Zoebisch


9:45 — Intermission.

10:00 — 9. Comparison of the simulated properties of N-methylacetamide and glycine in water obtained using different force fields. M. Kang, P. E. Smith


10:50 — 11. ReaxFF simulations on reactive processes at the water/metal/metal oxide interface. A. C. van Duin, V. S. Bryantsev, W. A. Goddard III


Section C

Unknown Site -- Unknown Room

**Antifreeze Proteins: A Memorial Symposium for Robert Feeney**

A. Wierzbicki, Organizer

8:30 — Introductory Remarks.

8:40 — 13. The quasi-liquid layer involvement in antifreeze function. Y. Yeh, K. Krishnan, W. H. Fink, Y. Duan


9:50 — 15. Antifreeze fundamentals: Explaining the dependence of freezing point upon concentration. C. A. Knight, A. L. DeVries

10:20 — Intermission.


11:35 — 18. Antifreeze Glycoproteins to function as intrinsically unstructured proteins. K. Krishnan, Y. Yeh, Y. Duan, W. H. Fink

Section D

Unknown Site -- Unknown Room

Recent Advances in Studies of Molecular Processes at Interfaces

Ultrafast and Reactions at Interfaces

L. X. Dang, Organizer
J. Hemminger, Presiding

8:30 — Introductory Remarks.

8:35 — 19. Dynamics of electrons at interfaces on ultrafast timescales. C. B. Harris


10:15 — Intermission.

10:35 — 22. Equilibrium and ultrafast phenomena at liquid interfaces. K. B. Eisenthal

11:15 — 23. Solute rotational dynamics at water surfaces. I. Benjamin


Section E

Unknown Site -- Unknown Room

Protein-Nucleic Acid Interactions: Experimental and Modeling Analysis

M. R. Mihailescu, Organizer


9:00 — 26. RNA and protein structural requirements in NCp7 chaperoned HIV-1 DIS maturation. J. P. Marino

10:00 — Intermission.


10:45 — 29. Dynamics of the assembling ribosome. J. R. Williamson


11:45 — 31. What can simulation tell us about protein-nucleic acid interactions? Successes, failures, and our approach to overcome the deficiencies. T. E. Cheatham III

Computational Actinide and Transactinide Chemistry: Progress and Perspectives

Actinide Chemistry Overview

Sponsored by NUCL, Cosponsored with COMP, and INOR

Computational Electrochemistry for New Energy

Redox Potentials

Sponsored by PHYS, Cosponsored with COMP

Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?

Nonadiabatic Dynamics

Sponsored by PHYS, Cosponsored with COMP

SUNDAY AFTERNOON

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

Biological
E. A. Carter and M. S. Gordon, Organizers

H. Gray, Presiding

2:00 — 32. Computational methods for protein design applications. S. L. Mayo

2:35 — 33. Use of protein-ligand docking methods to rank order ligand binding affinities. R. Friesner

3:10 — 34. My protein folds faster than yours: Using protein folding rates to test protein folding theory. K. W. Plaxco

3:45 — Intermission.

4:00 — 35. DNA: Not merely the secret of life. N. C. Seeman


Section B

Unknown Site -- Unknown Room

Drug Discovery

Docking

I. Visiers, Organizer
D. Ryan, Presiding

1:00 — Introductory Remarks.


1:50 — 39. All-atom semiempirical LocalSCF quantum-mechanical protein-ligand docking. V. M. Anisimov, V. L. Bugaenko

2:10 — 40. Improving the accuracy of MM-GBSA binding energy predictions through parameter optimization. B. W. Sherman, J. Duan, M. P. Repasky

2:30 — 41. Using diverse computational approaches to understand protein/ligand binding affinities in structure-based drug design: A cross-docking study. J. H. Voigt, C. Elkin, J. S. Duca

2:50 — Intermission.

3:05 — 42. TAE Augmented scoring functions, two approaches, atom and surface based. M. D. Ryan, T. Hepburn, N. Sukumar, S. Das, C. M. Breneman

3:45 — 44. Development of customized scoring function for the prediction of binding affinities of Aurora Kinase inhibitors. S. N. Rao, B. W. Sherman, R. Farid

4:05 — 45. Knowledge-based docking for kinases with minimal bias. S. Wittkopp, J. E. Penzotti, R. V. Stanton, S. A. Wildman

4:25 — 46. Species selectivity of the Urotensin II receptor: Molecular Modeling study. S.-K. Kim, Y. Li, C. M. Park, R. Abrol, W. A. Goddard III

4:45 — 47. Study of antimalarial activity of pyrimethamin and flavonoids by molecular docking. A. B., A. C. Mustapha BENCHARIF

Section C

Unknown Site -- Unknown Room

Quantum Chemistry

A. E. Roitberg, Organizer
E. R. Chan, Presiding

1:30 — 48. Design of small band gap conjugated ladder polymers using acetylenic crosslinks. M. Kertesz, S. Yang


2:45 — Intermission.

3:00 — 51. On the acidic properties of conventional and novel zeolitic materials: A DFT investigation. M. Elanany, D. P. Vercauteren


Section D

Unknown Site -- Unknown Room

Phil Magee Memorial Symposium: QSAR Reborn
The Foundations of QSAR

Cosponsored with CINF
J. H. Block and B. Clark, Organizers

1:30 —54. Philip S. Magee: A Life in QSAR. M. Charton

2:00 —55. Molecular surfaces, QSAR, QSPR and reactivity. T. Clark

2:30 —56. CoMFA investigation of Taft Es values. Y. C. Martin, K. H. Kim

3:00 — Intermission.

3:20 —57. Conformation independent QSAR Descriptor, scaffold hopping with surface property based eHiTS LASSO. Z. Zsoldos, D. Reid, B. S. Sadjad, A. Simon

3:50 —58. Approaches to the use of quantum mechanical modeling in QSAR analysis of agrochemicals. D. W. Boerth, T. C. Andrade, E. Eder

4:20 —59. QSAR without arbitrary descriptors: The electron-conformational method. I. B. Bersuker

Section E

Unknown Site -- Unknown Room

Emerging Technologies

Competition Symposium

C. M. Breneman, Organizer

1:00 — Introductory Remarks.

1:05 —60. New approaches to quantitative modeling that span the periodic table: The correlation consistent Composite Approach (ccCA). N. DeYonker, T. R. Cundari, A. K. Wilson


2:35 — Intermission.

2:50 —63. Conformational sampling by self-organization. F. Zhu, D. K. Agrafiotis


3:50 —65. Insights into peptide folding from a multiscale coarse-grained model. I. F. Thorpe, J. Zhou,
G. A. Voth


4:50 — Award Presentation.

Section F

Unknown Site -- Unknown Room

Recent Advances in Studies of Molecular Processes at Interfaces

Ions at Interface

L. X. Dang, Organizer
B. D. Kay, Presiding


2:10 — 68. Computational analysis of interfacial sum frequency generation spectroscopy. A. Morita, T. Ishiyama

2:50 — 69. Is the surface of neat water neutral, acidic, or basic? R. Vacha, V. Buch, A. Milet, J. P. Devlin, P. Jungwirth

3:10 — Intermission.

