SUNDAY MORNING

Unknown Site -- Unknown Room

Computational Phase Equilibria

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
J. I. Siepmann and J. K. Johnson, Organizers

8:00 — 1. Molecular modeling of complex fluids. C. McCabe

8:40 — 2. Phase diagram calculations of alloys using density functional theory. V. B. Warshasky, X. Song


9:40 — Intermission.


10:30 — 5. Modeling the kinetics of nanocrystal growth. S. K. Kumar, M. Tambasco

11:10 — 6. Simulation of pure component phase equilibrium properties using a modified Stockmayer potential. T. McKnight, K. Bolton

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Methods I

S. Rick, Organizer

8:00 — 7. Replica-Exchange Method and Its Generalizations. Y. Okamoto

9:20 — Intermission.

9:40 — 9. Improving the convergence of replica exchange simulations for complex systems. C. L. Simmerling


11:00 — 11. Biasing potential replica-exchange to enhance sampling of peptide and protein conformations during molecular dynamics simulations. M. Zacharias

Section C

Unknown Site -- Unknown Room

Drug Discovery

Docking and Scoring

Cosponsored by CINF
I. Visiers, Organizer
A. Tebben, Presiding

8:00 — 12. Abandoning the rigid receptor approximation: Side-chain flexibility in GOLD. P. Carlqvist, J. W. Liebeschuetz


8:50 — 14. Advances in induced-fit docking with applications toward predicting binding energies of diverse molecules. I. Alberts, R. B. Murphy, B. W. Sherman, R. Farid, R. Friesner

9:15 — 15. Improved water handling in structure-based molecular docking. A. Rumpl, C. Detering, H. Claußen

9:40 — Intermission.


10:45 — 18. Role of quantum mechanical energies in binding sites of metalloproteins. A. E. Cho, D. Rinaldo


Section D

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Organic and Biorganic**

A. Roitberg, *Organizer*

8:00 — 20. Cation binding and quadrupole moments of substituted cyclopentadienyl rings. **K. Cormier**, M. Lewis

8:25 — 21. Effects of the crystal environment on potential energy surfaces for proton transfer in aspirin. M. M. Francl, **M. Wampole**


9:40 — Intermission.


10:20 — 25. Minding the gap: Lowering the barrier to the bergman cyclization of enediynes. **C. A. Parish**


**SUNDAY AFTERNOON**

Section A

Unknown Site -- Unknown Room

**Computational Catalysis**

**Zeolites and Homogeneous**

*Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)*

A. M. Rappe and S. Linic, *Organizers*
1:30 — 27. ACE, a virtual screening tool for asymmetric catalysts. C. R. Corbeil, J. Schwartzentruber, N. Moitessier


2:30 — 29. Born-Oppenheimer molecular dynamics simulations of enzyme catalysis with ab initio QM/MM methods. Y. Zhang, S. Wang, P. Hu

3:00 — Intermission.


Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Computational Efficiency

S. Rick, Organizer

1:30 — 32. Comparison between regular and replica exchange molecular dynamics simulations and their applications in protein folding. W. Zhang, H. Lei, C. Wu, Z. Wang, Y. Duan

2:10 — 33. Enhanced Sampling via Replica Methods. A. E. Roitberg

2:50 — Intermission.


3:50 — 35. Exploring the energy landscape of protein folding using replica-exchange and conventional molecular dynamics simulations. V. Daggett


Section C

Unknown Site -- Unknown Room

Molecular Mechanics
Advancing Methodologies I

E. X. Esposito, Organizer


2:45 — Intermission.

3:00 — 40. Using wide-angle x-ray scattering and molecular mechanics to explore the conformational ensemble of a hexameric porphyrin macrocycle: Evaluating charmm's ability to reproduce large amplitude motions. K. L. Mardis, H. Sutton, D. M. Tiede


MONDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Phase Equilibria

II

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
J. I. Siepmann and J. K. Johnson, Organizers

8:00 — 42. Simulations of phase transitions and activity coefficients in ionic systems. A. Z. Panagiotopoulos


9:20 — 44. Free energy calculations of molecular solutes in polymeric microstructures. N. F. van der Vegt, B. Hess, T. A. Ozal, C. Peter

9:40 — Intermission.

