# 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

**11:35 —5.** How insights into bonding of molecules help explain high temperature evolution of materials. **E. A. Carter**

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**

**9:20 —8.** Canonical sampling through velocity rescaling. **G. Bussi**, D. Donadio, M. Parrinello

**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

**10:25 —10.** QTPIE: A new charge model for arbitrary geometries and systems. **J. Chen**, T. J. Martínez

**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

**11:15 —12.** Simulation of interfacial systems with isotropic periodical sum. **X. Wu**, J. B. Klauda, R. W. Pastor, B. R. Brooks

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

**9:20 —14.** A theoretical study of the kinetic effect of AFGP adsorption on ice. **E. Yokoyama**, S. Zepeda, Y. Furukawa

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

**10:20 —** Intermission.

**10:35 —16.** Fluorescence microscopy and microfluidic techniques for studying interactions between antifreeze proteins and ice surfaces. **I. Braslavsky**, N. Pertaya, Y. Celik, A. Groisman, J. Wettlaufer, P. L. Davies

**11:05 —17.** Behavior of antifreeze proteins and glycoproteins at the ice/solution interface and ice growth kinetics during one-directional growth. **Y. Furukawa**, S. Zepeda, H. Nakaya, Y. Uda, E. Yokoyama

**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**

**9:15 —20.** Modeling reaction dynamics at liquid surfaces. **G. C. Schatz**, D. Kim

**9:55 —21.** Role of molecular anisotropy in electrowetting. D. Bratko, C. D. Daub, K. Leung, **A. Luzar**

**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**

**11:55 —24.** Molecular dynamics simulations of ion adsorption at the mineral-water interface. **S. Kerisit**, S. C. Parker, E. S. Ilton, C. Liu

Section E

Unknown Site -- Unknown Room

**Protein-Nucleic Acid Interactions: Experimental and Modeling Analysis**

M. R. Mihailescu, *Organizer*

**8:30 —25.** Two-metal associative catalysis: Phosphodiester cleavage in ribonuclease H. **M. De Vivo**, M. Dal Peraro, M. L. Klein

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

**9:30 —27.** Structural studies of the RNA aptamer drug, Macugen, bound to the angiogenic protein vascular endothelial growth factor. **A. Pardi**, J -H. Lee, F. Jucker, N. K. Kruse

**10:00 —** Intermission.

**10:15 —28.** Computational prediction of the sequence specificity and binding energy of protein-RNA complexes. **G. Varani**, T. Robertson, S. Zheng, Y. Chen

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

**11:15 —30.** U1A-RNA Complex formation: Insights from combining experimental and computational approaches. **A. M. Baranger**

**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

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*
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**

**4:35 —36.** Millisecond-scale molecular dynamics simulations of proteins: Algorithms, architectures and applications. **D. E. Shaw**

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Docking**

I. Visiers, *Organizer*
D. Ryan, *Presiding*

**1:00 —** Introductory Remarks.

**1:10 —37.** A new implicit solvent model for protein-ligand docking. **A. R. Ortiz**

**1:30 —38.** Explicit and implicit solvation binding free energies of FKBP-12. **M. R. Shirts**, G. Jayachandran, C. D. Snow, V. S. Pande, R. A. Friesner

**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

**3:25 —43.** Docking ligands into challenging targets using single interactions and an appropriate metal description. C. Detering, C. Lemmen, M. Lilienthal, **M. Gastreich**

**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 flavonoïds 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

**1:55 —49.** Air-stable, high performance, rigid [:4,5]thieno[2,3-d]thiophene-derivative organic semiconductors. **J. Schrier**, S. Atahan, L -W. Wang, A. Aspuru-Guzik

**2:20 —50.** Electron transport through carbon nanotubes connected by conjugated molecules. **R. R. Pandey**, N. A. Bruque, R. K. Lake

**2:45 —** Intermission.

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

**3:25 —52.** Quantum chemical molecular dynamics simulations of carbon nanotube self-assembly on transition metal catalysts. **S. Irle**, Y. Ohta, Y. Okamoto, Z. Wang, G. Zheng, K. Morokuma

**3:50 —53.** Theoretical studies on phenyl cored thiophene dendrimers. **M. E. Kose**, K. Kim, S. E. Shaheen, G. Rumbles, N. Kopidakis