3:30 — 70. Interfacial reactions in salty glycerol. J. L. DeZwaan, A. H. Muenter, G. M. Nathanson

4:10 — 71. Structural order and dynamics at water/hydrocarbon and water/surfactant interfaces. B. M. Ladanyi, J. Chowdhary


Computational Actinide and Transactinide Chemistry: Progress and Perspectives

Structure and Bonding

Sponsored by NUCL, Cosponsored with COMP, and INOR

Computational Electrochemistry for New Energy
Electrocatalysis

Sponsored by PHYS, Cosponsored with COMP

Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?

Statistical Theories

Sponsored by PHYS, Cosponsored with COMP

SUNDAY EVENING

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Poster Session in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

E. A. Carter and M. S. Gordon, Organizers

7:30 - 9:30

73. Conversion of a plant chloroplast to a biological fuel cell: 1. Comparison of electron transfer from reduced ferredoxin to FAD and a gold electrode. S. P. Walch, J. D. Komadina, F. B. Prinz

74. Exploring conductance switching properties of molecular scale devices: A computational approach. B. D. Dunietz, T. Perrine, A. Prociuk

75. A bond energy bond order model for electronic energy. S. Tulyani, G. A. Petersson, P. R. Westmoreland


77. Advanced CCBB-MC method for polymer statistics. J. Sadanobu

78. Application of structure-based pharmacophore screening in ligand docking. D. Zhang

79. Bold advances in force fields: The ReaxFF reactive force field. A. C. van Duin, W. A. Goddard III

80. Coherent electron tunneling through 1-D fullerene channels. G. I. Lee, Y. H. Kim, J. K. Kang


82. Cyclic saturated hydrocarbons containing planar tetracoordinate carbon atoms. N. Pérez, G. Merino
83. Defects modifications of ferroelectric PVDF based polymers. Q. Zhang

84. Discovery of new NOx reduction, hydrocarbon SCR catalysts using high throughput technologies. R. J. Blint

85. DNA-dependent RNA polymerases: Common structures of the active sites and possible reaction mechanisms. D. R. Salahub, R. Zhu

86. Electron force field simulation of matter at extreme conditions. J. T. Su


88. High-throughput optical methods for the analysis of chirality. E. V. Anslyn, S. Shabbir

89. Hybrid density functional band structure calculations on the cuprate superconductors. J. K. Perry, J. Tahir-Kheli, W. A. Goddard III

90. Hydrated water-soluble dendrimer-grafted polymer membranes for application to polymer electrolyte membrane fuel cells. S. S. Jang, W. A. Goddard III

91. Improved methods for predicting the structure and function of G protein-coupled receptors. R. Abrol, W. A. Goddard III


94. Molecular-scale understanding and design of low friction and biocompatible surfaces. S. Jiang

95. Multiconfigurational study of tetrasilacyclobutadiene cobalt complex. S. Sok, M. S. Gordon


98. New assignment of parameters for charge equilibration approach. N. Nakayama, H. Goto


101. Palladium mediated activation of molecular oxygen: Pd(0) vs. direct insertion. J. M. Keith, J. Oxgaard, W. A. Goddard III
102. Predictions of thermoelectric materials from atomistic simulations. **G. Galli**

103. Predicting the properties of hydrated silica at extreme conditions. **K. E. Anderson**, J. I. Siepmann, M. M. Hirschmann


106. Protein unfolding free energy surfaces from Jaryznski’s equality. **N. Salwen**, C -H. Kiang, N. C. Harris

107. QTPIE: A minimal extension of Goddard's QEq model with correct dissociation. **J. Chen**, T. J. Martínez

108. Quantum chemistry and collisions in planetary atmospheres. **D. L. Huestis**

109. Quantum mechanical rapid screening of chemical sensing materials. **A. V. Shevade**, A. Ryan, M. Homer, M. Blanco, W. A. Goddard

110. Spin-orbit ab initio study of excited state of CH2CII cation. **J. Kim**, H. Ihee, Y. S. Lee


113. The photoinduced electron transfer on dye-sensitized solar cells: Modified Sakata-Hashimoto-Hiramoto model (MSHH). **O. Kitao**


**MONDAY MORNING**

Section A

Unknown Site -- Unknown Room

**Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday**

**Nanotechnology**

E. A. Carter and M. S. Gordon, **Organizers**
J. Tahir-Kheli, **Presiding**


10:45 — Intermission.


Section B

Unknown Site -- Unknown Room

Molecular Mechanics

Biological Systems

E. X. Esposito, Organizer
M. M. Layten, Presiding


8:55 — 121. Disruption of membranes by antimicrobial oligomers: An atomistic view. J. Henin, M. L. Klein


9:45 — 123. Coupling of fast and slow modes in the reaction pathway of the minimal hammerhead ribozyme cleavage. R. Radhakrishnan

10:10 — Intermission.


Section C

Unknown Site -- Unknown Room

Antifreeze Proteins: A Memorial Symposium for Robert Feeney

A. Wierzbicki, Organizer

8:30 — 128. Competing effects in hydrophobic hydration. D. Chandler

9:10 — 129. Effects of motion and aggregation of AFP segments on water molecules near an ice crystal. Y. Hagiwara, T. Nobekawa

9:40 — 130. From interfacial structure to antifreeze mechanism of antifreeze protein. X. Y. Liu, N. Du

10:10 — Intermission.

10:25 — 131. Interaction and dynamics in water-AFP-ice interfacial region and the thermodynamic effect on ice growth inhibition. Y. Ba, Y. Mao


11:25 — 133. Molecular dynamics study of growth kinetics of ice-water interfaces in the presence of winter flounder antifreeze protein. H. Nada, Y. Furukawa

Section D

Unknown Site -- Unknown Room

Recent Advances in Studies of Molecular Processes at Interfaces

Liquid Surfaces

L. X. Dang, Organizer
T. M. Orlando, Presiding

8:30 — 134. The surface of nitric acid solutions: Insights gained from a combined experimental and computational approach. G. L. Richmond

9:10 — 135. Hydrated protons at interfaces. G. A. Voth

10:10 — Intermission.

10:30 — 137. Application of inner-shell photoelectron spectroscopy to aqueous solutions. B. Winter

11:10 — 138. Computational study of SFG spectra of ice, water and acid solution. V. Buch, G. L. Richmond, M. J. Shultz

11:50 — 139. pH of the liquid water surface: Is hydroxide present at the interface? R. J. Saykally, P. B. Petersen

Section E

Unknown Site -- Unknown Room

Protein-Nucleic Acid Interactions: Experimental and Modeling Analysis

M. R. Mihailescu, Organizer
T. Evans, Presiding

8:30 — 140. Deducing the multiple binding modes of p53 tetramer – DNA interaction based on full-site palindrome of p53 response elements. B. Ma, A. J. Levine

9:00 — 141. How does a protein find its site on DNA? L. Mirny

9:30 — 142. Fragile X mental retardation syndrome: Structure of the KH1-KH2 domains of fragile X mental retardation protein. L. Regan, R. Valverde, I. Pozdnyakova, T. Kajander, J. Venkatraman

10:00 — Intermission.