9:50 — 45. Molecular simulation of equilibrium properties of fluids: From understanding toward quantitative predictions. V. Lachet

11:10 — 47. Discretized transferable Lennard-Jones united atom models for phase equilibria. J. Elliott, P. Stuhldreher

Section B
Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Methods II

S. Rick, Organizer

8:00 — 48. Problem Oriented Sampling Design via the Replica Exchange Strategy. W. Yang

8:40 — 49. Extrapolating to equilibrium from early simulation results of replica exchange calculations on proteins. W. C. Swope, J. W. Pitera


10:00 — Intermission.


11:00 — 52. Advanced sampling in exploring pH-dependent conformational transitions in proteins and peptides. C. L. Brooks III

11:40 — 53. Temperature intervals with global energy reassignment (TIGER): Algorithm development and application to protein folding. R. A. Latour

Section C
Unknown Site -- Unknown Room

Drug Discovery

Finding hits

Cosponsored by CINF
I. Visiers, Organizer
J. Woolfrey, Presiding

8:00 — 54. Identification of Pyk2 FERM ligands by combining protein similarity assessment,
mutagenesis study, pharmacophore prediction, and in silico screening. L. Wang, N. Meurice, J. Loftus, Y.-P. Pang, B. Clark, C. A. Lipinski


9:15 — 57. Fragment based de novo design using an existing fragment based docking program, eHiTS. D. Reid, Z. Zsoldos, A. P. Johnson

9:40 — Intermission.


10:45 — 60. Searching for new targets for the inhibition of Acetyl-CoA Carboxylase. M. E. McKenzie, G. L. Waldrop, B. Chen


Section D

Quantum Chemistry

Quantum-Methods I

A. Roitberg, Organizer

8:00 — 62. Computation of acidity constants in solution from vertical energy gaps. M. Sulpizi, A. Shah, M. Sprik


8:50 — 64. Semiempirical PM6 modeling of organic crystal structures. J. J. P. Stewart

9:15 — Intermission.


10:30 — 67. Multi-centered ONIOM method for weakly bound non-covalent clusters: Recent advances and applications. G. S. Tschumper

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Catalysis

Nano

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
A. M. Rappe, S. Linic, and J. W. Bennett, Organizers

1:30 — 68. First principles study on the effect of metal and interface identities on thin film surface activity. V. R. Cooper, A. M. Kolpak, A. M. Rappe


2:30 — 70. Surface chemistry of gold nano-structures deposited on oxides: oxide-specific O2 interactions with supported gold and the oxidation state of gold. S. Laursen, S. Linic

3:00 — Intermission.


4:00 — 72. First principle calculations of supported catalysts: CO binding on MgO supported gold clusters and nanoparticles. G. Mpourmpakis, D. G. Vlachos

Section B

Unknown Site -- Unknown Room

Thomas Kuhn Paradigm Shift Award Competition

A. Nicholls and A. G. Skillman, Organizers

1:00 — Introductory Remarks.

1:05 — 73. Believe it or not: Understanding prediction confidence in computational drug discovery. D. Debe
1:45 — 74. Exploration of Chemical Space for Drug Discovery by Database Generation. J-L. Reymond

2:25 — Intermission.


4:00 — Concluding Remarks.

Section C

Unknown Site -- Unknown Room

Quantum Chemistry

Quantum-Methods II

A. Roitberg, Organizer

1:30 — 77. Natural linear scaled coupled cluster theory with local transferable triple excitations: Applications to polymers. T. F. Hughes, N. Flocke, R. J. Bartlett

1:55 — 78. Dispersion in combined ab initio/effective fragment potential systems. T. Smith, L. V. Slipchenko, M. S. Gordon


2:45 — Intermission.

3:10 — 80. Pushing the limits of MCSCF. L. Roskop, M. S. Gordon


ADAPT'ing to Retirement: A Symposium Honoring Peter C. Jurs

Sponsored by CINF, Cosponsored by COMP and PROF
R. Guha, Organizer
R. Guha, Presiding

1:10 — Introductory Remarks.
1:15 — 47. Wavelet based search prefilters for spectral library matching. B. K. Lavine, N. Mirjankar, K. Nuguru


2:45 — Intermission.

