COMP
DIVISION OF COMPUTERS IN CHEMISTRY

H. Woodcock and J. Shen, *Program Chairs*

SUNDAY MORNING – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Immersive Virtual Reality for Molecular Design

Cosponsored by CHED, CINF and COMSCI
R. S. Paton, L. Whitehead, *Organizers, Presiding*

8:30 **1.** Development of a virtual reality interface for molecular simulations-driven interactive ensemble-based drug design. J. Juarez-Jimenez, S. Llabres, **J. Michel**
9:10 **2.** Nanome: Next generation molecular visualization, collaboration, and design. E. Leija, S. McCloskey, **K. Wang**
9:50 **3.** Development of a virtual reality platform for effective communication in drug discovery. **L. Kingsley**, G. Spraggon
10:30 Intermission.
10:50 **4.** Computational modeling of Novichok interaction with acetylcholinesterase in VR. **Z. Radic**
11:30 **5.** Use of VR for molecular structures. **J. Boström**

SECTION B
Omni San Diego Hotel
Gallery 3A

Advances in Multiscale Computational Modeling of Biomass Conversion Processes

R. Assary, V. Glezakou, S. Kim, *Organizers, Presiding*

8:30 Introductory Remarks.
8:35 **6.** Overview of the US Department of Energy's consortium for computational physics and chemistry. **G.J. Leong**, J. Parks
9:00 **7.** Computational studies of catalytic biomass conversion. **D.A. Dixon**
9:30 **8.** Catalytic mechanisms of butanediol conversion by metal phosphates. J. Alegre Requena, Y. Guan, X. Huo, J. Stunkel, S. Kim, D. Vardon, **R.S. Paton**
10:00 Intermission.
10:15 **9.** Multiscale modelling approach for the electrochemical hydrogenation of organic compounds. **R. Rousseau**, V. Glezakou, M. Lee, D.C. Cantu, S. Akhade, M. Nguyen, S. Yuk, D. Zhang
10:45 **10.** Multiscale modeling of hierarchical transport and chemical reaction in porous catalyst particles in fluidized and packed bed reactor systems. **P. Ciesielski**, V.S. Bharadwaj, B. Pecha, H. Sitaraman, L. Bu, A. Lattanzi, X. Gao, W. Rogers
11:15 **11.** Toward the optimal design of molybdenum carbide catalysts for vapor phase upgrading of bio-oil. **H. Doan**, M. Zhou, R. Assary

SECTION C
Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
H. Harb, *Presiding*

8:30 **12.** Impact of protein conformational changes and electrostatics on a BLUF photoreceptor. **J.J. Goings**, S. Hammes-Schiffer
9:00 **13.** Catalytic structure and function of CRISPR-Cas9 revealed by *ab intio* quantum mechanics/molecular mechanics (QM/MM) simulations. **G. Palermo**
9:30 **14.** Effect of ions on absorption spectra of green fluorescent protein (GFP) chromophore in aqueous solution. **S.V. Shedge**, T.J. Zuehlsdorff, M. Servis, A.E. Clark, C. Isborn
10:00 Intermission.
10:15 **15.** Quantum mechanics of how solvents alter the identity of chemical bonds. D.R. Widmer, **B.J. Schwartz**
10:45 **16.** Bond orders: Definition, evaluation, and physical meaning. **G. Knizia**, S. Bintrim
11:15 **17.** Rovibrational spectroscopy of magnesium acetylide (MgCCH) and its detection in the interstellar medium. J.E. Burns, Q. Cheng, R.C. Fortenberry, **N.J. Deyonker**
11:45 **18.** Static and dynamic approaches to computing spectral lineshapes. **T.J. Zuehlsdorff**, A. Montoya Castillo, J. Napoli, T. Markland, C. Isborn

SECTION D
Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
W. G. Noid, J. Shelley, *Organizers*
J. Li, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 **19.** Recent advances in coarse-graining. **G.A. Voth**
9:05 **20.** Relative entropy design of coarse-grained protein models. **M. Shell**, T. Sanyal
9:35 **21.** Systematic coarse-graining for thermodynamic properties and inhomogeneous systems. **W.G. Noid**
10:05 Intermission.
10:20 **22.** Consistent representation of structural and dynamical properties from coarse-grained simulation models. **J.F. Rudzinski**, T. Bereau
10:50 **23.** Developing transferable coarse-grained potentials for the prediction of multiproperties of polymer systems. **H. Guo**
11:20 **24.** Integrating dynamic ionization into membrane permeation free energy landscapes and macroscopic permeability calculations. Z. Yue, **J.M. Swanson**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Use of Predictive Computational ADME Tools to Enable Drug Discovery

F. Broccatelli, *Organizer*
D. F. Ortwine, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 **25.** 30 years of computational ADME: What have we learned?. **N. Hosea**
9:05 2 **6.** Comparison of matched molecular pairs, matched molecular series and machine learning models for the optimization of ADME endpoints. **C. Keefer**
9:35 **27.** Building a stronger *in silico* ADME program through partnership. **K.E. Desino**
10:05 Intermission.
10:20 **28.** Estimation of membrane permeation using implicit membrane models and machine learning. **B. Dutagaci**, S. Brocke, A.D. Mackerell, M. Feig
10:50 **29.** Advancing the quan/qual partnership for chemical design. **C. Kochansky**
11:20 **30.** Anticipating and addressing solubility and precipitation problems computationally. **R.D. Clark**, R. Fraczkiewicz

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

SUNDAY AFTERNOON – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Modeling Protein-Ligand Recognition in Aqueous Environment: Present & Future

E. Alexov, C. Chang, R. Luo, *Organizers*
H. Muddana, *Presiding*

1:30 Introductory Remarks.
1:35 **31.** Modeling water in molecular recognition and drug design. **M.K. Gilson**
2:05 **32.** Ligand-protein pose and affinity predictions: New perspectives and lessons learned from the drug design data resource (D3R). **R.E. Amaro**
2:35 **33.** Water, water everywhere, nor any drop to drink. **M.S. Head**
3:05 Intermission.
3:20 **34.** Molecular diffusion in biology. **J. McCammon**
3:50 **35.** Machine learning identifies chemical drivers of enzyme catalysis. N. Seelam, B.M. Bonk, J.W. Weis, **B. Tidor**
4:20 **36.** Modeling ligand-CDK8/CycC unbinding free energy barriers for designing drugs with preferred binding kinetics. **C. Chang**, Z. Tang, S. Chen, H.D. Pandey

SECTION B
Omni San Diego Hotel
Gallery 3A

Advances in Multiscale Computational Modeling of Biomass Conversion Processes

R. Assary, V. Glezakou, S. Kim, *Organizers, Presiding*

1:30 **37.** PETase: Engineering and characterization of a plastic "eating" enzyme. **H.L. Woodcock**, G. Beckham, J. McGeehan
2:00 **38.** Unraveling the oxidative coupling of methanol on Au(111) using first-principles-based kinetic modelling. R. Réocreux, I. Fampiou, **M. Stamatakis**

2:30 **39.** Computational fluid dynamic modeling and simulation of biomass pyrolysis vapor-phase upgrading process at reactor scale. **X. Gao**, T. Li, W. Rogers, R. Panday, C. Li, H. Ashfaq, B. Hughes

3:00 Intermission.

3:15 **40.** Computational scale-up of packed bed reactor and process for catalytic upgrading of pyrolysis vapors using COMSOL. **B. Adkins**, J. Parks, K. Iisa, K. Smith

3:45 **41.** Predicting hydroxymethylfurfural (HMF) formation rate in sugar upgrading through investigation of Lewis acid and organic solvent effects. **Y. Kim**, H.M. Pilath, D. Robichaud, D.K. Johnson, S. Kim

4:05 **42.** First-principle based microkinetic study of water effect in aldol condensation reaction on MgO(111) surface. **M. Zhou**, L.A. Curtiss, R. Assary

4:25 Concluding Remarks.

SECTION C
Omni San Diego Hotel
Gaslamp 1

Molecular Mechanics

J. Shen, *Organizer*
R. Teo, *Presiding*

1:30 **43.** From *ab initio* data to high-dimensional potential energy surfaces: Nuts and bolts of generating a general many-body potential energy function. **S.E. Brown**, F. Paesani

1:50 **44.** Effective fragment potentials made faster. **L.V. Slipchenko**, K.B. Bravaya, E. Epifanovsky

2:10 **45.** Modeling hydrogen-oxygen combustion via programmable potentials. **A.M. Avila**, **L. Bertels**, **M.P. Head-Gordon**, **I. Mezic**

2:30 **46.** Advanced electrostatic potential based methods to derive atomic charges and polarizabilities. **M. Schauperl**, P.S. Nerenberg, L. Wang, D.L. Mobley, C.I. Bayly, M.K. Gilson

2:50 **47.** MBX: Next generation molecular dynamics. **M. Riera Riambau**, D. Smith, A.C. Simmonett, F. Paesani

3:05 Intermission.