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**

**1:35 —61.** Accurate coarse-grain modeling of biomembranes. **J. Michel**, M. Orsi, W. Sanderson, J. W. Essex

**2:05 —62.** Reaction path methods based on holonomic constraints. **J -W. Chu**

**2:35 —** Intermission.

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

**3:20 —64.** Generalization of the Gaussian Electrostatic Model: A molecular density based force field. **G. A. Cisneros**, J -P. Piquemal, T. A. Darden

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

G. A. Voth

**4:20 —66.** Recore: A fast and versatile method for scaffold hopping. **P. C. Maass**, T. Schulz-Gasch, M. Stahl, M. Rarey

**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*

**1:30 —67.** Composition and chemistry at the liquid/vapor interface of aqueous solutions: Comparisons between experiment and MD simulations. **J. C. Hemminger**, M. A. Brown, M. J. Krisch, D. E. Starr, S. Mun, H. Bluhm

**2:10 —68.** Computational analysis of interfacial sum frequency generation spectrosopy. **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

**4:50 —72.** Dissociation of "buried" water on Pt(111). **J. P. Cowin**, Y. Lilach, M. J. Iedema

**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

Section A

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

**76.** A new generation of model chemistries based on pair natural orbital extrapolations to the CCSD (T)/CBS limit. **M. J. Spescha**, E. C. Barnes, G. A. Petersson

**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

**81.** Concentration effects in the Wacker process. **J. A. Keith**, R. J. Nielsen, J. Oxgaard, W. A. Goddard III

**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**

**87.** Electronic scaling properties in graphene nanoribbons. **H. Su**, Q. Li, Z. F. Wang, Q. Shi, J -L. Yang

**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

**92.** Molecular dynamics simulations of liposomes: From formation to fusion and fission. **P. Spijker**, A. J. Markvoort, K. Pieterse, A. F. Smeijers, R. A. van Santen, P. A. J. Hilbers

**93.** Molecular dynamics simulations of surfactant protein C mimic in phospholipid bilayers. **S. M. Dutz**, Z. Ramjan, P. W. Mobley, L. M. Gordon, F. J. Walther, B. Vovan, J. M. Hernandez-Juviel, M. A. Sherman, A. J. Waring, S. Sharma

**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

**96.** Multiscale simulations of block copolymers. **J. Andzelm**, F. L. Beyer, J. F. Snyder, P. W. Chung

**97.** Nature of chemical bonds between glycopeptide antibiotics and bacterial cell walls. **J -G. Lee**, C. Sagui, C. Roland

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

**99.** Novel adaptive grid for electronic structure calculations. **J. I. Rodríguez**, D. C. Thompson, P. W. Ayers

**100.** Oxidation pattern of small silicon oxide clusters. **W. Lu**, Q. J. Zang, Z. M. Su, C. Z. Wang, K. M. Ho

**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

**104.** Predicting the structure of family A GPCR TM domains. **M. Michino**, J. Chen, C. L. Brooks III

**105.** Prediction of Raman spectra in novel polyyne@SWNT peapods using dispersion-augmented density-functional-tight-binding. **S. Irle**, H. A. Witek, H. Shinohara, K. Morokuma

**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 CH2ClI cation. **J. Kim**, H. Ihee, Y. S. Lee

**111.** Structure-performance relationships for asymmetric carbenes in Pd-catalyzed chiral alcohol oxidations. **R. J. Nielsen**, W. A. Goddard III

**112.** Sulfur K-edge XAS and DFT studies of Fe-S bonds in models and protein active sites: Effects of H-bonds on covalency and redox properties. **E. I. Solomon**, A. Dey

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

**114.** TiO2 photoreduction of CO2 by H2O: A plausible CO2 sequestration model. **A. K. Rappe**, K. B. Ford

## 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*

**9:00 —115.** Quantum chemical molecular dynamics simulations of growth of fullerenes, metallofullerenes and carbon nanotubes. **K. Morokuma**, S. Irle, Z. Wang, G. Zheng, B. Y. Finck, B. Saha, Y. Ohta, Y. Okamoto

**9:35 —116.** Silicon nanowire thermoelectrics. **J. R. Heath**, A. Boukai, Y. Bunimovich, J. K. Yu, W. A. Goddard III, P. von Allmen, J. Tahir-Kheli, S. Lee, R. J. Nielsen, Y. Matsuda

**10:10 —117.** Chemical dynamics at metal surfaces: Electronic excitations. N. Shenvi, S. Roy, H. Cheng, **J. Tully**

**10:45 —** Intermission.

**11:00 —118.** Quantum conductance of silver nanowires and linearization of atomic gold chains. Y. C. Choi, W. Y. Kim, S. K. Min, H. M. Lee, **K. S. Kim**