3:00 — 50. QSAR at the undergraduate institution and a model of air-to-blood partition coefficients for small organic molecules. N. R. McElroy, S. D. Smith

3:30 — 51. Adapting in an ABCD world. E. P. Jaeger

MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix

E. X. Esposito, Organizer

8:00 - 10:00

116, 121, 127, 132, 136, 141, 143-144, 147, 151, 155, 157, 163, 199, 204. See subsequent listings.

TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Phase Equilibria

III

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
J. I. Siepmann and J. K. Johnson, Organizers

8:00 — 82. Coarse-grain simulations of complex systems. J. J. de Pablo

8:40 — 83. Optimized expanded ensembles for simulations involving molecular insertions and deletions. F. A. Escobedo, F. J. Martinez-Veracochea
9:20 — 84. Use of the AUA intermolecular potential to determine the solubility of hydrogen in oxygenated solvents. R. Lugo, N. Ferrando, C. Nieto-Draghi

9:40 — Intermission.

9:50 — 85. Monte Carlo simulations for phase equilibria: Polymer solubility and quantum effects. C. D. Wick

10:30 — 86. Thermodynamics of solvent reorganization in solvent/co-solvent mixtures. N. F. van der Vegt, M. Lee, T. A. Ozal

11:10 — 87. Structure of liquid water from ab initio molecular dynamics at the complete plane wave basis set limit. O. Isayev, L. Gorb, J. Leszczynski

11:30 — 88. Treatment and importance of conformations in COSMO-RS. A. Klamt, M. Diedenhofen

Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Applications to Protein Folding

S. Rick, Organizer

8:00 — 89. Computing properties determining the stability diagram of a miniprotein in dilute aqueous solution by full atomic detail computer simulation. D. Paschek, A. E. Garcia

8:40 — 90. Convergence of folding free energy landscapes via application of enhanced sampling methods in a distributed computing environment. V. S. Pande, X. Huang, G. Bowman

9:20 — Intermission.


10:20 — 92. Sampling sequences: Engineering protein structure and function with theoretical protein design. J. G. Saven

Section C

Unknown Site -- Unknown Room

Drug Discovery

Mostly about Ligands
8:00 — 93. Applications of target class pharmacophore fingerprint modeling and multi-objective genetic algorithm optimization to large-scale combinatorial library design for corporate compound collection enhancement. **Z. Yang**, G. P. Brady

8:25 — 94. Combining clique-detection, MOGUL and MOGA for pharmacophore generation. D. A. Cosgrove, **E. J. Gardiner**, V. J. Gillet, R. Taylor

8:50 — 95. Confirm: Connecting fragments in receptor molecules. D. C. Thompson, A. Denny, D. Joseph-McCarthy, C. Humblet, **E. Feyfant**


9:40 — Intermission.


**TUESDAY AFTERNOON**

Section A

Unknown Site -- Unknown Room

**Computational Catalysis**

**Surfaces**

_Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)_

A. M. Rappe, S. Linic, and V. R. Cooper, _Organizers_

1:30 — 99. Modeling the Fischer-Tropsch synthesis catalyzed on a Fe(1,0,0) surface. J. Lo, **T. Ziegler**

2:00 — 100. First-principles modeling of Ba(Ce1-xPdx)O3-x: redox, structure, and chemistry. **J. W. Bennett**, R. Seshadri, S. L. Scott, A. M. Rappe

2:30 — 101. First-principles investigations of oxygen vacancies, copper adatoms, and their interactions on TiO2 (110). **S. Lewis**

3:00 — Intermission.

3:30 — 102. Identification of surface intermediates through the combined use of molecular modeling and vibrational spectroscopy. **J. W. Medlin**
4:00 — 103. NO oxidation thermodynamics and kinetics at high O coverage on Pt(111). R. B. Getman, W. F. Schneider


Section B

Unknown Site -- Unknown Room

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of J. Andrew McCammon

J. D. Madura, Organizer

1:00 — Introductory Remarks.


1:50 — 106. Brownian dynamics with hydrodynamic interactions: Application to lipid bilayers and biomembranes. F. L. H. Brown

2:30 — 107. Ensemble approaches yeild new scaffolds and new binding sites. H. A. Carlson

3:10 — Intermission.