3:20 **48.** Implementing polarizable Gaussian multipole model for molecular dynamics simulations. H. Wei, **R. Qi**, R. Luo

3:40 **49.** Modeling vibrational Stark effects using polarizable force fields: KSI as an exemplar. **J.W. Essex**, R.T. Bradshaw, S. Fried

4:00 **50.** Assessing the performance of various binding-free-energy-prediction approaches on kinase/ligand complexes: Importance of the density-functional theory tight-binding method and atomic-charge calculations. **M. Ghaani**, O. Barker, N. English

4:20 **51.** Accuracy vs. efficiency? Towards ACKS2-based polarization in force fields. **P. Gütlein**, H. Oberhofer, K.U. Reuter, J. Blumberger

SECTION D
Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
J. Li, W. G. Noid, J. Shelley, *Organizers*
J. F. Rudzinski, *Presiding*

1:30 **52.** Polymer electrolytes statistics and thermodynamics. **M. Olvera De La Cruz**

2:00 **53.** Multiscale modeling for the materials and pharmaceutical industries. **J. Shelley**

2:30 **54.** Molecular and mesocale modeling for mechanical issues in composite interfaces. **N.E. Iwamoto**

3:00 Intermission.

3:15 **55.** Structure and dynamics of macromolecular systems on multiple scales. **M. Guenza**

3:45 **56.** Coarse-grained electron transfer model for reactive force fields. **I. Leven**, T.L. Head-Gordon

4:15 **57.** Coarse-graining electrons: Nonreactive many-body force fields for molecular dynamics. T.L. Head-Gordon, **A. Das**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Use of Predictive Computational ADME Tools to Enable Drug Discovery

F. Broccatelli, *Organizer*
D. F. Ortwine, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **58.** Dose optimization concepts in drug design. **F. Broccatelli**

2:05 **59.** Integration of machine learning models for ADME to enable drug discovery: Deep neural network vs. support vector machine. **P. Desai**

2:35 **60.** Incorporating ADME/Tox parameters in optimising multiobjective molecular design. **N. Brown**

3:05 Intermission.

3:20 **61.** Cross-company evaluation of *in silico* approaches to predict microsomal or hepatocyte binding. **S. Winiwarter**

3:50 **62.** Rationally controlling the chameleonic properties of beyond Rule of 5 (bRo5) compounds. **G. Caron**, G. Ermondi

4:20 **63.** Beyond ADME QSAR: Adapting physiologically-based PK simulations to lead optimization. **E.J. Martin**, B.D. Madej, M. Bolger, R. Clark, P.R. Daga

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

SUNDAY EVENING – COMP

Computational Methods for Lanthanides & Actinides: Theory & Applications

Sponsored by NUCL, Cosponsored by COMP

MONDAY MORNING – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Modeling Protein-Ligand Recognition in Aqueous Environment: Present & Future

E. Alexov, C. Chang, R. Luo, *Organizers*
M. S. Head, *Presiding*

8:30 **64.** Using structure to identify protein-protein and drug protein interaction networks. **B.H. Honig**
9:00 **65.** Challenges and improvements in modeling protein-ligand interactions. **D.L. Mobley**
9:30 **66.** Solvation structure and thermodynamic mapping (SSTMap): Open-source software package for the analysis of water in molecular dynamics trajectories. K. Haider, A. Cruz, S. Ramsey, M.K. Gilson, **T.P. Kurtzman**
10:00 Intermission.
10:15 **67.** Role of interfacial water in protein-ligand binding: Classical density functional perspective. **R.M. Levy**
10:45 **68.** Computational crystal structure and polymorph prediction. **H. Muddana**
11:15 **69.** Molecular simulation: Methodology advancements and applications to drug discovery. **R. Luo**
11:45 **70.** Constraining evolution —> Avoiding drug resistance: Lessons from viruses. **C.A. Schiffer**
12:15 Concluding Remarks.

SECTION B
Omni San Diego Hotel
Gallery 3A

Women Make COMP

Cosponsored by PROF and WCC
K. Armacost, M. C. Nagan, *Organizers*
G. Palermo, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 Panel Discussion.
8:50 Discussion.
8:55 **71.** Development of rare-event sampling methods for biomolecular transport systems. **N. Roussey**, A. Dickson
9:00 **72.** Tailoring the variational implicit solvent method (VISM) for new challenges: Heterogeneous hydration in biomolecular recognition. **C. Gravina Ricci**, B. Li, L. Cheng, J. Dzubiella, J. McCammon
9:05 **73.** Computational methodologies for the accurate simulation of Raman intensities in the low-frequency vibrational spectra of molecular crystals. **S.J. Dampf**, T.M. Korter
9:10 **74.** Structural basis for ligand modulation of the CCR2 conformational landscape. **B.C. Taylor**, C.T. Lee, R.E. Amaro
9:25 **75.** Identifying and quantifying allosteric pathways from molecular simulations. **H. Klem**, P. Lake, R.B. Davidson, R.S. Paton, M. McCullagh
9:30 **76.** Structural and dynamic properties of $A\beta_{21-30}$ with experiments and simulations. **D.B. Amirkulova**, M. Chakraborty, A. White
9:35 **77.** Targeting alpha isoform specificity in human topoisomerase II. **J.A. Akkarapattiakal Kuriappan**, N. Osheroff, M. Devivo
9:50 **78.** Elucidation of the mechanism for ethene hydrogenation over single metal cation catalysts: Combined modeling and experimental study. **H. Shabbir**, S.L. Pellizzeri, M. Ferrandon, I. Kim, M. Delferro, A.B. Martinson, R.B. Getman
9:55 **79.** Iridium(I) catalyzed α-C(sp^3)–H akylation of saturated azacycles: Experiment and theory. **P. Verma**, N. Chekshin, J. Yu
10:00 **80.** Putting force fields to the test: Mutual interaction of aminoacids, lipids, and carbohydrates with GPI-anchored proteins inserted into lipid bilayers and membranes. **P. Banerjee**, R. Lipowsky, M. Santer
10:05 **81.** Charge density in enzyme active site as a descriptor of electrostatic preorganization. **A. Alexandrova**, M. Eberhart
10:20 Intermission.
10:30 **82.** Towards a wavelength sensitive detector, based on ICD in a system of coupled quantum wells. **T.G. Goldzak**, N. Moiseyev

10:45 **83.** Hot ground state photochemistry of aldehydes in the atmosphere. **M. Corrigan**, B. Welsh, S. Kable, M. Jordan

10:50 **84.** Investigating the mechanical perturbations of asymmetric lipid bilayers on mechanosensitive Piezo ion channels through multiscale approach. **W. Jiang**, W.M. Botello-Smith, H. Zhang, J. Lacroix, Y.L. Luo

10:55 **85.** Enhancing side chain rotamer sampling using non-equilibrium candidate Monte Carlo. **K.H. Burley**, S.C. Gill, N.M. Lim, C. Goulding, D.L. Mobley

11:00 Panel Discussion.

11:15 **86.** Computational probing of the force-biased potential energy surface: Uncovering nonintuitive mechanochemical reaction pathways. **A.K. Roessler**

11:20 **87.** Enzyme engineering to computationally predict stereoselective products for biocatalysts. **S. Lenka**, P. Buteler, R.R. Watkins, J.D. Stewart, A.E. Roitberg

11:25 **88.** Towards the *de novo* design of functional metalloproteins. **K. Belsare**, W.F. Degrado, N. Polizzi

11:30 **89.** Machine-learning-aided *in silico* drug discovery: Machine-learning-based atom parameterization program for molecular mechanics force fields. **M. Charles**

11:45 **90.** Molecular simulation to accelerate discovery of $\alpha_V\beta_6$ integrin inhibitors. **E. Guest**, S. Oatley, S.J. MacDonald, J.D. Hirst

11:50 **91.** Solvent design strategies from computation and statistical modeling. **L.C. Gallegos**, J. Alegre Requena, R.S. Paton

11:55 **92.** Understanding and correcting DFT errors in transition metal chemistry. **F. Liu**, H.J. Kulik

12:00 **93.** Computational flavor chemistry: Towards the rational design of chemosensory GPCR-targeted food ingredients and drug candidates. **A. Di Pizio**, L. Waterloo, M. Behrens, P. Gmeiner, M. Niv

SECTION C
Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
A. Zamani, *Presiding*

8:30 **94.** Halogen-bonding interactions: Revised benchmarks and a new assessment of exchange vs. dispersion. **B.M. Wong**, L. Anderson, F. Aquino, A.E. Raeber, X. Chen

9:00 **95.** Compressibility of intramolecular dispersion interactions. **C.J. Mackie**, J. Gonthier, M.P. Head-Gordon

9:30 **96.** Accurate prediction of electronic coupling for hole and electron transfer problems using DFT-based approaches. **Y. Mao**, T. Markland

10:00 Intermission.