**11:35 —119.** Time-dependent density-functional theory for open systems and its calculation of transient currents through molecular devices. **G. Chen**

Section B

Unknown Site -- Unknown Room

**Molecular Mechanics**

**Biological Systems**

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

**8:30 —120.** A proposed structural model for human protein Z and its putative activated form (Za). **V. Chandrasekaran**, C. J. Lee, R. E. Duke, L. Perera, L. G. Pedersen

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

**9:20 —122.** An ionic network stabilizes the p53 tetramerization domain. **T -Z. W. Lwin**, C. Galea, R. W. Kriwacki, D. Bashford

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

**10:10 —** Intermission.

**10:25 —124.** Gating mechanisms in the ribosomal exit tunnel. **P. Petrone**, V. S. Pande

**10:50 —125.** Interaction of a type IIa bacteriocin with lipid bilayer and its immunity protein: A molecular dynamics simulation study. **K. Kaur**, W. Soliman, S. Bhattacharjee

**11:15 —126.** Molecular dynamics study for nitrous oxide in a DMPC bilayer. **E. Pinnick**, S. Erramilli, F. Wang

**11:40 —127.** Molecular simulation of RNA complexes: Searching for minimum binding sequences. **S. Mecozzi**

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

**10:55 —132.** Antifreeze protein from Japanese fish: An epoch in biotechnology. **S. Tsuda**

**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**

**9:50 —136.** Structure and dynamics of atmospherically relevant aqueous interfaces. **J. L. Thomas**, A. C. Moskun, L. M. Wingen, M. Roeselová, B. J. Finlayson-Pitts, D. J. Tobias

**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

**11:15 —145.** Design of a protein ring sequencer via SMD simulations of RNA translocation. **I. Cozmuta**, V. Stolc

**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**

**9:50 —148.** Benchmarking sets for molecular docking. **J. J. Irwin**, N. Huang, B. Shoichet

**10:25 —** Intermission.

**10:40 —149.** Comparison of topological, shape, and docking methods in virtual screening. **G. McGaughey**, R. P. Sheridan, C. Bayly, J. C. Culberson, C. Kreatsoulas, S. Lindsley, V. N. Maiorov, J - F. Truchon, W. D. Cornell

**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**

**2:35 —153.** Breakthroughs in oxidizing CH4 and prospects for the 21st century. **R. A. Periana**

**3:10 —154.** Virtually (im)possible: Computational design of novel C-H functionalization catalysts. **J. Oxgaard**, J. Gonzales, R. J. Nielsen, Z. Xu, J. M. Keith, J. A. Keith, S. Pudar, M -J. Cheng, W. A. Goddard III

**3:45 —** Intermission.

**4:00 —155.** Understanding bistable [2]rotaxanes in solid-state devices. **J. F. Stoddart**, W. R. Dichtel

**4:35 —156.** Using quantum chemical simulations to engineer new homogeneous catalysts. **C. B. Musgrave**, P. Ankan, L. P. C. Nielsen, E. N. Jacobsen

Section B

Unknown Site -- Unknown Room

**Drug Discovery**

**Virtual Screening**

I. Visiers, *Organizer*
L. Herman, *Presiding*

**1:00 —157.** A novel, efficient virtual screening algorithm using 3-D chemical feature pattern recognition. **G. Wolber**, F. Bendix, J. Kirchmair, T. Langer

**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

**1:40 —159.** Distributed docking: An improved structure-based virtual screening combined with ligand-centric shape matching. **S. Yoon**, H. Lee, J. Choi, Y. Ko

**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**

**2:55 —162.** Strategies for docking “fragments” and lead-like molecules. **D. Joseph-McCarthy**, D. C. Thompson, J. Jacob, D. Tsao, C. Humblet

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

**3:35 —164.** Maximum common binding modes: A novel consensus scoring concept using multiple ligand information. **S. Renner**, S. Derksen, S. Radestock, T. Weil

**3:55 —165.** Screening very large virtual libraries using structure-based docking. **B. W. Sherman**, C. Higgs, M. Shelley

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**

**1:55 —167.** Hidden Jahn-Teller effect. **I. B. Bersuker**

**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 $C_3H^+$ and $HO_2^+$. **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