10:15 — 143. Mechanism of RNA binding by RNA recognition motifs. K. B. Hall

10:45 — 144. Probing the structure and activity of DNA-/RNA-processing enzymes with the 2,4-difluorotoluyl/ribo-2,4-difluorotoluyl (dF/rF) nucleoside, an apolar thymidine/uridine analog. M. Egli, P. S. Pallan, F. Li, A. Irimia, R. L. Eoff, J. Xie, A. Noronha, K. G. Rajeev, F. P. Guengerich, E. Rozners, M. Manoharan


11:45 — 146. On nucleic acid flexibility using continuum solvent models. Y. J. Bomble, D. A. Case

Section F

Unknown Site -- Unknown Room

Evaluation of Computational Methods: Insights, Philosophies and Recommendations

Focus on Docking
A. Nicholls and A. N. Jain, *Organizers*

9:00 — Introductory Remarks.

9:15 — 147. Methodological performance reporting: To confuse or to enlighten. **A. N. Jain**


10:25 — Intermission.


11:15 — 150. Insights into the setup of the GSK docking evaluation. **N. Nevins**, M. S. Head

11:50 — 151. On how (not) to do an evaluation. **P. Hawkins**

**Computational Actinide and Transactinide Chemistry: Progress and Perspectives**

**Solvation and Spectroscopy**

*Sponsored by NUCL, Cosponsored with COMP, and INOR*

**Computational Electrochemistry for New Energy**

**Charge Transfer**

*Sponsored by PHYS, Cosponsored with COMP*

**Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?**

**Water and Solvent Effects**

*Sponsored by PHYS, Cosponsored with COMP*

**MONDAY AFTERNOON**

Section A

Unknown Site -- Unknown Room

**Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill**
Goddard, on the Occasion of his 70th Birthday

Homogeneous Catalysis

E. A. Carter and M. S. Gordon, Organizers
R. G. Parr, Presiding

2:00 —152. Stitching with nitrogen. K. B. Sharpless


3:45 — Intermission.


Section B

Unknown Site -- Unknown Room

Drug Discovery

Virtual Screening

I. Visiers, Organizer
L. Herman, Presiding


1:20 —158. Automated combinatorial alignment for 3-D similarity searching. J. H. Nettles, J. L. Jenkins, Z. Deng, A. Bender, J. W. Davies, M. Glick


2:00 —160. Electrostatic similarity as an orthogonal approach to atom-based methods. P. Hawkins

2:20 — Intermission.

2:35 —161. Improving scoring for virtual screening of fragment-sized molecules. B. W. Sherman

3:15 — 163. FlexX-Screen: Interactive virtual screening. H. Claußen


Section C

Unknown Site -- Unknown Room

Quantum Chemistry

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

1:30 — 166. Basis set convergence of correlation energy contributions from connected triple, quadruple, and higher excitations. J. M. Martin


2:20 — 168. Ensemble-based electron propagator calculations of electron binding energies. J. V. Ortiz

2:45 — Intermission.

3:00 — 169. Highly accurate ab initio quartic force fields of C₃H⁺ and HO₂⁺. X. Huang, T. J. Lee

3:25 — 170. Principles and applications of the general-purpose reactivity indicator: Beyond the classic reactivity paradigms. J. S. M. Anderson

3:50 — 171. Self-consistent polarization of the boundary in the redistributed charge and dipole scheme for combined quantum mechanical and molecular mechanical calculations. H. Lin, Y. Zhang, D. G. Truhlar

Section D

Unknown Site -- Unknown Room

Phil Magee Memorial Symposium: QSAR Reborn

Theory

Cosponsored with CINF
J. H. Block and B. Clark, Organizers
1:30 — 172. QSAR applied in systems biology. **D. E. Patterson**

2:00 — 173. The role of alignment in 3-D QSAR. **R. D. Clark**, R. Cramer


3:00 — Intermission.


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**Section E**

Unknown Site -- Unknown Room

**Computational Science & Engineering Advances Supported by NSF Resource**

**Engineering Sciences**

_Cospresented with PHYS_

J. Towns, Organizer

1:30 — 178. Multiscale models for biomolecular engineering. **Y. Kaznessis**

2:00 — 179. All-atom and multiscale modeling of silicon nanobiodevices. **A. Aksimentiev**


3:00 — 181. Improvement in structure model accuracy and molecular replacement through high-resolution protein structure refinement. **B. Qian**, D. Baker

3:30 — Intermission.

3:45 — 182. Performing simulations at the terascale today and at the sustained petascale "tomorrow". **J. A. Nichols**

4:15 — 183. Screened hybrid DFT and the Mott transition in MnO. **R. L. Martin**

4:45 — 184. Advances in ab initio and density functional approaches: From a methodological and basis set perspective. **A. K. Wilson**

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**Section F**
Evaluation of Computational Methods: Insights, Philosophies and Recommendations

Focus on Docking

A. Nicholls and A. N. Jain, Organizers

1:30 —185. Can we use docking and scoring for hit optimization? I. J. Enyedy, W. Egan


2:40 —187. Protein crystal structures: Are they really as precise or accurate as we think? G. L. Warren

3:15 — Intermission.

3:30 —188. Diverse, high-quality test set for the validation of protein-ligand native and cross-docking performance. P. N. Mortenson

4:05 —189. Evaluating docking programs: Keeping the playing field level. J. W. Liebeschuetz

4:40 —190. Panel Discussion of Computational Methods Evaluation, Moderated by Marti Head. M. S. Head

Computational Actinide and Transactinide Chemistry: Progress and Perspectives

Relativistic Quantum Chemistry

Sponsored by NUCL, Cosponsored with COMP, and INOR

Computational Electrochemistry for New Energy

Transport

Sponsored by PHYS, Cosponsored with COMP

Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?

Nuclear Quantum Dynamics

Sponsored by PHYS, Cosponsored with COMP
MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix

E. X. Esposito, Organizer

6:00 - 8:00

268, 329-346, 349. See subsequent listings.

TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

Theory

E. A. Carter and M. S. Gordon, Organizers
R. P. Muller, Presiding

9:00 — 191. Reading the map while walking through the minefield: An ab initio excursion into high temperature superconductivity. J. Tahir-Kheli, W. A. Goddard III

9:35 — 192. Recent advances and ongoing challenges in accelerated molecular dynamics methods. A. F. Voter


10:45 — Intermission.

11:00 — 194. A general approach to intermolecular interactions. M. S. Gordon


Section B

Unknown Site -- Unknown Room

Molecular Mechanics
Protein-Ligand Interactions

E. X. Esposito, Organizer
V. Chandrasekaran, Presiding

8:30 — 196. The dynamic behavior of some hairpin loops in rRNA upon ligand binding. A. Rakic, P. M. Mitrasinovic

8:55 — 197. Ligand binding affinity estimate by amoeba polarizable force field. P. Ren, D. Jiao

9:20 — 198. Trypanosoma cruzi trans-sialidase binding investigated by molecular dynamics simulations. Ö. Demir, A. Roitberg

9:45 — 199. A computational approach toward combating pandemic influenza: Molecular dynamics and docking studies of ligand binding with neuraminidase. R. C. Rizzo, R. Chachra, J. E. Shipman, N. A. Carrascal, S. Mukherjee

10:10 — Intermission.