10:15 **97.** Conformational exploration of aromatic amino acids: Assessment of DFT levels by comparison of vibrational frequencies with experimental data. **T. Dinadayalane**, D.A. Daggag

10:45 **98.** Methane combustion studied using the *ab initio* nanoreactor approach combined with kinetic modeling. **J. Meisner**, X. Zhu, H. Hirai, K. Thompson, T.J. Martinez

11:15 **99.** Modeling the photodetachment processes of lanthanide oxide and boride clusters. **H. Harb**, H.P. Hratchian

11:40 **100.** Spin state ordering in metal-based compounds using the localized active space self-consistent field method. **R. Pandharkar**, M. Hermes, C.J. Cramer, L. Gagliardi

SECTION D
Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
J. Li, J. Shelley, *Organizers*
W. G. Noid, *Organizer, Presiding*

8:30 **101.** Combining enhanced sampling with machine learning in the generation of high-dimensional free energy landscapes of complex molecular systems. **M.E. Tuckerman**

9:00 **102.** Machine learning of coarse-grained molecular dynamics force fields. **F. Noe**, C. Clementi

9:30 **103.** Coarse-graining molecular models with machine learning and experimental data. **C. Clementi**

10:00 Intermission.

10:15 **104.** Nanoscale simulations to enable mRNA delivery. **M.L. Hall**

10:45 **105.** High-throughput molecular dynamics of drug-membrane thermodynamics. **T. Bereau**

11:15 **106.** Bridging the scales: Machine learning directed macro-to-micro scale simulation to model KRAS initiation of cancer. **T.S. Carpenter**, F.C. Lightstone, D.V. Nissley, F. Streitz, H. Ingolfsson

11:45 **107.** Top-down multiscale modeling to design nanomaterials from peptide self-assembly. **J. Li**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Cosponsored by MEDI
L. Whitehead, *Organizer*
J. Shen, *Organizer, Presiding*

8:30 **108.** In pursuit of elusive allosteric pathways in protein kinases. **A.P. Kornev**
9:00 **109.** Harnessing allostery for selective targeting of Aurora kinase A in cancer. **N. Levinson**
9:30 Intermission.
9:40 **110.** Innovative technologies packages for kinase drugs with diverse inhibition modes. **L. Neumann**, **D. Witte**, L. Lercher, K. von König, E. Schneider
10:10 **111.** Conformational plasticity and covalent hotspots: New computational tools for assisting targeted kinase inhibitor design. **J. Shen**, C. Tsai, R. Liu

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

MONDAY AFTERNOON – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Membrane Systems & Water Phase

E. Alexov, C. Chang, R. Luo, *Organizers*
A. V. Onufriev, *Presiding*

1:30 **112.** Water facilitated proton transport in biomolecular systems: Remarkably complex and collective phenomenon. **G.A. Voth**
2:00 **113.** How proteins use hydration as a kinetic control knob in coupled ion exchange. **J.M. Swanson**
2:30 **114.** Modeling studies of water interaction with magnesium and calcium ions and inhibitors in selective ion channels. **M.G. Kurnikova**
3:00 Intermission.
3:15 **115.** Ras signaling: PI3K and Raf activation at the membrane. **R. Nussinov**, M. Zhang, H. Jang
3:45 **116.** Preferential solvation of membrane surfaces in the presence of protein crowders. **M. Feig**

SECTION B
Omni San Diego Hotel
Gallery 3A

Women Make COMP

Cosponsored by PROF and WCC
M. C. Nagan, G. Palermo, *Organizers*
K. Armacost, *Organizer, Presiding*

1:30 Panel Discussion.
1:45 **117.** DNA can do it! Catalytic mechanism of the 8-17 DNAzyme. **S. Ekesan**, D.M. York
1:50 **118.** Linking multiscale data analyses, ligand- and structure-based modeling to explore ligand interactions with hepatic organic anion transporting polypeptides. **A. Tuerkova**, S. Jain, U. Norinder, C. Özvegy-Laczka, G. Szakács, B. Zdrazil
1:55 **119.** BioSimSpace: Interoperable molecular software framework. **A. Mey**, L.O. Hedges, C. Woods, J. Michel
2:00 **120.** Excited states of the photosystem II reaction center. **M. Kavanagh**, I.R. Gould, L. Barter
2:05 **121.** Women in science: What can you do to close the gap?. **A. Krylov**
2:20 **122.** Electron transfer in transition metal complexes. **H. Carson**, T. Keane, J.A. Weinstein, A.J. Meijer
2:25 **123.** Linking the ligand modulation of the binding site to the function of HCN ion channels. **F. Tofoleanu**, B. Brooks
2:30 **124.** Structural basis for group 1 influenza fusion inhibition by Arbidol characterized with a cell-scale, ensemble based Markov state model. **S.E. Kochanek**, R.E. Amaro
2:35 **125.** Deriving a modern fixed partial charge set for the nucleic acids using the IPolQ scheme. **E.A. Rosenzweig**, D.S. Cerutti, D.A. Case
2:50 Intermission.
3:05 **126.** On the many roles played by lipids in the activation TRPV1, the noxious heat and capsaicin receptor. **E. Gianti**, A. Yazici, M.A. Kasimova, T. Rohacs, M.L. Klein, V. Carnevale

3:20 **127.** MD in protein design: Investigation of binding determinants for design strategies and screening. **E. Pecora de Barros**, J. Schiffer, A.A. Vorobieva, J. Dou, D. Baker, R.E. Amaro

3:25 **128.** Extending molecular kinetics modeling tools to nonreversible dynamics. **B.E. Husic**

3:30 **129.** Efficient prediction of binding affinity for reversible covalent inhibitors. **H. Zhang**, W. Jiang, P. Chatterjee, P. Edwards, Y.L. Luo

3:35 **130.** Modelling the aggregation-induced emission phenomena: Challenge for computational chemistry. **L. Le Bras**, L. de Thieulloy, C. Adamo, A. Perrier

3:50 **131.** Computational investigation of reaction selectivity in non-heme Fe(II) and alphaketoglutarate dependent halogenase SyrB2. **R. Mehmood**, H. Qi, A.H. Steeves, H.J. Kulik

3:55 **132.** Multi-task modeling of antiviral activity for small organic compounds. **E.A. Sosnina**, S. Sosnin, D.I. Osolodkin, M. Fedorov

4:00 **133.** Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. **Y.M. Huang**, G. Huber, N. Wang, S.D. Minteer, J. McCammon

4:05 **134.** Mechanistic insights into photodecarboxylation of fatty acids from classical and QM/MM simulations. **A. Walker**, T.J. Lane, H. van den Bedem, T.J. Martinez

4:20 **135.** Modeling actinide chemistry with spin-orbit coupled auxiliary field quantum Monte Carlo. **H. Hao**, R. Nanguneri, B. Marston, B.M. Rubenstein

4:25 **136.** Transcription initiation machinery functional dynamics and genetic disease. **C. Yan**, T. Dodd, J.A. Tainer, S.E. Tsutakawa, I.N. Ivanov

4:30 Panel Discussion.

4:45 Discussion.

4:50 Concluding Remarks.

SECTION C
Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
A. Abou Taka, *Presiding*

1:30 **137.** Multicomponent wave function based methods for describing nuclear quantum effects in molecular systems. **F. Pavosevic**, S. Hammes-Schiffer

2:00 **138.** Simulating photoionisation phenomena in DNA/RNA pyrimidine nucleobases. **J. Segarra-Martí**, T. Tran, T.A. Mackenzie, M. Bearpark

2:30 Intermission.

2:45 **139.** MolSSI quantum chemistry archive project. **D. Smith**, L. Naden, D. Altarawy

3:15 **140.** Understanding the vibrational solvatochromism of the ester carbonyl vibration in dilute PCBM solutions. **Y. Yu**, L. Shi

3:45 **141.** Computational NMR characterization of chiral $Au_{25}(SMeBut)_{18}^{0}$. **S. Gelpi Dominguez**, J. Gascon

SECTION D
Omni San Diego Hotel
Gaslamp 2

Advances in Multiscale Modeling

Financially supported by Schrödinger
J. Li, W. G. Noid, *Organizers*
J. Shelley, *Organizer, Presiding*

1:30 **142.** Atomistic and coarse-grained analyses of membrane remodeling by proteins and nanoparticles. **Q. Cui**

2:00 **143.** Simulations at multiple scales reconcile lipid membrane structure with the barrier function of mammalian skin. **G. Fiorin**, C.M. MacDermaid, R. Devane, M.L. Klein

2:30 **144.** Multiscale modeling of mechanochemistry during protein synthesis: Challenges and insights. **E. O'Brien**, C. Deutsch, S. Leininger

3:00 Intermission.