3:30 — 108. Molecular simulations of macromolecular behavior in physiological conditions. A. H. Elcock

4:10 — 109. Adventures in computational chemistry. J. A. McCammon

Section C

Unknown Site -- Unknown Room

Molecular Mechanics

Advancing Methodologies II

E. X. Esposito, Organizer

1:30 — 110. The generalized Born model: Past, present, future? A. V. Onufriev

1:55 — 111. Salt Effects and explicit ions in continuum representations of water. S. A. Hassan

2:45 — Intermission.

3:00 —113. Molecular dynamics with generalized effective fragment potentials. J. M. Mullin, M. S. Gordon


Careers in Chemical Information

Sponsored by CINF, Cosponsored by CHAL, PROF, COMP, CEPA, and WCC
L. M. Balbes, Organizer

1:30 — Introductory Remarks.

1:35 —81. Chemist-librarian: The best of both worlds. F. B. Culp

2:00 —82. You know you're a Chemical Information Searcher if. B. M. Bridgewater

2:25 —83. Information highway to drug discovery. L. P. Greenblatt

2:50 — Intermission.

3:00 —84. Path less traveled: From the periodic table to public relations. J. E. Mears

3:25 —85. Breaking news: Chemistry is everywhere. I. Amato

3:50 —86. Careers in patent law: Going beyond the bench with your chemistry degree. J. J. Hasford

4:15 — Networking Discussion.

TUESDAY EVENING

Unknown Site -- Unknown Room

Poster Session

E. X. Esposito, Organizer
116. On the applicability of GPCR homology modeling to drug discovery: A comparison between crystal structure and in silico model of the β2 adrenergic receptor complexed with carazolol. S. Costanzi

117. Decomposition of high-energy density materials using high-level coupled-cluster theory. A. G. Taube, R. J. Bartlett

118. Building aromatic oligoamide foldamers. J. A. Geer, Z. Liu, V. Pophristic

119. Salt effects on the conformational preferences of alanine peptides. E. Asciutto, J. D. Madura

120. Molecular dynamics of the RNA-binding domain of Influenza A NS1. C. Young, R. Manetsch, E. Rivera, A. van Olphen, A. E. Cardenas

121. TAE augmented scoring functions: Application to enzymatic and non-enzymatic proteins. S. Das, C. M. Breneman, N. Sukumar, M. D. Ryan

122. A novel computational strategy for identifying peptides that bind pancreatic lipase. J. Audie, A. Spock


124. Theoretical Study of the Glutamate Receptor Ligand Binding Domain Flexibility and Conformational Reorganization. T. Mamonova, M. Kurnikova

125. A New Strategy to Drug Discovery - Systems-Based Drug Discovery. Z. Hu

126. Ab initio calculation of reaction between series of gilman cuprates and CH3I. J. Liu, J. P. Snyder

127. Acute toxicity of polynitroaromatics and products of their biotransformation on Vibrio fischeri: 2D QSAR study. A. Artemenko, A. V. Lyakhovskij, V. E. Kuz'min, E. N. Muratov, L. Gorb, M. Quasim, J. Leszczynski

128. Amyloidogenic intermediates: A computational study of the conversion of the β-sheet to α-sheet structure. A. M. Canfield, S. Huo, H. Wu

129. Analysis of polarization effects in protein-water simulations. S. Urahata, J. W. Ponder

130. Analysis of torsional effects and ring flipping in heavily substituted oxazolidine rings. P. M. Spoutz, M. C. Milletti

131. Application of the fault-injection system algorithm for chips coated with silsesquioxanes. Q. Pan, B. Hong, Q. Pan, L. Hu

132. Artificial neural network prediction of metal hydride properties with experimental and/or computational data. W. O. Griffin, J. A. Darsey

133. Atomic level computational identification of ligand migration pathways between solvent and binding site in myoglobin. J. Z. Ruscio, M. G. Prisant, T. Murali, A. V. Onufriev


137. Calculation of rotational barriers for two iminium cation stereoisomers. **L. A. Lello**, M. C. Milletti

138. Calculations of the acidities of n-butylbenzene protons in aqueous media under normal and supercritical conditions. **P. R. Alburquerque**, T. Junk, B. Ramachandran

139. CCl$_4$ adsorption and dissociation on Si($111$)-$\sqrt{3}\times\sqrt{3}$-Ag surface from first principles. **X. Liu**, H. Guo, C. Meng