**2:30 —174.** Realizing Prospective QSAR through data fusion and modern descriptors. **C. M. Breneman**, N. Sukumar, M. J. Embrechts, K. P. Bennett, C. M. Sundling, M. Krein, T. Hepburn

**3:00 —** Intermission.

**3:20 —175.** QSAR model assessment. **D. M. Hawkins**, J. J. Kraker

**3:50 —176.** On some aspects of validation of predictive QSAR models. **K. Roy**, J. T. Leonard, P. P. Roy

**4:10 —177.** Proof of the pudding: How predictive are QSAR models? **T. I. Oprea**, T. K. Allu, D. C. Fara, O. Ursu

Section E

Unknown Site -- Unknown Room

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

**Engineering Sciences**

*Cosponsored 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**

**2:30 —180.** High-performance, multiscale simulation of engineered tissue mechanics. **V. H. Barocas**, T. Stylianopoulos, X. Luo, M. S. Shephard

**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**

Section F

Unknown Site -- Unknown Room

**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

**2:05 —186.** RMSD comparisons, enrichment and decoy selection for virtual screening: What can we learn from earlier mistakes? **J. Kirchmair**, G. Wolber, S. Ristic, K. Eder, P. Markt, C. Laggner, T. Langer

**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**

**10:10 —193.** Hypervalency in molecules. **T. H. Dunning Jr.**, D. E. Woon

**10:45 —** Intermission.

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

**11:35 —195.** Revisiting the concepts of chemical bond, resonance and hyperconjugation. **M. A. C. Nascimento**, F. P. Fleming, A. G. H. Barbosa

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.

**10:25 —200.** Probing flexibility in the activation loop of kinases. **B. W. Sherman**, J -C. Mozziconacci, S. N. Rao, R. Farid

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

**11:15 —202.** Specificity in SH2 domain mediated protein-protein interactions: Insights from binding free energy calculations. **W. Gan**, B. Roux

**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

Section C

Unknown Site -- Unknown Room

**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**

**9:10 —205.** Antifreeze proteins and assorted crystals: The memory effect and remembrance. **V. K. Walker**, H. Zeng, Z. Wu, G. R. Palmer, E. Huva, J. A. Ripmeester

**9:40 —206.** Characterization of Ca2+-dependent herring type II antifreeze protein. **Z. Li**, Y. Liu, Q. Lin, J. M. Bujnicki, J. Sivaraman, C -L. Hew

**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

**11:25 —209.** Structural basis of antifreeze protein action. **C. S. Strom**, X. Y. Liu, Z. Jia

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

**11:50 —215.** Water in nonpolar pores and protein cavities. **G. Hummer**, J. C. Rasaiah, H. Yin

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.

**10:15 —220.** Mechanistic studies of nucleic acid chaperone activity of retroviral nucleocapsid proteins. **K. Musier-Forsyth**, M. Mitra, K. M. Stewart-Maynard, M -N. Vo, M. Cruceanu, F. Wang, R. J. Gorelick, M. C. Williams, I. Rouzina

**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**

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*

**9:00 —** Introductory Remarks.

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

**9:40 —225.** Virtual high-throughput screening, enrichment, and the "early recognition" of actives. **C. I. Bayly**, J -F. Truchon

**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**

**11:25 —228.** Development and use of a small representative benchmark suite for thermochemical kinetics. **J. Zheng**, Y. Zhao, B. J. Lynch, D. G. Truhlar

**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**

**4:35 —233.** Theoretical approaches to actinide complexes and cerium oxide materials using density functional theory. **P. J. Hay**, R. L. Martin, E. R. Batista, J. Uddin, G. E. Scuseria

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.

**2:55 —239.** Surflex-dock: Effects of protomol generation and fragment matching on docking results. **E. Metwally**, J. K. Shepphird

**3:15 —240.** The Shiraz Challenge: The unlovable in search of the undruggable. **K. Branson**, G. L. Warren

**3:35 —241.** TrixX-BMI: Fast virtual screening using compressed Bitmap Index Technology for efficient prefiltering of Compound Libraries. **J. Schlosser**, M. Rarey

**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**

**1:55 —244.** Nature of ligand binding in HCV polymerase: Characterization of specific interactions from QM/MM calculations. **J. M. Parks**, H. Hu, R. Kondru, W. Yang