3:15 **145.** Coarse-grained models for liquid-liquid phase separation of intrinsically disordered proteins. **T.L. Head-Gordon**

3:45 **146.** Coarse-grained models of cellular environments to study dynamics and phase behavior. **M. Feig**

4:15 **147.** Multiscale simulations of G-protein coupled receptors. **P. Carloni**

4:45 Concluding Remarks.

SECTION E
Omni San Diego Hotel
Gaslamp 3

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Cosponsored by MEDI
J. Shen, *Organizer*
L. Whitehead, *Organizer, Presiding*

1:15 **148.** What makes a kinase promiscuous for inhibitors?. S. Hanson, G. Georghiou, M.K. Thakur, J. Rest, W.T. Miller, J.D. Chodera, **M. Seeliger**

1:40 **149.** How, when and why do small molecules unbind: Insights from predictive all-atom simulations. **P. Tiwary**

2:05 **150.** Allosteric regulation and reversible covalent drug design for serine/threonine kinase. **Y.L. Luo**, W. Botello-Smith

2:30 Intermission.

2:45 **151.** Targeting the r-spine: Design, synthesis, and biological evaluation of novel type I½ p38α MAP kinase inhibitors with excellent selectivity, high potency, and prolonged target residence time. Implication for cancer- and CNS-applications. **S.A. Laufer**, H.K. Wentsch, N.M. Walter, M. Laemmerhofer, R. Buijsman, D. Rauh, L. Zender

3:10 **152.** Application of ensemble based simulations and machine learning for the prediction of binding free energies and personalized drug selection. S. Wan, **P.V. Coveney**

3:35 **153.** Leveraging synthetically-aware enumeration strategies and free energy simulations in drug discovery campaigns. **J.L. Knight**, K. Konze, P. Bos, S. Bhat, R. Abel, L. Wang

4:00 **154.** Modeling covalent modifiers of kinase proteins. E. Awoonor-Williams, **C.N. Rowley**

4:25 **155.** Connection between protein conformational dynamics and catalysis in protein kinases: Insights from multiscale simulations. **K. Nam**

Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

Metabolomics in Forensics: Applications, Technical Barriers & Emerging Approaches for Chemical Identification Using In Silico Reference Libraries

Sponsored by ANYL, Cosponsored by COMP

MONDAY EVENING – COMP

SECTION A

San Diego Convention Center
TBD

Sci-Mix

H. L. Woodcock, *Organizer*

8:00 - 10:00

156. Water purification with nanoscale turing structures. **R. Chakraborty**

212, **213**, **214**, **215**, **216**, **225**, **229**, **231**, **233**, **238**, **240**, **242**, **247**, **249**, **255**, **260**, **263**, **264**, **271**, **274**, **278**, **281**, **282**, **286**, **294**, **302**, **308**, **309**, **310**, **311**, **312**, **313**, **314**, **315**, **316**, **347**, **348**, **349**, **391**, **392**, **393**, **394**, **403**, **404**, **405**, **406**, **407**, **409**, **410**, **411**.

See Subsequent Listings.

TUESDAY MORNING – COMP

SECTION A

Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Enzyme Mechanisms & pH-Dependence Processes

E. Alexov, C. Chang, R. Luo, *Organizers*
M. Feig, *Presiding*

8:30 **157.** Simulations and force fields with quantum mechanics/molecular mechanics and machine learning. **W. Yang**

9:00 **158.** Importance of modeling water in enzyme function elucidation and protein-ligand scoring function development. **Y. Zhang**

9:30 **159.** Exploring pH- and redox-dependent properties of biomolecules. **A.E. Roitberg**

10:00 Intermission.

10:15 **160.** Role of aqueous pH in modulating biological function. **C.L. Brooks**

10:45 **161.** How ligand protonation state controls water in protein-ligand binding. **J. Shen**, J. Henderson

11:15 **162.** Modeling pKa without solute-water boundary: DelPhiPKa and its applications to protein-protein binding. **S. Pahari**, E. Alexov

SECTION B
Omni San Diego Hotel
Gallery 3A

Drug Design

Novel Methods & Lightning Talks

Y. Tseng, *Organizer*
M. R. Landon, *Organizer, Presiding*

8:30 **163.** Drug discovery by molecular dynamics: Role of the free energy landscape. **S. Leoni**, A. Casini
8:55 **164.** Electrostatic-field and surface-shape similarity for ligand-based drug design. **A.N. Jain**, A.E. Cleves
9:20 **165.** PickR: Pick diverse R-groups for library design using 3D electrostatics and shape. **P. Tosco**, M.D. Mackey, T. Cheeseright
9:45 Intermission.
10:00 Discussion.

SECTION C
Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, N. Mayhall, *Organizers*
H. P. Hratchian, *Organizer, Presiding*

8:30 **166.** Theoretical studies of spectroscopic properties of transition metal complexes. **J. Autschbach**
9:05 **167.** Computational EPR spectroscopy of transition metal complexes with DMRG. **E. Sayfutyarova**, G.K. Chan
9:40 **168.** Magnetic anisotropy in mono- and binuclear complexes: Theoretical insight and prospects. **N. Guihéry**, R. Maurice, B. Cahier, N. Suaud
10:15 Intermission.
10:35 **169.** Towards a uniform black-box framework for computing magnetic properties: Theory and applications to single molecular magnets. **A. Krylov**
11:10 **170.** Diffuse and magnetic Dyson orbitals in the Rydberg anions and solvated-electron precursors of transition-metal chemistry. **J.V. Ortiz**
11:45 **171.** Embedding relativistic 2-component Kohn-Sham density functional theory in a non-relativistic quantum environment. **C. Hoyer**, D. Williams-Young, C. Huang, X. Li

SECTION D
Omni San Diego Hotel
Gaslamp 2

Protein Degradation Computational Design

L. Xiao, *Organizer, Presiding*

8:30 Introductory Remarks.
8:40 **172.** Principles of small molecule mediateed ubiquitin ligase targeting. **E.S. Fischer**
9:10 **173.** Design and optimization of targeted protein degraders: Leveraging computational tools. **Y. Che**
9:40 **174.** Computational modeling of PROTAC-mediated ternary complexes: Applications and insight. **M.L. Drummond**
10:10 Intermission.
10:30 **175.** Development and validation of a computational modeling workflow to characterize the structure of bi-functional degraders-protein-protein ternary complex. **D.R. Weiss**, P. Novick, A.C. Parente, M. Lawrenz, D.W. Robbins, A. Kelly, M.G. Cardozo
11:00 **176.** PROTAC-mediated protein degradation: New therapeutic modality. **G. Burslem**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Recent Advances in Kinase Drug Discovery: A Joint Venture Between Medicinal, Biological & Computational Chemists

Cosponsored by MEDI
L. Whitehead, *Organizer*
J. Shen, *Organizer, Presiding*

8:30 **177.** Exploring chemical space to discover novel BRD4 inhibitors. **C. Lemmen**
9:00 **178.** Is using a 2D drawing application to design for kinase selectivity an oxymoron?. **P. Tosco**, M.D. Mackey, T. Cheeseright, H. Jubb
9:30 **179.** Kinase atlas: Predicted regulatory hot spots in kinases. **S. Vajda**, C. Yueh, D. Kozakov
10:00 Intermission.
10:15 **180.** Multi-target pharmacology of kinase inhibitors, beneficial off-targets and allosteric sites. **R. Abagyan**, I. Kufareva, K. Chahal, D. Shi
10:45 **181.** Rational design of cross-gene family multitarget kinase inhibitors for multi-indication polypharmacology. **L. Xie**
11:15 **182.** Strategies to design conformation-specific kinase inhibitors. **A. Schlessinger**

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Biomolecular Recognition

E. Alexov, C. Chang, R. Luo, *Organizers*
W. Jiang, *Presiding*

1:30 **183.** Long-timescale protein motion coupled solvation dynamics. **W. Yang**
2:00 **184.** Simulation of amyloid formation and propagation. **U. Hansmann**
2:30 **185.** Energy-flow perspective on activated dynamics in biomolecules. **A. Ma**
3:00 Intermission.
3:15 **186.** Why some atomistic simulations are very sensitive to the water model. **A.V. Onufriev**
3:45 **187.** Revealing the essential role of protein-protein interactions in viral capsid assembly. Y. Xian, C. Karki, **L. Li**
4:15 **188.** Effect of water on the entropy of protein-protein binding. **A. Chakravorty**, J. Higham, E. Alexov, R.H. Henchman

SECTION B
Omni San Diego Hotel
Gallery 3A

Drug Design

Novel Methods & Lightning Talks

Y. Tseng, *Organizer*
M. R. Landon, *Organizer, Presiding*

1:30 **189.** MDockPeP2: Predicting protein-peptide complex structures by accounting for peptide flexibility in long peptides. **X. Xu**, X. Zou
1:55 **190.** Dynamic docking to investigate thermodynamics and kinetics of drug-target binding. **A. Cavalli**
2:20 **191.** Design in 2D, model in 3D: Live 3D pose generation from 2D sketches. **P. Tosco**, M.D. Mackey, T. Cheeseright
2:45 **192.** Protein-ligand binding mode prediction from the apo-protein structure using a molecular dynamics-based pocket generation approach. **M. Araki**, Y. Okuno
3:10 Intermission.
3:25 Discussion.