141. Comparing the thermodynamic stability of skipped diene radicals: A model for the peroxidation of arachidonic acid. **C. E. Tornow**, M. C. Milletti

142. Comparison of density functionals and semiempirical methods for protonated creatinine. **N. Settergren**, E. A. Amin, P. Buhlmann


147. Computational study of the interaction of sulfoindocyanine dye Cy3 with single- and double-stranded DNA. **E. Dolghih**, J. Krause, A. E. Roitberg


151. Design of peptidomimetic ligands using core hopping. **M. Shelley**


155. Docking based pharmacophore modeling of combined AT1-PPAR gamma ligands. **F. Shah**, P. Mukherjee, M. A. Avery

156. Doublet-quartet gaps of substituted carbynes. **K. A. Daniel**, E. V. Patterson


158. Efficient extrapolation to the CCSD(T)/CBS limit using pair natural orbitals. **E. C. Barnes**, G. A. Petersson

159. Enhanced stacking interactions between nucleic acid base pairs upon hydrogenation. **M. Mandziuk**, J. Landers, F. Duffy

160. Enthalpies of formation of TNT derivatives by homodesmotic reactions. **A. Sood**, D. H. Magers

161. Establishing a balance between prediction accuracy and applicability domain of QSAR models. **L. Ye**, H. Zhu, A. Golbraikh, A. Tropsha

162. Evaluation of density functionals, semiempirical methods, SCC-DFTB and molecular mechanics force fields for prolyl-leucyl-glycinamide (PLG) analogs designed as dopamine D2 receptor modulators. E. A. Amin, **R. L. Wood**, R. L. Johnson, B. J. Young-Dixon


164. Fast folding of peptides and small proteins using the “temperature intervals with global energy reassignment” (TIGER) method. **X. Li**, S. J. Stuart, R. A. Latour

165. Finding the right path: Computational approach to DNA base eversion. **C. Bergonzo**, C. L. Simmerling

166. FITTED: A docking-based virtual screening tool for flexible and complex systems. **C. R. Corbeil**, J. Schwartzentruber, N. Moitessier


170. How do SET-domain Protein Lysine Methyltransferases Achieve the Methylation State Specificity? An ab initio QM/MM Molecular Dynamics Study. **P. Hu**, S. Wang, Y. Zhang


173. Iterative refinement of parameters for computer simulation of peptides and proteins. **P. J. Steinbach**

174. Kinetic aspects of the oxygenation reaction mechanism in COX-1. **M. A. Lukowski**, M. C. Milletti


177. Mechanistic study of inosine monophosphate dehydrogenase. **D. E. Mendes**, A. Cook, S. Braun-Sand


184. QSPR predictions of an aqueous solubility for military compounds using SiRMS. **E. N. Muratov**, V. E. Kuz'min, A. G. Artemenko, L. Gorb, M. Quasim, J. Leszczynski


188. Reduced point charge approximation for speeding up the computation of electrostatic potential in biomolecular systems. **R. Anandakrishnan**, A. V. Onufriev


194. Simulations of polypeptide folding using new efficient replica exchange methods. **A. J. Lee**, S. Rick

195. Strain energies in isomers of 1,3-cycloheptadiene and bicyclo[3.2.0]hept-6-ene. **B. Magers**, S. R. Davis, D. H. Magers

196. Structural Effects of Interstrand Crosslinks on DNA through Molecular Dynamic Simulations. **A. J. Campbell**, K. Song, A. Guainazzi, O. D. Scharer, C. L. Simmerling

197. Surflex-Docking into the minor groove of DNA. **L. Wang**, T. E. Mansley


200. The free energy and entropy of a water molecule in hydrophobic cavities. **H. Yu**, S. Rick

201. The radical enhanced nucleation of water. **S. J. Keasler**, B. Chen, J. S. Francisco, R. B. Nellas

202. The role of the active site solvent in the thermodynamics of factor Xa-ligand binding. **R. Abel**, T. Young, R. Farid, B. Berne, R. A. Friesner

203. Unusual participation of the counterion in charge transfer copper(I) complexes. **L. M. Matosziuk**, T. Pintauer, J. D. Evanseck