**2:20 —245.** Exploring QM/MM paths for mapping reaction mechanisms. **H. L. Woodcock III**, M. Hodoscek, B. R. Brooks

**2:45 —** Intermission.

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

**3:25 —247.** Evaluation of different quantum mechanics methods applied to biological molecules: Potential and free energy surfaces of alanine and glycine dipeptides in vacuum and in water. **G. D. M. Seabra**, R. C. Walker, A. E. Roitberg

**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

Section D

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/ olored 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**

**2:30 —251.** Hierarchical QSAR technology on the base of simplex representation of molecular structure. **E. N. Muratov**, V. E. Kuz'min, A. G. Artemenko

**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**

**4:20 —254.** Workflows based quantitative structure-activity relationship modeling. **S. K. Dogra**, R. Hariharan

Section E

Unknown Site -- Unknown Room

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

**Molecular Sciences**

*Cosponsored 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**

**2:30 —258.** Multi-terascale molecular modeling of biological systems. R. DeVane, W. Shinoda, J. Henin, M. Dal Peraro, A. Kohlmeyer, **M. L. Klein**

**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

Section A

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 microfludic 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. Qinqin, 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

**288.** Computer-aided design of vancomycin analogs for efficient binding of both D-Ala-D-Ala and D-Ala-D-Lac. **S. S. F. Leung**, J. Tirado-Rives, W. L. Jorgensen

**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

**293.** Efficient parallel Fock matrix construction on the Grid. **H. Umeda**, Y. Inadomi, T. Watanabe, T. Ishimoto, U. Nagashima

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

**295.** Evaluation of pharmacophore modeling based virtual screening: comparative assessment of catalyst, phase and MOE at the example of HRV coat protein. M. Mangold, G. M. Spitzer, T. M. Steindl, H. G. Wallnoefer, C. Laggner, T. Langer, **K. R. Liedl**

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

**297.** Experimental and molecular docking simulation studies of Histone deacetylases (HDACs) enzyme inhibitors. **K. Yelekci**, G. Bora, D. Dayangac-Erden, P. Ayhan, S. Dalkara, A. S. Demir, H. Erdem-Yurter

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

**299.** How to improve structure-based pharmacophores by modeling the binding site shape. S. Grona, P. Markt, J. Kirchmair, D. Schuster, T. Langer, **C. Laggner**

**300.** Identification of non-peptidic cell recognition motifs applying hybrid structural based computational methods: Development of an in vitro validation assay. **R. J. Perez**

**301.** Improved multistate empirical valence bond model for aqueous proton transport. **H. Chen**, Y. Wu, F. Wang, P. Liu, G. A. Voth

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

**303.** Interaction analysis between EGF receptor and EGF by fragment molecular orbital calculation. **T. Watanabe**, T. Ishimoto, Y. Tamura, Y. Inadomi, H. Umeda, U. Nagashima

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

**305.** Investigation of MDM2-inhibitor interactions by molecular dynamics and free energy calculations. **Y. Lu**, D. Qin, C -Y. Yang, K. Ding, Z. Nikolovska-Coleska, S. Wang

**306.** Modeling the flexibility of alpha helices in protein interfaces: Structure based design and prediction of helix mediated protein-protein interactions. **J. R. Apgar**, X. F. Stowell, K. N. Gutwin, A. E. Keating

**307.** Molecular dynamics simulations of bound VEGF. **B. A. C. Horta**, R. B. Alencastro

**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

**309.** Nature of stacking interactions between imidazoacridone intercalators and DNA Base Pairs. **I. E. Weidlich**, S. G. Tarasov, C. J. Michejda, M. C. Nicklaus

**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

**312.** Novel approach to structure-based pharmacophore search using computational geometry and shape matching techniques. **J. O. Ebalunode**, Z. Ouyang, J. Liang, W. Zheng

**313.** Pharmacophore-based virtual screening: How to obtain the best enrichment rates. **J. Kirchmair**, S. Ristic, K. Eder, P. Markt, G. Wolber, T. M. Steindl, C. Laggner, T. Langer

**314.** Prediction of blood-air and tissue-air partition coefficients: Calculated molecular descriptors vs. experimentally determined properties. **D. Mills**, S. C. Basak, B. D. Gute

**315.** Prediction of pH-dependent aqueous solubility of histone deacetylase (HDAC) inhibitors. **S. M. Vadlamudi**, F. Bjorkling, I. Kouskoumvekaki, N. T. Hansen, S. Ó. Jónsdóttir