SECTION C
Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, H. P. Hratchian, *Organizers*
N. Mayhall, *Organizer, Presiding*

1:30 **193.** Magnetic properties and hyperfine tensors of $TbPc_2$-type single-molecule magnets. **K. Park**
2:05 **194.** Density-functional perturbation theory for excited states from constrained DFT. **D.A. Strubbe**
2:40 **195.** Calculations of transition metal clusters and complexes using self-interaction corrected energy functional. **H. Jonsson**
3:15 Intermission.
3:35 **196.** Interfacial proton-coupled electron transfer at nanoparticles and electrodes composed of transition metals. **S. Hammes-Schiffer**
4:10 **197.** Computational catalysis on amorphous silicates. **M. Caricato**

SECTION D
Omni San Diego Hotel
Gaslamp 2

Protein Degradation Computational Design

L. Xiao, *Organizer, Presiding*

1:30 Introductory Remarks.
1:35 **198.** New activities for cereblon modulators: Low molecular weight inducers of targeted protein degradation. **P. Chamberlain**
2:05 **199.** Reimagining druggability using chemoproteomic platforms. **D. Nomura**
2:35 **200.** Inhibition and degradation of drug targets using bioPROTAC mRNAs: Novel approach with broad therapeutic potential. **S. Ng**, J. Chang, S. Lim, R. Khoo, P. Gopal, B. Henry, A. Partridge
3:05 Intermission.
3:25 **201.** Targeting the undruggables: Design of highly potent and efficacious STAT3 degraders with absolute selectivity over other STAT proteins. **S. Wang**
3:55 **202.** Targeted protein degradation. **A. Phillips**
4:25 Concluding Remarks.

SECTION E
Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics

J. Shen, *Organizer*
P. Buteler, *Presiding*

1:30 **203.** Tracking the allosteric signaling in CRISPR-Cas9 by leveraging accelerated molecular dynamics, solution NMR and artificial intelligence. **G. Palermo**, V.S. Batista, G.P. Lisi
1:50 **204.** Computational quest of full-length apobec3B. **O. Demir**
2:10 **205.** Mechanical coupling in the nitrogenase complex. **Q. Huang**, L.E. Johnson, B. Ginovska, S. Raugei
2:30 **206.** Temperature-modulated allostery in the IGPS enzyme of a thermophile. **F. Tofoleanu**, U. Morzan, J. Loria, A. Chaudhuri, B. Brooks, V.S. Batista
2:50 **207.** Molecular dynamics study on the stability of G-quadruplexes in the presents of incorporated mono-valent metal ions and small drug molecules. **U. Schnupf**, M. Caterino, A. Cesaro, J. Brady
3:10 Intermission.
3:20 **208.** Dissociation mechanism of processive cellulases explored through molecular simulation. **J.V. Vermaas**, R. Kont, G. Beckham, M.F. Crowley, M. Sandgren, J. Ståhlberg, P. Väljamäe, B. Knott
3:40 **209.** From Markov state models to absolute binding free energies. **B. Xie**, D.D. Minh
4:00 **210.** Binding free energies computed using emerging force fields from the Open Force Field Initiative. **D. Slochower**, N.M. Henriksen, M.K. Gilson
4:20 **211.** Markov models of functional dynamics of histone methyltransferases by millisecond-timescale molecular simulation and chemical probing. **R.P. Wiewiora**, S. Chen, M. Luo, J.D. Chodera

Elucidating Reaction Mechanisms with Computational & Experimental Chemistry

Sponsored by CMA, Cosponsored by COMP and PROF

TUESDAY EVENING – COMP

SECTION A
San Diego Convention Center
TBD

Chemical Computing Group Graduate Student Travel Awards

K. N. Kirschner, C. L. Simmerling, *Organizers*

6:00 - 8:30

212. Unraveling functional hole hopping pathways in the [4Fe4S]-containing DNA primase. **R. Teo**, A. Migliore, D.N. Beratan
213. Development of excited state quantum chemistry methods capable of describing photodissociation of single bonds. **D. Hait**, A. Rettig, M.P. Head-Gordon
214. Multifidelity methods for the design of transition metal complexes. **J.P. Janet**, H.J. Kulik
215. Rapid RNA structure determination through cryo-EM, high-throughput biochemistry, and computational modeling. **K. Kappel**, K. Zhang, Z. Su, G. Pintilie, W. Chiu, R. Das
216. High fidelity ultra-coarse-graining of soft matter systems. **J. Jin**, G.A. Voth

SECTION A
San Diego Convention Center
TBD

COMP Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:30

217. Electron transfer model for reactive force fields. **I. Leven**, T.L. Head-Gordon
218. Bottom-up coarse graining of inhomogeneous environments. **M. DeLyser**, W.G. Noid
219. Capturing the H2–metal interaction in the M-MOF-74 series using classical polarization. **T. Pham**, K. Forrest, B. Space
220. Compound libraries on Chemspace: An approach to chart useful regions in available chemical space. **Y. Moroz**, O. Gavrylenko
221. Crystal-structure prediction via basin-hopping global optimisation employing tiny periodic simulation cells and multipole expansion. **C. Burnham**, P. Samanta, M. Ghaani
222. Degradation of high energy molecules using biological reduction: Rational way to reach bioremediation. **S. Aguero**
223. Building upon a mean field platform for excited state quantum chemistry. **J. Shea**, E. Neuscamman

224. Design and integration of mutual supply network for ethylene feedstock. **Q. Li**
225. Predicting protein degradation through computational modeling of PROTAC-mediated ternary complexes. **M.L. Drummond**
226. Docking study of thymine-dimer containing DNA decamer on translesion DNA polymerase zeta from *Dictyostelium discoideum*. **D. He**, S.K. Mauldin
227. Computational exploration of spectroscopic and electronic properties of various 2,7-disubstitions of 4,10-dihydropyrrolo[3',2':9,10] phenanthro[4,5-*efg*]indole (DPPAI). **B. Wex**
228. Consistent method to calculate diffusion coefficients from molecular dynamics simulation. **D. Yu**
229. Predicting protein-ligand binding affinity with gnina. **P. Francoeur**, D. Koes
230. Classification and analysis of privileged scaffolds in protein families. **O.B. Scott**, A.E. Chan, X. Zhang
231. Assessment and preparation of crystal structures for drug design. **C. Williams**
232. Protocol for the analysis of vibrational circular dichroism spectra of small molecules using Gaussian and MOE. **A. Ajamian**
233. Application of extended Hückel theory to pharmacophore modeling. **A. Ajamian**
234. Computational analysis of the dimer interface of p53 bound to DNA. **T. Qiu**
235. Prediction of fluorescence and absorbance of cytidine analogues using time-dependent density functional theory (TDDFT). **S. Bachori**, A. Cooksy
236. Development of massively parallel software for quantum chemistry calculations: SMASH. **K. Ishimura**
237. New red-emitting phosphor $K_{3-x}Rb_xSiF_7:Mn^{4+}$: DFT study and its synthesis. **S. Jang**, J. Park, C. Kim, H. Chang
238. Molecular dynamics study of the hydrophobic effect in ethanol-water mixtures. **B. Liu**, T. Ichiye
239. Meta-dynamics-based conformational sampling with semi-empirical tight-binding methods. **P. Pracht**, S. Grimme
240. Quantum cluster growth: Explicit approach towards solvation free energies. **S. Spicher**, S. Grimme
241. Geometric approach toward identifying stable parameters for network Hamiltonians governing amyloid fibril formation. **G. Grazioli**, Y. Yu, C.T. Butts
242. Fragment-based *de novo* design targeting FABP5 and nSMase2. **L.E. Prentis**, P. Shanbhogue, Y.A. Hannun, R.C. Rizzo
243. Enhanced sampling of hydration states and binding modes in protein-ligand structures with nonequilibrium candidate Monte Carlo simulations. **M.L. Samways**, H. Bruce Macdonald, J.W. Essex
244. Protein-ligand pose and affinity prediction: Case study on BACE1 cyclic ligand dataset in D3R Grand Challenge 4. **C. Yang**, J. Lu, Y. Yang, Y. Zhang
245. Modelling electric double layers at metal/water interfaces from density functional theory based molecular dynamics. **J. Le**, J. Cheng
246. Conformational analysis and small molecule ligand recognition of the human-specific CHRFAM7A nicotinic receptor implicated in neuropsychiatric disorders. **D. LIU**, J. de Souza Cunha, A. Bronowska
247. Examination of factors affecting the accuracy of quantum chemical frequency calculations for first-row transition metal compounds. **A. Abou Taka**, L.M. Thompson, H.P. Hratchian
248. Effect of chemical functionalization on the thermal transport in the boron nitride nanosheets/polyvinyl alcohol composite. **J. Lu**, R. Sun, C.P. Wong
249. Evaluation of alchemical non-equilibrium free energy calculations. **H. Baumann**, D.L. Mobley
250. DFT study on the relative stabilities of double nitrogen doped graphene systems. **N.F. Alzaaqi**, T. Dinadayalane
251. Cooperativity effects in multivalent systems: Case study. **A.J. Achazi**, L.K. von Krbek, M. Solleder, M. Weber, C.A. Schalley, B. Paulus
252. Dynamics and molecular interactions of ssDNA in nucleic acid biosensors with varied surface properties. **T. Cholko**, S. Kaushik, C. Chang
253. Revealing the optoelectronic properties of non-fullerene acceptors and benzodithiophene based polymer donors: Molecular dynamics simulation approach. **J.K. Roy**, A. Golius, J.R. Leszczynski
254. Intermolecular interactions in human HDAC8 crystal structures and the stability of binding modes of co-crystallized inhibitors. **K. Yelekci**, A.I. Uba
255. LASSOing the atom-typing problem: Statistical method for ligand force field model selection. **J.J. Cherian**, R.T. McGibbon, P. Angelikopoulos, A.G. Taube, J.L. Klepeis, B. Cole, D.E. Shaw
256. How does glycosylation affect small molecule binding on influenza? Roles of electrostatics and sterics examined through Brownian dynamics simulations. **C. Seitz**, L. Casalino, G. Huber, J. McCammon, R.E. Amaro
257. Density functional theoretical study on the C-Cl oxidative addition reaction at POP Rh center. **S. Hwang**