Section B
Chemical Computing Group Excellence Award

A. Good, Organizer

7:00 - 9:00


209. Using computer simulations to explore pressure effects on proteins. S. Sarupria, S. Garde

HP Scholar Award Poster Session

C. M. Breneman, Organizer

7:00 - 9:00


211. Predictive electronic and vibrational many-body methods. S. Hirata

212. Advances in potentials of mean force methodology for organic and biological simulations. O. Acevedo

213. Integration of a bioinformatics approach to high-throughput docking and its application to the discovery of novel TNF receptor-associated factor 6 (TRAF6) inhibitors. S. Zhang, B. Darnay, L. Ducuny

WEDNESDAY MORNING

Computational Evaluation of Rate Constants
Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
T. N. Truong and H. DaCosta, Organizers

8:00 — Introductory Remarks.

8:05 —214. A Fast Semi-Empirical Approach to Accurate Rate Constants. N. S. Ostlund, J. R. Barker


9:35 — Intermission.


10:20 —217. Kinetic analysis of the pyrolysis of phenethyl phenyl ether with different substituents: Computational prediction of α/β-selectivities. A. Beste, A. C. Buchanan III, R. J. Harrison


Section B

Unknown Site -- Unknown Room

Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems

Methods III

S. Rick, Organizer

8:00 —220. Parallel tempering techniques for simulation of proteins. U. H. Hansmann, W. Nadler


10:00 — Intermission.

10:40 —223. A different architecture for expanded ensemble simulation: Adaptive AIS. E. Lyman, D. M. Zuckerman

11:20 —224. Protein folding network, and energy landscape, studied by parallel Wang-Landau sampling. S. Takada
12:00 —225. Protein folding using replica exchange and mechanism-based conformational searching. M. S. Shell, B. Ozkan, V. Voelz, A. Wu, K. A. Dill

Section C

Unknown Site -- Unknown Room

Drug Discovery

Drug Discovery

_Cosponsored by CINF_

I. Visiers, _Organizer_

P. Carlqvist, _Presiding_


8:50 —228. Virtual screening for superior R-groups. R. D. Cramer


WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Computational Catalysis

Electro-catalysis and the Impact of Environment

_Cosponsored by ACS Division of Computers and Chemistry and AIChe CoMSEF (Group 21)_

A. M. Rappe and S. Linic, _Organizers_

1:30 —231. Surface segregation in nanoalloys under reaction conditions. P. B. Balbuena, Y. Ma, G. Ramirez-Caballero, J. R. Callejas-Tovar

2:00 —232. First principles studies of electrochemical oxidation reactions at model solid oxide fuel cell (SOFC) anodes. D. Ingram, J. Mukherjee, S. Linic

2:30 —233. Why PtVFe nanoparticles are better catalysts for oxygen reduction. T. Lin, J. Williams, L. Wang
3:00 — Intermission.

3:30 — 234. Configurational correlations in the adsorption properties of atomic adsorbates on transition metal surfaces. J. R. Kitchin

4:00 — 235. First-principles prediction of switchable stoichiometry at interfaces. S. V. Levchenko, A. M. Rappe


Section B

Unknown Site -- Unknown Room

Model Applicability Domains: When Can I Use my Model?

Cosponsored by CINF
C. M. Breneman and D. F. Ortwine, Organizers

1:00 — Introductory Remarks.

1:10 — 237. Domain applicability of ligand and structure-based virtual screening. A. Nicholls, M. McGann, P. Hawkins

1:35 — 238. Testing the limits of a QSAR model: How many cases are actually needed to develop a reliable predictive model? C. M. Sundling, C. M. Breneman, M. J. Embrechts, C. Huang, X. Wu, N. Sukumar


2:25 — Intermission.

2:40 — 240. Combining global and local approaches to model domain applicability. R. Guha, D. T. Stanton

3:05 — 241. QSAR model stability: How much information is in the data? D. Ryan, M. McLellan, C. M. Breneman


Section C

Unknown Site -- Unknown Room

Molecular Mechanics
Biomolecular Simulations

E. X. Esposito, Organizer


1:55 — 244. Examination of proposed intercalation models for imidazoacridone related compounds. I. E. Weidlich, S. G. Tarasov, I. V. Filippov, M. C. Nicklaus


2:45 — Intermission.