**316.** Prediction of pKa values for amino acids and peptides. **S. Zhang**, J. Baker, P. Pulay

**317.** QSAR approach to modeling membrane permeability. **B. D. Gute**, J. Riviere, R. E. Baynes, S. C. Basak

**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

**321.** Structure-LD50 correlations: DFT study on substituted 3-carboethoxy-4-aminoquinolines. **T. C. Cordova de Sintjago**, L. Escalante, J. Posada, M. Rodriguez, G. Cabrera

**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. Szegezdi**, 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

**325.** Theoretical studies on pillared covalent organic frameworks for the hydrogen storage material. D. Kim, D. H. Jung, **S -H. Choi**, S. B. Choi, J. Yoon, Y. H. Jhon, J. Kim

**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

**329.** A classical/quantum chemical approach for quantitative structure activity of flavonoids. **I. A. Shehadi**, D. K. Al Jayousi, A. Al Mehdi

**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

**332.** Brownian dynamics simulations of lactate dehydrogenase isoforms with actin. **E. N. Njabon**, **K. L. Carlson**, K. A. Thomasson

**333.** Comparison of semi-empirical quantum mechanics methods applied to biological molecules: Potential and free energy surfaces of alanine and glycine Dipeptides in vacuum and in water. **G. D. M. Seabra**, R. C. Walker, A. E. Roitberg

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

**335.** Density Functional Theory studies of the interaction of sulfur oxides with large water clusters. **J. M. Standard**, R. D. Quinn, M. T. Van der Hoven

**336.** Evaluation of docking performance: Comparison of Surflex-Dock with five docking algorithms using the Johnson & Johnson data set. **T. E. Mansley**, J. K. Shepphird, L. Wang

**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

**340.** Molecular dynamics simulations of a DNA-biosensor. N. Le Bouch, J. Brisson, **M. Leclerc**

**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**

**343.** Predicting absolute binding free energies in a model binding site. **D. L. Mobley**, A. P. Graves, J. D. Chodera, A. McReynolds, B. K. Shoichet, K. A. Dill

**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

**345.** QSAR modeling of blood–brain barrier permeability of diverse organic compounds. **L. Zhang**, H. Zhu, T. I. Oprea, A. Tropsha

**346.** Topomer CoMFA: Investigation of scope. **G. Stahl**, R. D. Cramer, B. Wendt

**347.** Structure-based design of a novel class of beta-secretase (BACE) inhibitors. **C. H. Reynolds**, B. A. Tounge, A. B. Reitz, E. W. Baxter

**348.** Trends in ligand efficiency: Where do they come from? **C. H. Reynolds**, B. A. Tounge, S. D. Bembenek

**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

**354.** Improving generalized Born model in protein side chain and loop prediction. **K. Zhu**, M. R. Shirts, R. Friesner

**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**

**9:35 —358.** Multiscale modeling of deformation and fracture: Integrating chemistry and mechanics. **M. J. Buehler**

**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. K. 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

**10:50 —367.** Using inter-residue distances to predict protein structure. **C. R. Crecca**, A. E. Roitberg

**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**

**9:30 —371.** ATR-FTIR study of the secondary structure of antifreeze glycoproteins adsorbed at the ice/solution interface. **Y. Uda**, F. Kaneko, S. Zepeda, Y. Matsuura, Y. Furukawa

**10:00 —372.** Molecular dynamics simulations of antifreeze proteins at a lipid/water interface. **E. J. Smith**, P. Dalal, J. D. Madura, A. Haymet

**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*

**8:30 —374.** Atmospheric reactions in water clusters: Mechanisms, dynamics and rates. **R. B. Gerber**, Y. Miller, M. A. Kamboures

**9:10 —375.** Growth, structure, and dynamics of nanoscale water films on various substrates. **B. D. Kay**, G. A. Kimmel, N. G. Petrik, Z. Dohnálek, R. S. Smith

**9:50 —376.** Structure and dynamics of water near the interface with oligo(ethylene oxide) self-assembled monolayers. **A. E. Ismail**, G. S. Grest, M. J. Stevens

**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**

**9:20 —380.** Efficient dynamic boundary solvation models for biomolecular simulations. **W. Zhu**, G. Krilov

**9:40 —381.** Fast polarizable force field for molecular simulations. **G. A. Kaminski**

**10:00 —382.** Classical CHARMM Drude oscillator polarizable force field for nucleic acid bases. **V. M. Anisimov**, P. E. M. Lopes, A. D. MacKerell Jr.