258. Computational insights in generation mechanism of metal-hydrides. **H. Li**

259. Investigating the effects of mutations and post-translational modifications on intrinsic EGFR dynamics using molecular simulations in improved solvation model. **M. Kondal**, A. Ahmad, J. de Souza Cunha, A. Bronowska

260. Next generation of ADMETox dashboard for drug discovery: Learnings and recommendations. **B. Bhhatarai**, G. Gerebtzoff, J. Berghausen

261. Conformational analysis and investigation of energetics of the human AhR PAS-B domain: Impact on druggability. **S. Reznikov**, J. de Souza Cunha, A. Bronowska

262. Explicit solvent effects on the excited state of p-phenylene vinylene. **D.A. Tracy**, A.E. Roitberg

263. Force field complexity assessed via Bayesian inference and reversible jump Monte Carlo sampling. **O. Madin**, R. Messerly, M.R. Shirts

264. Targeting glioblastoma cancer stem cell derived neurospheres: From phenotypic screen to target identification. **S. Bahmanyar**, D.S. Mortensen, V. Plantevin-Krenitsky, b. whitefield, E. Torres, V.H. Grant, J. Parnes, J. Brazeau, J. Young, K. Leftheris, S.E. Swift, B. Gaffney, D. Zhu, D. Mikolon, G. Deyanat-Yazdi, L. Wong, T. Tran, J. Boylan, A. Wurmser

265. D3R Grand Challenge 4: Pose prediction and affinity ranking for BACE-1 inhibitors using ligand similarity and MM-GBSA calculations. **L. El Khoury**, S. Sasmal, D.L. Mobley

266. Data analysis of various homo-peptide repeats in proteins associated with degenerative diseases. **Q. Price**, D. Tandabany

267. Effects of electrostatic fields on the stability and reactivity of iron-sulfur clusters. **S. Gaughan**, J.D. Hirst, A. Croft, C.M. Jaeger

268. How does prenylated flavin mononucleotide biosynthesis occur? Computational study. **S. Zaczek**, A. Dybala-Defratyka

269. Band-gap opening and optical properties of graphene binding with low-concentration fluorine. **Y. Duan**, B. Chorpening, C. Stinespring

270. Influenza virus glycosylation: Impact on virulence and transmissibility revealed by all-atom mesoscale simulations. **L. Casalino**, C. Seitz, M.O. Altman, I.A. Wilson, R.E. Amaro

271. D3R Grand Challenge 4: Blind prediction of protein-ligand poses and affinity predictions. **Z. Gaieb**, C. Parks, M. Chiu, H. Yang, C. Shao, P. Walters, R.A. Lewis, S.D. Bembenek, S.K. Burley, R.E. Amaro, M.K. Gilson

272. Controlling emission energies in functionalized carbon nanotubes. **B.J. Gifford**, S.K. Doorn, S. Tretiak

273. Modeling coordinated conformational changes and interaction networks in alpha subunit of tryptophan synthase. **Y. Bosken**, D.D. Boehr, C. Chang

274. MB-nrg doesn't work by accident!. **C. Egan**, B. Bizzarro, M. Riera, F. Paesani

275. Computational predictions of drug binding kinetics with a multiscale molecular dynamics, Brownian dynamics, and milestoning approach. **B.R. Jagger**, C.T. Lee, R.E. Amaro

276. viewSq: VMD module for visualizing and quantifying periodic atomic ordering underlying static structure factors from molecular dynamics simulations. **T. Mackoy**, B. Kale, M.E. Papka, R.A. Wheeler

277. Structure-property relationship of high-spin state donor-acceptor (DA) polymers: Computational study. **M. Sabuj**, O. Muoh, N. Rai

278. Improving force fields by identifying and characterizing small molecules with parameter inconsistencies. **J. Ehrman**, V.T. Lim, C.C. Bannan, N. Thi, D. Kyu, D.L. Mobley

279. Multi-state QM/QM extrapolation of UV/Vis absorption spectra with point charge embedding. **K. Zhang**, S. Ren, M. Caricato

280. Modeling crystallization pathways of polymorphic materials: Enhanced sampling techniques and method development. **T.D. Janicki**, J.R. Schmidt

281. Curious case of DMSO: A computational study. **L. Olive** , E.V. Dornshuld, C.E. Webster

282. Virtual screening and *de novo* drug design with machine learning. **C. Parks**, Z. Gaieb, R.E. Amaro

283. Identification and characterization of small molecule inhibitors of Zika virus glycoprotein E. **S. Telehany**, M. Humby, D. McGee, A. Jacobs, R.C. Rizzo

284. Connecting wave function and ensemble DFT methods through inversion of model systems. **V. Martinetto**, A. Pribram-Jones

285. Efficient fitting of a density function theory energy curve using active learning. **T. Loeffler**, H. Chan, S. Sankaranarayanan

286. Optimizing Lennard-Jones parameters by coupling nano- and macroscale target data using user-guided numerical algorithms. **R. Strickstrock**, M. Huelsmann, D. Reith, K.N. Kirschner