10:50 — 201. Computational determination of the binding and insertion of PR3 to mixed lipid membranes. E. Hajjar, M. Mihajlovic, T. Lazaridis, N. Reuter


11:40 — 203. Molecular dynamics simulations suggest a way to stabilize von Hippel-Lindau tumor suppressor protein and rescue its function. J. Liu, R. Nussinov

Antifreeze Proteins: A Memorial Symposium for Robert Feeney

A. Wierzbicki, Organizer

8:30 — 204. Lessons from recent additions to the antifreeze protein portfolio. P. L. Davies


10:10 — Intermission.
10:25 —207. Probing the origin of the hyperactivity of the two-domain type III antifreeze protein RD3. 
N. B. Holland, Ö. Can, S. Tsuda, F. D. Sönnichsen

10:55 —208. Significance of non-polar interactions at the water/ice interface for non-equilibrium 
antifreeze activity. A. Wierzbicki, C. A. Knight, C. N. Henderson


Section D

Unknown Site -- Unknown Room

Recent Advances in Studies of Molecular Processes at Interfaces

Biological Interface

L. X. Dang, Organizer
R. B. Gerber, Presiding

8:30 —210. Simulations of water interfacial behavior. M. J. Stevens

9:10 —211. Modulating ligand-receptor binding at the lipid membrane interfaces. P. S. Cremer, H. Jung

9:50 —212. Calculation of diffusion coefficients of water and alkanes through single-walled carbon 
nanotubes from simulations. J. K. Johnson, Y. Wang, J.-C. Liu, D. S. Sholl

10:10 — Intermission.

10:30 —213. Insertion, folding and oligomerization of peptides at water-membrane interfaces. C. L. Brooks III

11:10 —214. Low-energy electron elastic scattering theory and an experimental description of water and 
water:DNA interfaces. T. M. Orlando, D. Oh, Y. Chen, A. Alexandrov


Section E

Unknown Site -- Unknown Room

Protein-Nucleic Acid Interactions: Experimental and Modeling Analysis

M. R. Mihailescu, Organizer
L. Menon, Presiding

8:00 —216. Polyelectrolyte behavior and dynamics of three-way RNA junctions and random RNA
sequences. **U. Mohanty**

**8:30 — 217.** Isostructural does not mean isoenergetic: Computational studies of the mechanism of recognition of oxidative DNA damage. **C. L. Simmerling**, K. Song

**9:00 — 218.** Single molecule folding reveals mechanism of ribozyme action. **N. G. Walter**, C. de Silva

**9:30 — 219.** The smn complex: A molecular assembly machine for rNPs. **G. Dreyfuss**

**10:00 —** Intermission.


**10:45 — 221.** Using structural superposition for the analysis of protein-RNA. **Y. Shamoo**

**11:15 — 222.** RNA structural bioinformatics of RNA-Protein interactions. **N. B. Leontis**

**11:45 — 223.** On the dynamics of some small structural motifs in rRNA upon ligand binding. A. Rakic, **P. M. Mitrasinovic**

Unknown Site -- Unknown Room

**Evaluation of Computational Methods: Insights, Philosophies and Recommendations**

**Focus on Ligand-Based Methods**

A. Nicholls and A. N. Jain, *Organizers*

**9:00 —** Introductory Remarks.

**9:05 — 224.** What do we know and when do we know it: Lessons from information theory. **A. Nicholls**


**10:15 — 226.** Ligand-based modeling: To confuse or enlighten. **A. N. Jain**

**10:50 — 227.** Issues in comparing shape similarity methods: KISS helps. **R. D. Cramer**


**Computational Actinide and Transactinide Chemistry: Progress and Perspectives**
Transactinide Chemistry

Sponsored by NUCL, Cosponsored with COMP, and INOR

Computational Electrochemistry for New Energy

Materials and Processes

Sponsored by PHYS, Cosponsored with COMP

Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?

Electronic Structure Theories

Sponsored by PHYS, Cosponsored with COMP

RNA Interference Based Therapeutics

Sponsored by CARB, Cosponsored with BIOL, BIOT, COMP, MEDI, ORGN, PMSE, POLY, and BTEC

TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

Heterogeneous Catalysis

E. A. Carter and M. S. Gordon, Organizers
M. A. C. Nascimento, Presiding

2:00 — 229. Selectivity issues in ammoxidation catalysis: MoV(Nb,Ta)(Te,Sb)O System. R. K. Grasselli

2:35 — 230. Theoretical heterogeneous catalysis, limitations and challenges. R. A. van Santen

3:10 — 231. Understanding electrochemical systems from first principles. T. Jacob

3:45 — Intermission.
4:00 — 232. Rational design of molecular catalysts applied in hydrogen storage, production and hydrogen fuel cell. W.-Q. Deng


Section B

Unknown Site -- Unknown Room

Drug Discovery

Virtual Screening

I. Visiers, Organizer
D. Joseph-McCarthy, Presiding

1:00 — 234. FITTED 2.0: A program for flexible protein-flexible ligand docking. N. Moitessier, C. R. Corbeil, P. Englebienne

1:20 — 235. DOVIS: A high performance computing tool for virtual screening using AutoDock. X. Jiang, K. Kumar, A. Wallqvist, J. Reifman

1:40 — 236. Finding the best protocol for enzyme activity modeling. S. A. Wildman, R. V. Stanton

2:00 — 237. Can we improve the structure-based virtual screen hit rate by proposing limited number of VS hits? S.-B. Rong, J. van Drie

2:20 — 238. Identification of weak leads with virtual screening. N. Brooijmans, C. Humblet

2:40 — Intermission.


3:55 — 242. Understanding false positives in reporter gene assays: In silico chemogenomics approaches to prioritize cell-based HTS data. M. Glick

Section C

Unknown Site -- Unknown Room
Quantum Chemistry

A. E. Roitberg, Organizer
A. J. Campbell, Presiding

1:30 —243. Computation of electron transfer energies for redox proteins by combining QM/MM and classical molecular dynamics simulation. J. Blumberger


2:45 — Intermission.

3:00 —246. A design atom approach for the QM/MM covalent boundary. Y. Zhang, C. Xiao


3:50 —248. QM/MM study of orotidine-5'-monophosphate decarboxylase. I. F. W. Kuo, C. L. Stanton, C. J. Mundy, T. Laino, K. N. Houk

Unknown Site -- Unknown Room

Phil Magee Memorial Symposium: QSAR Reborn

Methods

Cosponsored with CINF
J. H. Block and B. Clark, Organizers

1:30 —249. New pharmacophore constrained Gaussian shape/electrostatic/oroed force field similarity searching tools: Feeding the synthetic beast with KIN. A. C. Good, A. Tebben, B. Claus

2:00 —250. Application of pharmacophore fingerprint QSAR to 7TM drug design. Z. Yang


3:00 — Intermission.