**10:20 —** Intermission.

**10:35 —383.** Unraveling the behavior of DNA through multiscale modeling. **T. A. Knotts IV**, S. Deublein, J. J. de Pablo

**10:55 —384.** Multiproperty parametrization of a coarse grained model for proteins. **R. DeVane**, W. Shinoda, M. L. Klein

**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*

**8:30 —387.** Potency and selectivity of hydroxy hydantoins, a novel class of MMP-12 inhibitors: Structure-based QSAR analysis. **B. O. J. Nordén**, I. Shamovsky, B. Gabos, M. Munck af Rosenschöld, M. Lepistö, G. Carlström, J. Evenäs, D. Musil, K. Stenvall

**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

**11:10 —392.** Using homology models and structure-based design to improve the MAO-A safety profile of oxazolidinone antibacterials. **C. Eyermann**, P. Fleming, M. Gravestock, T. Jones, G. Kern, R. Ramsay, F. Reck, F. Zhou

**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

Unknown Site -- Unknown Room

**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

**1:20 —401.** Molecular modeling of drug binding to CYP 3A4. **J. Li**, C. H. Reynolds

**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**

**3:15 —406.** New approach to lead optimization and core hopping. **M. Shelley**, L. L. Frye, B. W. Sherman, S. N. Rao, H. Beard, J -C. Mozziconacci, P. S. Shenkin

**3:35 —407.** Structure-based design of aminohydantoins as highly potent, selective and orally active BACE1 inhibitors. **M. S. Malamas**, J. Erdei, I. Gunawan, N. Pawel, K. Barnes, M. Johnson, A. J. Robichaud, P. Zhou, J. Bard, J. Turner, Y. Hu, E. Wagner, S. Aschmies, T. Comery, R. Chopra, K. Fan

Section C

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

**1:55 —409.** Peptide bond non-planarity affects vibrational spectra of short peptides. **N. S. Myshakina**, **Z. Ahmed**, S. V. Bykov, J. K. Vries, **S. A. Asher**

**2:20 —410.** Density functional theory study on the protonation of guanine quadruplex. J. W. Gauld, **H. Liu**

**2:45 —** Intermission.

**3:00 —411.** Multistep cluster chemistry involved in SN2@P reaction systems. **M. A. van Bochove**, M. Swart, F. M. Bickelhaupt

**3:25 —412.** Reaction mechanism of direct gas phase synthesis of H2O2 catalyzed by Au3. **B. Njegic**, M. S. Gordon

**3:50 —413.** Theoretical study on the hydrolysis mechanism of 1-substituted silatranes in the gas phase. **S. Sok**, M. S. Gordon

Section D

Unknown Site -- Unknown Room

**Phil Magee Memorial Symposium: QSAR Reborn**

**Methods**

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

**1:30 —414.** A new paradigm for pattern recognition of drugs. **M. A. Grishina**, V. Potemkin, E. S. Pereyaslavskaya

**2:00 —415.** Intrinsic descriptors. **G. D. Purvis III**

**2:30 —416.** 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**

**3:00 —** Intermission.

**3:20 —417.** Molecular topology as a tool for the design of new drugs. **J. Galvez Sr.**

**3:50 —418.** Evaluation of descriptors and classification schemes to predict drug metabolism in terms of chemical information. **J. H. Block**, D. Henry

**4:20 —419.** Gaussian processes: A method for automatic QSAR and ADME modelling. **O. Obrezanova**, J. M. Gola, M. D. Segall

Section E

Unknown Site -- Unknown Room

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

**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.** Atronomy 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.

**3:45 —424.** Numerical study of Quantum Chromodynamics. **R. L. Sugar**

**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**

**4:50 —432.** Liquid-vapor interfaces of hydrogen bonded fluids using density functional theory interaction potentials. **C. J. Mundy**, S. M. Kathmann, W. I -F. Kuo

**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

**9:35 —434.** Is the band gap problem truly a problem: Defects in semiconductors. **P. A. Schultz**

**10:10 —435.** Density functional theory with accurate bond-breaking and band-gaps using generalized valence bond wave functions via the optimized effective potential method. **R. P. Muller**

**10:45 —** Intermission.

**11:00 —436.** Accurate density functionals addressing the self-interaction error and potential functional formalism. A. J. Cohen, P. Mori-Sánchez, T. Heaton-Burgess, F. A. Bulat, **W. Yang**

**11:35 —437.** TDDFT studies of resonance Raman processes: Understanding SERS. L. Jensen, C. M. Aikens, **G. C. Schatz**