287. Withdrawn

288. Mechanisms for the transduction of light and chemical energy into molecular motion. **M. Feng**, M.K. Gilson

289. Probing binding modes of dye molecules on semiconductor surface and their dynamics. **M. Huda**, N. Rai

290. Computational investigations on the structure-function relationship of rubisco activase from tobacco. **P. Khakbaz**, D. Shukla
291. Thermal adiabatic connection for the uniform gas. **B. Harding**, A. Pribram-Jones
292. Waterkit: Fast method for estimating receptor desolvation free energy. **J. Eberhardt**, S. Forli
293. Comparing the stability of the sarcin/ricin domain and A-form RNA using adaptively biased molecular dynamics. **J.M. Imamoto**, M.F. Bruist
294. Effects of spin contamination on the potential energy surfaces of water splitting catalysis by tungsten-oxide clusters. **A. Zamani**, H.P. Hratchian
295. Reduced RAM access algorithm for molecular orbital electron repulsion integrals with resolution of the identity applied in post Hartree-Fock methods. **J. Lew Yee**, R. Flores Moreno, J. Martín del Campo Ramírez
296. Calculating 1-octanol/water and hexadecane/water partition coefficients for small molecules. **S. Sasmal**, A. Nguyen, D.L. Mobley
297. Molecular insights into the activity and structural impacts of enzymes across the changing pH environment in marine aerosol particles. **N.A. Wauer**, A. Dommer, R.E. Amaro
298. Effects of the crystal packing of homo-halogenated benzenes on their electronic properties. **K. Pearce**, B. Schatschneider
299. Fitting improper torsion parameters for atomistic force fields. **J. Maat**, C.C. Bannan, V.T. Lim, D.L. Mobley, B. Tjanaka, L. Wang, C.I. Bayly
300. Intrinsic conductivity and small polaron formation in normal spinel ZnFe2O4 from first-principles. **R. Leano**, T. Smart, Y. Ping
301. Computational models for activated human MEK1: Identification of key active site residues and interactions. **K.R. Sabsay**, R.T. Lee, L.M. Ravatt, J.P. Oza, A. Ringer McDonald
302. Towards improved accuracy in calculation of binding thermodynamics. **S. Kantonen**, H. Muddana, M.K. Gilson
303. New integrator framework for GROMACS. **P.T. Merz**, M.J. Abraham, M.R. Shirts
304. Determining the effect of hydration shell on the spectra of proteolysis targeting chimera MD-224 by efficiently sampling conformations using the effective stochastic potential method. **J. Scher**, A. Chakraborty
305. Characterization of active site and distal residues in the human ornithine transcarbamylase. **S. Watson**, P.J. Beuning, M. Ondrechen
306. Mechanistic study of isotactic propylene oxide polymerization by a flexible bimetallic Cr(III) catalyst. **A.K. Roessler**
307. Assessment for the inclusion of liquid-phase chemistry in automatic kinetic model generation. K. De Ras, **R. Van de Vijver**, F.H. Vermeire, G.B. Marin, K. Van Geem
308. Withdrawn
309. Many-body effect in the selectivity of calcium-binding proteins. **Z. Jing**, P. Ren
310. Withdrawn
311. Computational design of foldamer based water channels. **S. Houshyar Azar**, V. Pophristic, Z. Liu
312. Natural transition orbitals for complex 2-component TDDFT. **J.M. Kasper**, X. Li
313. Excited state calculations using multiconfiguration pair-density functional theory: Successes and challenges. **P. Sharma**, V. Bernales, D.G. Truhlar, L. Gagliardi
314. Multiconfigurational pair-density functional theory: Strong-correlation method in quantum chemist's toolbox. **M. Mostafanejad**, A.E. DePrince
315. Deciphering biomolecular corona formation on coated nanoparticles through all-atom molecular dynamics and dissipative particle dynamics simulations. **G. Chong**, M. Wu, I.U. Foreman-Ortiz, C. Allen, E. Tollefson, E.E. Carlson, J.A. Pedersen, C.J. Murphy, R. Hernandez
316. Using coarse-graining and maximum entropy method to study Aβ aggregation. **D.B. Amirkulova**
317. Building accurate and fast implicit solvation models. **I.S. Tolokh**, A. Mukhopadhyay, A.V. Onufriev
318. Towards predictive chromatography: Computationally directed separations for efficient drug design and production. **L.D. Bishop**, N. Moringo, A. Misiura, C.F. Landes
319. SkeleDock: New scaffold docking based algorithm. **A. Varela Rial**, G. De Fabritiis
320. LigVoxel: Inpainting binding pockets using 3D-convolutional neural networks. **A. Varela Rial**, G. De Fabritiis
321. Reactive docking: HTVS of covalent binders for *in silico* proteomics. **S. Forli**, G. Bianco, K.M. Backus
322. Drug design using virtual reality: Free energy calculation of pathways generated from interactive molecular dynamics. **S.R. Hare**, D.R. Glowacki, B.K. Carpenter
323. Exploration of the potential of mean force (PMF) method applied to the study of protein:ligand binding using the movable type method. **L. Westerhoff**, Z. Zheng, K.M. Merz
324. Predicting plasticity of ligand-unbinding transition states for a library of minutes-scale k_d inhibitors. **S.D. Lotz**
325. Non-covalent interactions in carbonyl complexes of Mn: Theoretical QTAIM study. **J.F. Van Der Maelen**, J. Ruiz

326. Withdrawn
327. Mechanism of spin-dependent electron transfer on ferromagnetic interfaces: *Ab initio* study. **S. Ghan**, K.U. Reuter, H. Oberhofer
328. Electronic structure of metal-organic frameworks. **R. Chakraborty**, J.R. Long, M.P. Head-Gordon
329. Spin-flip EOM-CCSD investigation of g-tensors in spin-frustrated systems. **S. Kaehler**, A. Krylov
330. Beyond property prediction: What can machine learning do for virtual screening of transition metal complex space?. **J.P. Janet**, C. Duan, A. Nandy, H.J. Kulik
331. Quantum mechanical studies of the depolymerization of lignin by the $ZnCl_2$: Ethylene glycol deep eutectic solvent (DES). **A. Landera**, A. George, L. Das, J. Gladden
332. Automated generation of metal-doped amorphous silica clusters. **A. Jystad**, P.N. Wimalasiri, W.H. Thompson, M. Caricato
333. Streamlining the exploration of chemical space for aqueous molecular metal oxides as thin film precursors. **A.J. Achazi**, P. Miro
334. Exploring magnetic responses of transition metal complexes. **S. Sun**, X. Li
335. Strong correlation in transition metals with adaptive sampling configuration interactions. A. Aldossary, **R. Chakraborty**, N. Tubman, D. Hait, M.P. Head-Gordon
336. Multiconfigurational calculations on bimetallic decorated NU-1000 for C–H activation and comparison with DFT. **C. Gaggioli**, J. Sauer, L. Gagliardi
337. Spin-flip Bethe–Salpeter equation approach and applications to simple molecular systems. **B.A. Barker**, D.A. Strubbe
338. Computational study of the reactivity and stability of dinuclear heterogeneous catalysts on metal oxide supports. **K. Yang**, V.S. Batista
339. Computational investigation of domain registration of membrane rafts. **P.B. Moore**, N. Chen
340. Mechanistic elucidation of transition metal-catalyzed bond activations by quantum chemical simulation. **X. Hong**
341. Chemical activation and allosteric modulation of mechanosensitive Piezo1 channel. **Y.L. Luo**
342. Advancing nonadiabatic molecular dynamics methods and software for condensed matter and nanoscale systems. **A.V. Akimov**
343. Clean and simple wave function interpretation with intrinsic bond orbitals: From [F-H-F]– to proton coupled electron transfer in enzymes. **G. Knizia**
344. On the role of noncovalent interactions in the initial aggregation of dipeptide-based nanostructures. **M.L. Mayes**, L. Perreault, B. Visayas
345. Absolute binding free energies from binding free energies to multiple rigid receptor conformations. **D.D. Minh**
346. Withdrawn
347. Enhanced sampling methods to resolve thermodynamics and kinetics of slow and rare biophysical processes. **H. Vashisth**
348. Identifying metrics governing the non-native structure evolution in ionic liquid-ionic liquid mixtures from molecular simulations. **J. Shah**, U. Kapoor
349. Modeling electron detachment in metal oxide and metal boride clusters. **H.P. Hratchian**
350. Combinatorial reaction searches on the PES using KinBot. **R. Van de Vijver**, J. Zádor, G.B. Marin, K. Van Geem
351. Modelling nonelectrostatic solute-solvent interactions in continuum embedding. C. Hille, S. Ringe, **J. Filser**, M. Deimel, C. Kunkel, W.E. Acree, K.U. Reuter, H. Oberhofer
352. Excitation energies from linear response theories with localized orbitals scaling correction in density functional theory. **J. Li**, N. Su, Y. Jin, W. Yang
353. Application of computational reaction modeling to the development of pharmaceuticals. **C. Lam**
354. How to fix CO_2 with four amino acids: Enoyl-CoA carboxylase/reducase QM/MM study. **E. Vohringer-Martinez**, D. Saez
355. Understanding the nature of weak interactions between functionalized boranes and N_2/O_2, promising functional groups for gas separations. **J. Townsend**, K.D. Vogiatzis
356. Efficient and accurate estimation of free energy profiles for Kemp elimination reactions. **X. Pan**, Y. Mei, Y. Shao
357. Theoretical design and analysis of high-spin state donor-acceptor (DA) polymers. **M. Sabuj**, M. Huda, N. Rai
358. Towards density functional approximations from coupled cluster correlation energy densities. J. Margraf, **C. Kunkel**, K.U. Reuter
359. Withdrawn
360. Performance of Dunning, Jensen, and Karlsruhe basis sets on computing relative energies and geometries of mimima and transitions states. **K.N. Kirschner**, D. Reith, W. Heiden
361. Impurities limit the capacitance of carbon-based supercapacitors. **T.T. Duignan**, X. Zhao
362. *In silico* prediction of O^6-methylguanine-