3:20 —252. Informatics-based to structure-based ADME/tox modeling. A. J. Hopfinger

3:50 —253. A novel technique for virtual discovery for study of multistage bioprocesses. V. Potemkin

Section E

Unknown Site -- Unknown Room

Computational Science & Engineering Advances Supported by NSF Resource

Molecular Sciences

Co-sponsored with PHYS
J. Towns, Organizer

1:00 — 255. From megaflops to teraflops: From molecules to cells. K. Schulten

1:30 — 256. Classical and quantum/classical biological modeling using the TeraGrid. A. E. Roitberg

2:00 — 257. Biomolecular simulation toward the petascale: Performance, workflow, and application to nucleic acid structure and dynamics. T. E. Cheatham III


3:00 — Intermission.

3:15 — 259. Using NSF supercomputer resources to study biomolecular structure and function. J. D. Madura

3:45 — 260. New discoveries in biomolecular systems enabled by high performance computing. G. A. Voth

4:15 — 261. Using large-scale computing to investigate dynamic aspects of biomolecular structure and function. C. L. Simmerling

4:45 — 262. Integrated computational biology: From the molecule to the cell. J. A. McCammon

Section F

Unknown Site -- Unknown Room

Evaluation of Computational Methods: Insights, Philosophies and Recommendations

Focus on Ligand-based Methods

A. Nicholls and A. N. Jain, Organizers

1:30 — 263. Computational model validation—conducting a fair trial. G. Pearl, S. Bhal, E. Kolovanov
2:05 — 264. Practicing best practices in developing predictive QSAR models. A. Golbraikh, A. Tropsha

2:40 — Intermission.

2:55 — 265. Validation and the downside of the law of large numbers. R. D. Clark, M. A. Dolan

3:30 — 266. Virtual screening enrichment studies: A help or hindrance in tool selection? A. C. Good, T. I. Oprea

4:05 — 267. Panel discussion of computational methods evaluation, Moderated by Terry Stouch. T. R. Stouch

4:35 — Concluding Remarks.

Computational Actinide and Transactinide Chemistry: Progress and Perspectives

Gas- and Condensed-Phase Actinide Chemistry

*Sponsored by NUCL, Cosponsored with COMP, and INOR*

Computational Electrochemistry for New Energy

Biological Applications

*Sponsored by PHYS, Cosponsored with COMP*

Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?

Materials and Surfaces

*Sponsored by PHYS, Cosponsored with COMP*

RNA Interference Based Therapeutics

*Sponsored by CARB, Cosponsored with BIOL, BIOT, COMP, MEDI, ORGN, PMSE, POLY, and BTEC*

**TUESDAY EVENING**
Unknown Site -- Unknown Room

**Poster Session**

J. D. Madura, *Organizer*

6:00 - 8:00

**268.** Molecular dynamic simulations of peptide nucleic acids modified with cycloalkanes. **A. K. Manukyan,** J. L. Poutsma

**269.** A microfluidic device to study ice crystal growth and interactions of antifreeze proteins with ice crystals. **Y. Celik,** N. Pertaya, J. Wettlaufer, P. L. Davies, I. Braslavsky

**270.** A novel use for protomols in Surflex-Dock: Searching for binding sites with a global protomol. **E. Metwally,** J. Begemann

**271.** Accurate sampling using stochastic dynamics. **G. Bussi,** M. Parrinello

**272.** New methods for efficient direct calculation of drug binding free energies. **M. R. Shirts,** J. D. Chodera, R. A. Friesner

**273.** Analysis of protonic and deuteronic basis functions using Gaussian-type functions. **T. Ishimoto,** M. Tachikawa, Y. Inadomi, H. Umeda, T. Watanabe, U. Nagashima

**274.** Analysis of solvent-solute interactions and its effect on crystal morphology. **C. Acquah,** A. T. Karunanithi, L. E. Achenie, J. A. Gascon, S. Sithambaram, S. L. Suib

**275.** Antiviral drug design: Cross-docking to influenza neuraminidase. **J. E. Shipman,** R. C. Rizzo

**276.** Are enzyme active sites built in multiple layers? **H. Brodkin,** M. J. Ondrechen, D. Ringe

**277.** Artificial neural network models for prediction of intestinal permeability of oligopeptides. E. Jung, J. Kim, **M. Kim,** D. H. Jung, S -H. Choi, S -K. Kang, M -K. Kim, Y -J. Choi

**278.** Brownian dynamics simulations of glycolytic enzymes interacting with tubulin. **E. N. Njabon,** N. Y. Forlemu, K. A. Thomasson

**279.** Charge-ELF: Addressing conformational dependency of small-molecule atomic charges for biomolecular simulations. **D. J. McKay,** C. I. Bayly

**280.** Comparative analysis of the molecular recognition within ATP binding pockets of GHKL-family proteins. **M. Song,** W. Ying, L. Sun

**281.** Computational analysis of the peptide bond formation mechanism in peptidyl transferase. **W. A. Tian,** P. M. Kiefer, R. Bianco, J. T. Hynes

**282.** Computational analysis of the search and recognition mechanism of the formamido-pyrimidine DNA glycosylase. **K. Song,** C. De los Santos, A. P. Grollman, C. L. Simmerling
283. Computational binding models for ligands with EGFR: Characterizing the basis of resistance. T. E. Balius, R. C. Rizzo

284. Computational characterization of amyloidogenic mutations in protein sequences. J. Choi, H. S. Lee, M. Qinquin, S. Yoon

285. Computational modeling of a crystal structure. M. L. Mihajlovic, P. M. Mitrasinovic

286. Computational study of Bacillus anthracis glutamate racE2. W. Fu, S. Mehboob, M. E. Johnson

287. Computational study of interaction between argadin and acidic mammalian chitinase. H. Gouda, S. Hirono


289. Correction of charge-transfer indices for multifunctional amino acids. F. Torrens, G. Castellano

290. Design of quantum sieves for seperation of hydrogen isotopes. Y. Ping

291. Docking studies of cytochrome P450-2D6 inhibitors. R. J. Unwalla, J. Cross, S. Salaniwal, J. Kao, A. Shilling, L. Leung

292. Downfolding and N-ization of a localized AO or LCAO basis set. E. D. Zurek, J. Autschbach, O. K. Andersen


294. Enhancing sampling and relating kinetics rates from all-atom explicit solvent accelerated molecular dynamics simulations. C. A. F. de Oliveira, D. Hamelberg, J. A. McCammon


296. Examining the role of conformational changes in HIV protease drug resistance. M. M. Layten, F. Ding, C. L. Simmerling


298. Exploration of the sequence dependent stability of helical content using short alanine peptides. F. Ding


302. Inactivation mechanism of [FeFe]-Hydrogenase H-cluster by oxygen. **D. Dogaru**, S. Motiu, V. Gogonea


304. Interactions of antifreeze proteins with ice crystals and cell membranes. **Ö. Can**, S. Essampally, N. B. Holland


308. Molecular mechanics force fields for modeling small, drug-like molecules compared to wave function, density functional, and semi-empirical molecular orbital theories. **B. White**, E. A. Amin, C. R. Wagner, D. G. Truhlar