3:00 — 246. Computational study of the interaction of sulfoindocyanine dye Cy3 with single- and double-stranded DNA. E. Dolghih, J. L. Krause, A. E. Roitberg


THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

Computational Evaluation of Rate Constants

Computational Evaluation of Rate Constants

Cosponsored by ACS Division of Computers and Chemistry and AIChE CoMSEF (Group 21)
T. N. Truong and H. DaCosta, Organizers

8:00 — Introductory Remarks.


8:50 — 249. The Determination of Reaction Rate Constants for H-atom Abstraction from N2H4 by H, NH2, CH3, C2H5 and NO2. C. Chiung-Chu, M. Michael

9:35 — Intermission.

9:50 — 250. Rate constants from biased and unbiased reactive path ensembles. B. M. Dickson, G. Henkelman, D. E. Makarov

10:20 — 251. Rate estimation rules for H abstraction reactions by H and CH3 from pure and oxygenated hydrocarbons. H. Carstensen, A. M. Dean


Section B

Unknown Site -- Unknown Room

**Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems**

Applications

S. Rick, *Organizer*

8:00 —254. Simulations of hydrogen clathrate hydrates. **D. L. Freeman**, W. Cardoen, E. Curotto, J. D. Doll


9:20 — Intermission.


10:40 —258. Novel Ligand-induced Survivin Dimer Conformation via Replica Exchange Molecular Dynamics (REMD) and Receptor-Based Reverse Virtual Screening. **I. H. Park**, C. Li

Section C

Unknown Site -- Unknown Room

**Quantum Chemistry**

**Quantum-Materials**

A. Roitberg, *Organizer*

8:00 —259. Testing, validation, and parameterization of density functionals and molecular orbital theory for zinc bio- and nanocenter coordination chemistry. **E. A. Amin**, D. G. Truhlar, A. Sorkin

8:25 —260. Methane and silane dimer potentials from quantum chemistry calculations. **S. D. Chao**, A.
H.-T. Li

8:50 — 261. Nonequilibrium DFT properties of intramolecular hydrogen bonding in malonaldehyde, aminoacrolein, iminopropenylamine and derivatives. J. N. Woodford

9:15 — Intermission.

9:30 — 262. Origin of Lewis acid strength within mixed boron halides. J. A. Plumley, J. D. Evanseck

9:55 — 263. Quantum chemical calculations of surface photovoltages: Applications to adsorbates on Si (111). D. S. Kilin, D. A. Micha


THURSDAY AFTERNOON

Unknown Site -- Unknown Room

Molecular Modeling Applied on DPP-4 Inhibitor Programs

Y.-D. Gao, Presiding

1:00 — 265. 3D structural insights for DPP-IV inhibition with Abbott compounds. K. Longenecker

1:30 — 266. Structural biology and molecular modeling in the design of novel DPP-4 inhibitors. G. Scapin


2:30 — 268. Structure, function and inhibitors of prolyl dipeptidase DPP8. X. Chen

3:00 — 269. Homology models of Dipeptidyl Peptidases 8 and 9. C. Rummey, G. Metz

Unknown Site -- Unknown Room

Model Applicability Domains: When Can I Use my Model?

Part II

Cosponsored by CINF
C. M. Breneman and D. F. Ortwine, Organizers

1:00 — Introductory Remarks.
1:05 —270. Applicability domains, space coverage, and predictive power of QSAR models. A. Tropsha, A. Golbraikh, H. Zhu

1:30 —271. Testing the validity range of QSAR models using one-class support vector machines. M. J. Embrechts, C. M. Breneman, C. Huang, N. Sukumar


2:20 — Intermission.


3:00 —274. Localizing uncertainty in PLS predictivity. R. D. Clark, G. Stahl, T. E. Mansley


Section C

Unknown Site -- Unknown Room

Molecular Mechanics

Advancing Methodologies III

E. X. Esposito, Organizer

1:00 —276. Advanced multicanonical replica exchange simulations. D. J. Sindhikara, A. Roitberg


2:15 — Intermission.

2:40 —279. Predicting protein structure using inter-residue distances. C. R. Crecca, A. E. Roitberg

3:05 —280. The Coordination Environments of Cu(I) in Proteins: Cu(I) Parameter Development for CHARMM. M. Harrison, A. Loccisano, C. T. Dameron, J. D. Evanseck

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