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

**10:25 —442.** Molecular dynamics study of liquids confined to sol-gels and their vibrational spectra. **C. M. Morales**, W. H. Thompson

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

**11:15 —444.** Single chain in mean-field Monte Carlo simulations of block copolymer self-assembly. **J. W. Pitera**, G. Srinivas

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

**9:25 —446.** Accurately computed hydrogen bond energies using density functional theory with dispersion corrected atom centered potentials. **J. S. Arey**, I -C. Lin, P. Aeberhard, U. Rothlisberger

**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

**10:55 —449.** Effective fragment potential modeling of substituted benzene dimers. **T. Smith**, L. V. Slipchenko, M. S. Gordon

**11:20 —450.** IR Spectra by DFT for glucose and its epimers: A comparison between vacuum and solvated spectra. **W. B. Bosma**, U. Schnupf, J. L. Willett, F. A. Momany

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**

**9:50 —453.** EXAFS analysis of aqueous interfaces. **G. K. Schenter**, C. J. Mundy, L. X. Dang

**10:10 —** Intermission.

**10:30 —454.** Some new nonlinear spectroscopic findings of the aqueous interfaces. **H -F. Wang**, R -R. Feng, Z. Zhang, H -T. Bian, Y. Guo

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

**11:50 —456.** Interaction of atmospheric oxidants with the air-liquid interface of organic coated electrolytic solutions: A molecular dynamics study. **R. D'Auria**, E. Knudsen, D. J. Tobias

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

**9:20 —458.** Sampling of rare protein aggregation events in explicit water. **M. Chopra**, A. S. Reddy, J. J. de Pablo

**9:40 —459.** Bridging timescales between atomistic simulation and experiments with master equation models of protein folding and dynamics. **J. D. Chodera**, N. Singhal, W. C. Swope, J. W. Pitera, I. Haque, K. A. Dill, V. S. Pande

**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**

**10:55 —462.** Obtaining converged conformational ensembles for biomolecules in explicit water. **C. L. Simmerling**, **C. Simmerling**

**11:15 —463.** Free-energy landscapes from combined parallel-tempering and metadynamics. **G. Bussi**, F. L. Gervasio, A. Laio, M. Parrinello

**11:35 —464.** WHAM without histograms: Statistically optimal free energy estimates. **M. R. Shirts**, J. D. Chodera

## 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**

**2:35 —466.** Elastic properties of DNA under high stretching force at various pulling rates. **P. K. Maiti**, K. Sen

**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*

**1:00 —470.** Validating crystallographic ligands. **B. Kelley**, J. H. Nettles, G. Warren

**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.

**2:20 —473.** Tackling the cellular drug resistance of thymidylate synthase – disruption of an obligate dimer. **O. M. Salo-Ahen**, P. M. Costi, R. C. Wade

**2:40 —474.** Analysis and comparison of multiple sar models from regression and classification methods. **R. R. Gupta**, E. A. Jamois, K. Subramanian

**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

**1:25 —477.** Complexation of copper (II) ion in aqueous solution: New insight from DFT and cosmo solvation model. **V. S. Bryantsev**, M. Diallo, W. A. Goddard III

**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

**3:20 —481.** Tautomer stability and pKa evaluation. **Z. Zhu**, M. Shalaeva, M. P. Pollastri, R. V. Stanton

**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. Sprous**, F. Salemme

**2:50 —** Intermission.

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

**3:40 —488.** Modeling fluorophilicity: A hybrid method. **M. Charton**

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

Section E

Unknown Site -- Unknown Room

**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**

**1:25 —491.** Atomistic and continuum modeling of deformation of coiled-coil vimentin intermediate filaments. **M. J. Buehler**, T. Ackbarow

**1:50 —492.** Caught in atomistic detailed action: Modeling of protein-G monomers forming oligomers. **J. M. Bui**, J. Gsponer, J. C. Wooley, M. Vendruscolo, J. A. McCammon, C. M. Dobson

**2:15 —** Intermission.

**2:30 —493.** Intricate role of water molecules in protein dynamics. **D. Hamelberg**, T. Shen, J. A. McCammon

**2:55 —494.** Reducing false-negatives in computational protein design: Moving beyond a single-backbone model. **D. F. Green**

**3:20 —495.** Tautomers, conformers, and computation of chemical similarity. **J. H. Nettles**, J. L. Jenkins, Z. Deng, A. Bender, J. Scheiber, J. W. Davies, M. Glick

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