310. New insight into the design of effective Bcl-xl inhibitors. **W. J. Novak**, G. Krilov

311. New scoring functions for discovery of lead peptides reversible inhibitors of thrombin. **C. C. Clement**, M. Philipp, J. Gingold


318. Quantum effective potentials: An efficient strategy for quantum dynamics. **D. Z. Goodson**
319. Quantum mechanics/molecular mechanics study of the catalytic mechanism of Trypanosoma cruzi trans-sialidase. Ö. Demir, A. Roitberg

320. Structure-based virtual screening against SARS-3CLpro: Identification of hits and insights into the process of lead development. P. Mukherjee, P. V. Desai, L. Ross, L. White, M. A. Avery


322. Support vector machines and THEMATICS for precise prediction of interaction sites in proteins from 3-D structure. W. Tong, M. J. Ondrechen, R. J. Williams

323. Tautomer generation. pKa based dominance conditions for generating the dominant tautomers. J. Szegedzi, F. Csizmadia

324. The foundation of the approach of Active Thermochemical Tables: The analysis and manipulation of the Thermochemical Network Graph. A. Fernandez, B. Ruscic


326. Thermal rearrangement of 2-acetoxy-2,6,6 trimethylbicyclo[3.1.0]hexane: Theoretical elucidation of the mechanism. K. Yelekci, S. Sag Erdem

327. Title 3-D-QSAR combined theoretical study of 5-HT1A-receptor agonists. E. Bartashevich, V. Potemkin

328. Understanding the binding mechanism of a new class of PTEN inhibitors. Q. Wang, M. Mottamal, G. Krilov


330. Ab initio molecular dynamics of visual pigment chromophore models. I. Schapiro, O. Weingart, V. Buss

331. Benchmarking a variety of QM methods in the calculation of relative conformational and pair-wise energies: Just how reliable are the "shortcut methods"? A close look at LMP2, RI-MP2 and other correlated methods. K. A. Rossi, D. L. Cheney


334. Data mining the drug database: Is there such a thing as drug-like space? C. Yang, G. Sun, D. Bower, J. F. Rathman


337. Investigate the fluorescence quenching and recovering process of beta-cyclodextrin anchored quantum dots. M. Ning, R. E. Brown

338. Investigating the predominant factors which drive receptor-ligand binding for inhibitors selective for MMP-13. N. A. Carrascal, R. C. Rizzo

339. Investigation of the inhibitory pathways of [FeFe]-hydrogenase by means of Quantum Mechanics/Molecular Mechanics. S. Motiu, D. Dogaru, V. Gogonea


341. Molecular dynamics studies of zeolites functionalized with transition metal ions. E. Jaramillo, E. C. Garcia, R. Guzman

342. Molecular mechanisms of gas surface interactions in hypersonic flow. I. Cozmuta


344. Prediction of the adsorption orientation of Human Serum Albumin on hydrophobic surfaces using theoretical thermodynamic analysis. H -J. Hsu, S -Y. Sheu, R -Y. Tsay


349. 3-D-QSAR Combined theoretical study of 5-HT1A-receptor agonists. E. Bartashevich, V. Potemkin

350. Multiway QSPR analysis of the acidity constant of some phenolic compounds utilizing quantum topological molecular similarity descriptors. B. Hemmateenejad, T. Khayamian, M. Esteki, A. Mohajeri

351. Quantitative structure-retention relationship for the Kovats retention indices of a large set of terpenes: A combined data splitting-feature selection (CDFS) strategy. B. Hemmateenejad, K. Javidnia, M. Elyasi

Section B
Unknown Site -- Unknown Room

Chemical Computing Group Excellence Award

A. C. Good, Organizer

6:00 - 8:00

352. Development of scoring functions for protein-ligand binding based on frequent geometric and chemical patterns of inter-atomic interactions at their interfaces. **R. Khashan**, W. Zheng, A. Tropsha

353. How much experimental data is needed to predict a protein's structure? **C. R. Crecca**, A. E. Roitberg


355. Novel basis-set free approaches to solving the electronic-Schrödinger equation. **J. S. M. Anderson**

356. To be native or not to be native, that is the question: Studies of the unfolded state structure of the Villin Headpiece Helical Subdomain. **L. Wickstrom**, D. P. Raleigh, C. L. Simmerling

WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

Molecular Dynamics

E. A. Carter and M. S. Gordon, Organizers
C. Mailhiot, Presiding

9:00 — 357. Coarse grain models for self-assembling systems. **M. L. Klein**


10:10 — 359. Atomic-level control of chemical doping for nanoelectronics through first principles modeling. **G. S. Hwang**

10:45 — Intermission.

11:00 — 360. Hamiltonian and non-Hamiltonian formulations for molecular dynamics simulations in materials chemistry. **T. Cagin**
11:35 —361. Multimillion atom simulations of nanorods, dynamics of wing cracks, hypervelocity impact damage, and planar shock on RDX. P. Vashishta, R. Kalia, A. Nakano

Section B

Unknown Site -- Unknown Room

Molecular Mechanics

Exploring Proteins

E. X. Esposito, Organizer
S. Sharma, Presiding

8:30 —362. Coarse master equations for peptide folding kinetics from atomistic molecular simulations. N.-V. Buchete, G. Hummer

8:55 —363. Exploring folding free energy landscapes of biomolecules via Serial Replica Exchange and Simulated Tempering methods using a distributed computing environment. X. Huang, V. S. Pande

9:20 —364. Folding pathways of three-helix proteins. H. Lei, Y. Duan

9:45 — Intermission.

10:00 —365. Multiscale studies of non-natural peptides. X. Zhu, A. Yethiraj, Q. Cui

10:25 —366. To be native or not to be native, that is the question: Studies of the unfolded state structure of the Villin Headpiece Helical Subdomain. L. Wickstrom, D. P. Raleigh, C. L. Simmerling


11:15 —368. Folding of helical structures of alternating pyridinedicarboxamide/M-(phenylazo) azobeneze oligomers. P. Tao, J. R. Parquette, C. M. Hadad

Section C

Unknown Site -- Unknown Room

Antifreeze Proteins: A Memorial Symposium for Robert Feeney

A. Wierzbicki, Organizer

8:30 —369. Antifreeze glycoprotein adsorption at the ice/solution interface. S. Zepeda, E. Yokoyama, Y. Uda, Y. Furukawa

9:00 —370. Antifreeze glycoproteins: Design of mimics and interaction with membranes. J. E. Stok, P. M. Abeysinghe, Y. Han, J. Garner, S. R. Inglis, M. M. Harding


10:30 — 373. Simulations of Type I AFPs at the ice/water interface. **J. D. Madura**

**Section D**

Unknown Site -- Unknown Room

**Recent Advances in Studies of Molecular Processes at Interfaces**

**Ice Surface**

L. X. Dang, *Organizer*
G. K. Schenter, *Presiding*


10:10 — Intermission.

10:30 — 377. Ions at water interfaces. **A. Haymet**, T. Bryk

11:10 — 378. Interaction of alkali halides and organic molecules with amorphous solid water. S. Bahr, O. Höfft, **V. Kempter**

**Section E**

Unknown Site -- Unknown Room

**Current Techniques in Molecular Simulation of Biological Systems**

*Cosponsored with PHYS, and BIOHW*
N. Rathore and T. A. Knotts IV, *Organizers*

9:00 — 379. Continuum solvents in polarizable force fields: A Poisson-Boltzmann approach. **R. Luo**


10:20 — Intermission.


11:15 —385. Molecular simulation of supported lipid bilayers on a coarse grained level. C. Xing, R. Faller

11:35 —386. Implicit modeling of membranes: How much physics can we incorporate? M. Feig

Section F

Unknown Site -- Unknown Room

Phil Magee Memorial Symposium: QSAR Reborn

Applications

Cosponsored with CINF
J. H. Block and B. Clark, Organizers


9:00 —388. PepT1 substrate QSAR and pharmacophore definition. T. R. Stouch, B. S. Vig

9:30 —389. 3-D-QSAR study of submandibular gland tripeptide FEG and its analogs. E. Metwally, R. D. Mathison, J. S. Davison, R. D. Clark

10:00 —390. Inorganic QSAR and imaging. D. E. Reichert

10:20 — Intermission.

10:40 —391. 3-D-QSAR models and activity predictions of human TRPV1 channel antagonists: Comparative molecular field analysis (CoMFA) and comparative molecular similarity analysis (CoMSIA) of cinnamide analogs. V. N. Viswanadhan, Y. Sun, M. H. Norman

**11:40 — 393.** Neural network-based QSAR and the discovery of the next generation spinosyn insecticide: Spinetoram (DE-175). **T. C. Sparks,** G. D. Crouse, J. E. Dripps, P. B. Anzeveno, J. Martynow, J. Gifford

**Cheminformatics Techniques in Bioinformatics-Related Applications**

*Sponsored by CINF, Cosponsored with COMP, and BIOHW*

**Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?**

**QM/MM Methods and Applications**

*Sponsored by PHYS, Cosponsored with COMP*

**WEDNESDAY AFTERNOON**

Section A

Unknown Site -- Unknown Room

**Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday**

**Biological**

E. A. Carter and M. S. Gordon, *Organizers*
R. A. Friesner, *Presiding*

1:30 — 394. On the mechanisms of photosynthesis and respiration. **P. E. Siegbahn**

2:05 — 395. Computer-aided drug design. **J. A. McCammon**

2:40 — 396. Predictions and experimental verification of conformational flexibility and ligand efficacy in G-protein coupled receptors. **N. Vaidehi**

3:15 — Intermission.

3:30 — 397. Solution theory formulations for biomolecules and interfaces. **B. M. Pettitt**

4:05 — 398. Redesigning photoactive proteins from first principles. **T. J. Martinez**

4:40 — 399. Dynamics of ternary complex EF-Tu(GTP)aa-tRNA on the ribosome. **U. Mohanty**

Section B
Drug Discovery

Rational Drug Design

I. Visiers, Organizer
A. C. Cheng, Presiding

1:00 — 400. A reactivity and recognition component-based methodology for computational prediction of likely sites of CYP 450 3A4-mediated metabolism. J. Zaretzki, C. M. Breneman, C. Bergeron, N. Sukumar, M. Krein


1:40 — 402. ACE, a computational tool for virtual screening of asymmetric catalysts. N. Moitessier, C. R. Corbeil, S. Thielges

2:00 — 403. Bisphosphonates: Teaching old drugs new tricks. E. Oldfield

2:20 — Intermission.

2:35 — 404. Determining a minimum yet sufficient training set size for QSAR modeling. S. K. Dogra

2:55 — 405. Developing QSAR models for multiple CNS activities. S. Mente


Unknown Site -- Unknown Room

Quantum Chemistry

A. E. Roitberg, Organizer
L. Wickstrom, Presiding

1:30 — 408. Why does the electron density sometimes go down when you add electrons to a molecule? J. Melin, P. W. Ayers, J. V. Ortiz

Density functional theory study on the protonation of guanine quadruplex. J. W. Gauld, H. Liu

Intermission.

Multistep cluster chemistry involved in SN2@P reaction systems. M. A. van Bochove, M. Swart, F. M. Bickelhaupt

Reaction mechanism of direct gas phase synthesis of H2O2 catalyzed by Au3. B. Njegic, M. S. Gordon

Theoretical study on the hydrolysis mechanism of 1-substituted silatranes in the gas phase. S. Sok, M. S. Gordon

Phil Magee Memorial Symposium: QSAR Reborn

Methods

Cosponsored with CINF
J. H. Block and B. Clark, Organizers

A new paradigm for pattern recognition of drugs. M. A. Grishina, V. Potemkin, E. S. Pereyaslavskaya

Intrinsic descriptors. G. D. Purvis III

The development of novel fragment descriptors of molecular structure using frequent common subgraph mining approach: applications to QSAR and protein structure function relationship modeling. A. Tropsha

Intermission.

Molecular topology as a tool for the design of new drugs. J. Galvez Sr.

Evaluation of descriptors and classification schemes to predict drug metabolism in terms of chemical information. J. H. Block, D. Henry


Computational Science & Engineering Advances Supported by NSF Resource

http://oasys.acs.org/acs/234nm/comp/staff/program.cgi?format=expanded&password=combi
General Sciences

*Cosponsored with PHYS*
J. Towns, *Organizer*

1:30—420. Where does it all go? How $70M in NSF cyberinfrastructure is leveraged. **J. Towns**

2:00—421. Astronomy and astrophysics. **J. P. Ostriker**

2:30—422. Large-scale simulations of complex flow phenomena. **S. Dong**

3:00—423. Transforming our understanding and prediction of thunderstorms through dynamic adaptation: People and technologies interacting with weather. **K. K. Droegemeier, M. Xue**

3:30 — Intermission.


4:15—425. Petascale computational cosmology. **T. Quinn**

4:45—426. Using the TeraGrid to advance earthquake system science. **P. Maechling**

Section F

Unknown Site -- Unknown Room

**Recent Advances in Studies of Molecular Processes at Interfaces**

**Liquid Surfaces**

L. X. Dang, *Organizer*
J. I. Siepmann, *Presiding*

1:30—427. Alkyl bromides at the air/water interface. **M. Roeselová, B. Minofar**

2:10—428. Specific and nonspecific solvation at liquid interfaces. **R. A. Walker, M. R. Brindza**

2:50—429. Theoretical study of small water clusters of dicarboxylic acids. **F.-M. Tao**

3:10 — Intermission.

3:30—430. Structure and dynamics of charge defects in methanol/water mixtures and at the liquid/vapor interface of NaOH solutions probed by ab initio molecular dynamics. **M. E. Tuckerman, J. A. Morrone, H.-S. Lee**

4:10—431. Influence of liquid structure on interfacial ion distributions. **M. L. Schlossman**

Cheminformatics Techniques in Bioinformatics-Related Applications

Sponsored by CINF, Cosponsored with COMP, and BIOHW

Quantum Mechanics and Statistical Mechanics: Can One Avoid the Other?
Free Energies and Sampling

Sponsored by PHYS, Cosponsored with COMP

THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday

Theory

E. A. Carter, Organizer
M. S. Gordon, Organizer, Presiding

9:00 — 433. New density functionals for making bold predictions. D. G. Truhlar, Y. Zhao


10:45 — Intermission.


Section B

Unknown Site -- Unknown Room

Molecular Mechanics
Material Science

E. X. Esposito, Organizer
A. J. Campbell, Presiding

8:30 — 438. Atomistic predictions for clay exfoliation relevant to nanocomposites formation. I. Cozmuta, M. Blanco, W. A. Goddard III

8:55 — 439. Development of the reaxFF water potential to describe reactions involving proton transfer in the aqueous phase. A. C. van Duin, V. S. Bryantsev, Z. Xu, W. A. Goddard III

9:20 — 440. Gas sorption and barrier properties of polymeric membranes from molecular dynamics and Monte Carlo simulations. I. Cozmuta, M. Blanco, W. A. Goddard III

9:45 — Intermission.

10:00 — 441. Modeling of sulfonated triblock copolymers with metal ions. J. Andzelm, J. M. Sloan, E. Napadensky, D. M. Crawford


10:50 — 443. Salt permeation in water-filled dipolar nanopores. K. Leung


Section C

Unknown Site -- Unknown Room

Quantum Chemistry

A. E. Roitberg, Organizer
M. M. Layten, Presiding

9:00 — 445. Solvent effects on nuclear shieldings: Frozen-density embedding in large MD generated solutions. R. Bulo, C. R. Jacob, L. Visscher


9:50 — 447. DFT studies of DP-3 amylose fragments. U. Schnupf, J. L. Willett, W. B. Bosma, F. A. Momany

10:15 — Intermission.

10:30 — 448. DNA replication: Estimating the effects and interplay of solvation, pi-stacking and
hydrogen bonding. **J. Poater**, M. Swart, C. Fonseca Guerra, F. M. Bickelhaupt


Section D

Unknown Site -- Unknown Room

**Recent Advances in Studies of Molecular Processes at Interfaces**

**Ions at Interface**

L. X. Dang, *Organizer*
M. Roeselová, *Presiding*

8:30—451. Ions at interfaces: Thermodynamic consequences and two-state molecular description of accumulation or exclusion. L. M. Pegram, K. VanderMeulen, M. W. Anderson, I. A. Shkel, D. J. Felitsky, R. Erdmann, **M. T. Record Jr.**

9:10—452. Structure and reactivity on the surface of aqueous electrolyte solutions. **D. J. Tobias**


10:10 — Intermission.


11:10—455. Effect of size and polarizability on ion partitioning at the aqueous liquid-vapor interface. **J. I. Siepmann**, B. L. Eggimann


Section E

Unknown Site -- Unknown Room

**Current Techniques in Molecular Simulation of Biological Systems**

*Cosponsored with PHYS, and BIOHW*
N. Rathore and T. A. Knotts IV, *Organizers*

9:00—457. Predicting bound protein-peptide conformations: Application to MHC-peptide complexes. **I. Antes**, T. Lengauer


10:00 — 460. Studying the activation mechanism of a signaling protein by transition path sampling and umbrella sampling. **L. Ma**, Q. Cui

10:20 — Intermission.

10:35 — 461. Optimization and convergence metrics for replica exchange molecular dynamics. **A. E. Roitberg**


**THURSDAY AFTERNOON**

Section A

Unknown Site -- Unknown Room

**Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday**

**Multiscale**

E. A. Carter and M. S. Gordon, *Organizers*
M. L. Klein, *Presiding*

2:00 — 465. Combustion chemistry: The evanescent NCCO radical. **H. F. Schaefer III**


3:10 — 467. Atomistic and mesoscale modeling of chemical and thermo-mechanical processes in molecular crystals. **A. Strachan**

3:45 — Intermission.
4:00 — 468. Multiscale modeling in automobile materials research: For engines, door panels and fuel cells. **Y. Qi**

4:35 — 469. mW: A coarse-grained model of water with tetrahedral interactions. **V. Molinero**

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Rational Drug Design**

I. Visiers, *Organizer*
S. Mente, *Presiding*


1:20 — 471. Non-additivity in structure-activity relationships. **J. van Drie**

1:40 — 472. Structure-based prediction of small-molecule druggability. **A. C. Cheng**

2:00 — Intermission.


3:00 — 475. DNA Minor groove pharmacophores describing sequence specific properties. **G. M. Spitzer**, B. Wellenzohn, C. Laggner, T. Langer, K. R. Liedl

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

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

1:00 — 476. Structural and dynamical properties of hydrogen bonded fluids from first principles molecular dynamics simulations in the isobaric-isothermal ensemble. **I. F. W. Kuo**, J. Schmidt, C. J. Mundy, M. J. McGrath, J. I. Siepmann

1:50 — 478. Cis-trans isomerization of a small peptidic fragment studied by ab initio and empirical simulation techniques. **Y. A. Mantz, D. Branduardi, G. Martyna, M. Parrinello**

2:15 — Intermission.

2:30 — 479. DFT studies of hydrated carbohydrates: DFT molecular dynamics simulations at the B3LYP/6-31+G* level of theory. **F. A. Momany, U. Schnupf, J. L. Willett, W. B. Bosma**

2:55 — 480. Structural, electronic and spectroscopic properties of the natural luteolin and apigenin pigments: A DFT/TDDFT investigation. **S. Fantacci, A. Amat, C. Miliani, F. De Angelis, A. Sgamellotti**


3:45 — 482. The reaction mechanism for the organocatalytic ring opening polymerization of L-lactide using bifunctional catalysts. **H. W. Horn, J. Rice**

Section D

Unknown Site -- Unknown Room

**Phil Magee Memorial Symposium: QSAR Reborn**

**Applications**

_Cosponsored with CINF_

J. H. Block and B. Clark, _Organizers_

1:00 — 483. Random forest ensembles applied to MLSCN screening data for toxicity prediction and feature selection. **R. Guha, S. Schurer**

1:30 — 484. On the importance of topological descriptors in understanding structure-property relationships in QSAR and QSPR models. **D. T. Stanton**

2:00 — 485. Predicting allergic contact dermatitis: alternative statistical approaches to chemical classification. **S. C. Basak, D. Mills, B. D. Gute, D. M. Hawkins**

2:30 — 486. A comparison of the chemical properties of drugs and FEMA/FDA notified GRAS chemical compounds used in the food industry. **D. Sprouse, F. Salemme**

2:50 — Intermission.

3:10 — 487. A QSAR model for hERG based on multiple 1-D alignments. **D. J. Diller**


4:10 — 489. "Inductive" descriptors: Ten successful years in QSAR. **A. Cherkasov**

Section E
Molecular Mechanics

Advancing Methodology

E. X. Esposito, Organizer
L. Wickstrom, Presiding

1:00 — 490. Polarizable force fields for biomolecular simulations: Bulk liquid properties using the CHARMM fluctuating charge force field. S. Patel


2:15 — Intermission.


3:45 — 496. Extending the scope of relative binding free energy calculations. J. Michel, J. W. Essex