DNA methyltransferase inhibitory potency of base analogs with QSAR and machine learning methods. **S. Guohui**, T. Fan, X. Sun, Y. Hao, X. Cui, L. Zhao, T. Ren, Y. Zhou, R. Zhong, Y. Peng

363. Scaling up quantum chemistry simulation: Error control and automation. **F. Liu**, H.J. Kulik

364. Modeling the interaction between EG_6 coated gold nanoparticles and cytochrome *c*. **C.A. Daly**, C.R. Allen, N. Rozanov, G. Chong, J.A. Pedersen, C.L. Haynes, E.E. Carlson, R. Hernandez

365. Exploring large combinatorial chemical spaces to accelerate drug discovery with multisite λ-dynamics. **J.Z. Vilseck**, R. Hayes, N. Sohail, K. Armacost, C.L. Brooks

366. Improvement of the GEM polarizable water model: Importance of the dispersion energy. **S. Naseem Khan**, G.A. Cisneros

367. Design principles for gas activation, storage, and transport in metal organic frameworks. **R. Chakraborty**, J.R. Long, M.P. Head-Gordon

368. Withdrawn

369. Computational structure prediction of arylamide foldamer helices encapsulating monosaccharides. **S. Makeneni**, Z. Liu, V. Pophristic

370. Computational study of water oxidation on metal oxide surfaces and its implication for efficient solar fuel production. **K. Yang**, V.S. Batista

371. Withdrawn

372. Investigating the role of linkers in the conformation of triazine-based sequence-defined polymers. **S. Ahn**, J.W. Grate

373. Quantum calculations of reactions on interstellar ice-covered surfaces. **A. Lamberts**

374. Improvements in symmetry-adapted perturbation theory (SAPT): Accurate separation of polarization and charge transfer terms. **S. Naseem Khan**, N. Gresh, A.J. Misquitta, J.A. Piquemal

375. Methane activation by an iron atom supported on graphene. **C. Wu**, I.D. Gates

376. Secret dance in Parkinson's disease: *In situ* structure determination of a pathological mutant of LRRK2 bound to microtubules. **M. Audagnotto**, K. Lasker, R. Watanabe Castillon, R.E. Amaro, R. Buschauer, J. Bohning, D. Boassa, S.S. Taylor, E. Villa

377. Using domain-aware machine learning to forecast aqueous iodine reactions. **J. Bilbrey**, C. Ortiz Marrero, M. Schram, R. Rallo

378. Modeling the effects of protein mutations towards target specificity in CRISPR/Cas9-based genome editing. **A. Ray**, R. Di Felice

379. Absolute binding free energy predictions for heat shock protein 90 (Hsp90) complexes. **L. El Khoury**, J. Hariyanto, D.L. Mobley

380. Parameterization of lamotrigine using quantum mechanical calculations. **S. Darancou**, S.T. Shipman

381. On the origin of circularly-polarized luminescence from achiral polymers. **B. Laidlaw**, T. Penfold

382. Withdrawn

383. Sampling binding modes of flexible ligands using nonequilibrium candidate Monte Carlo. **S. Sasmal**, D.L. Mobley

384. Pressure and temperature effects in *Escherichia coli* and *Moritella profunda* dihydrofolate reductase. **Q. Huang**, J.M. Rodgers, R.J. Hemley, T. Ichiye

385. From structure to molecular flux: Predicting compound permeability in Gram-negative bacteria. **S. Acosta-Gutierrez**

386. Protracted colored noise dynamics in polymer simulation. A. Peters, B. Nation, C. Henderson, **P.J. Ludovice**

387. Probing the early stage of aggregation of low molecular weight gelator (12-hydroxyoctadecanamide) in organic solvents. **M. Huda**, N. Rai

388. Molecular dynamics simulations reveal the mechanism of agonist ligand binding to ERRα. **L. Hegazy**

389. Highly efficient conformational sampling of *in vivo* SERCA activator CDN1163 for determination of thermal and solvent effects on its excited state properties. **J. Scher**, A. Chakraborty

390. Divergent ligand binding mechanisms in *Arabidopsis thaliana* and *Striga hermonthica* strigolactone receptors. **J. Chen**, D. Shukla

391. Microphysical climate-relevant properties of model marine aerosols surfaces explored with GPU-accelerated all-atom molecular dynamics. **A. Dommer**, R.E. Amaro

392. Exploring sequence-to-sequence learning methods for end-to-end, complete protein structure prediction. **J. King**, P. Francoeur, D. Koes

393. Rational engineering of CRISPR-based genome editors using computational methods. **K. Rallapalli**, F. Paesani

394. Molecular basis of glucose transport in plants. **B. Selvam**, D. Shukla

395. Characterizing the structural and chemical features of biological short hydrogen bonds. S. Zhou, **L. Wang**

396. Molecules mimicking atoms: Case of solvated electron precursors. I. Ariyarathna, N. Khan, N. Almeida, **E. Miliordos**

397. Embedded cluster density approximation for exchange-correlation energy. **C. Huang**

398. Evidence for nitrogen-fluorine halogen

bonding in silver-initiated fluorination reactions. **S. Bidwell**, A.M. Hua, S. Baker, R. Baxter, H.P. Hratchian

399. Using computational chemistry to understand genomes. C.L. Mills, L.A. Ruffner, P.J. Beuning, **M.J. Ondrechen**

400. Improving precision in absolute binding free energy calculations by increasing the number of alchemical intermediates. **B. Xie**, D.D. Minh

401. Assessing the conformational equilibrium of carboxylic acid via quantum mechanical and molecular dynamics studies on acetic acid. **V.T. Lim**, C.I. Bayly, L. Fusti-Molnar, D.L. Mobley

402. Rapid evaluation of protein hydration layer dynamics using hydration shell structure. **J.N. Dahanayake**, E. Shahryari, K.M. Roberts, M.E. Heikes, C. Kasireddy, K.R. Mitchell-Koch

SECTION A
San Diego Convention Center
TBD

NVIDIA GPU Award

M. E. Berger, C. L. Simmerling, *Organizers*

6:00 - 8:30

403. Efficient implementation of flexible integral-based Generalized Born implicit solvent model. **Y. Wang**, C.L. Brooks

404. GPU-accelerated constant pH and redox potential molecular dynamics: Exploring electrochemistry in AMBER. **V.D. Cruzeiro**, A.E. Roitberg

405. Revealing ALK-drug resistance mechanisms using GPU-driven molecular dynamics sampling. **Z. Zhao**, P. Bourne

406. Accelerating MM/PBSA calculation of protein-ligand binding on graphics processing units. **R. Qi**, A. Luo, H. Wei, R. Luo

407. Improving REMD efficiency with Monte Carlo moves using a structure reservoir. **K. Kasavajhala**, K. Lam, C.L. Simmerling

SECTION A
San Diego Convention Center
TBD

OpenEye Outstanding Junior Faculty Award

C. L. Simmerling, *Organizer*

6:00 - 8:30

408. Hierarchical simulation: Two different approaches and their applications to design complex biomaterials. X. Zhao, J. Ferrell, C. Liao, **J. Li**

409. Computational modeling of polariton chemistry. **J. Yuen Zhou**

410. Exploring graphene oxide-water interfaces: Computational investigation. **R. Kumar**

411. Wepy: Tool for exploring rough free energy landscapes. S.D. Lotz, N. Donyapour, N. Roussey, T. Dixon, **A. Dickson**

SECTION A
San Diego Convention Center
TBD

Wiley Computers in Chemistry Outstanding Postdoc Award

M. Cavalleri, C. L. Simmerling, *Organizers*

6:00 - 8:30

412. Photochemistry of conjugated systems with "black-box" multireference methods. **E. Sayfutyarova**, S. Hammes-Schiffer

WEDNESDAY MORNING – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Role of Water Phase in Molecular Biology: Importance of Water in Folding, Binding & Transport Phenomena

Biomolecular Recognition

E. Alexov, C. Chang, R. Luo, *Organizers*
A. Ma, *Presiding*

8:30 **413.** Can Google's Alphafold discover new drugs?. **G. Wei**

9:00 **414.** Predicting direct and water-mediated interactions in protein-protein complexes. **X. Zou**

9:30 **415.** Accelerating convergence of free energy computations with Hamiltonian simulated annealing of water. **W. Jiang**

10:00 Intermission.

10:15 **416.** Regulating protein-protein interactions by phosphorylation: New mechanism involving solvated electrostatic interactions. **C.B. Post**, D.P. Hua, C. Feng

10:45 **417.** Predicting metal ion dehydration in RNA structures. **S. Chen**

11:15 **418.** Roles of water molecules and shapes of compounds and DNA sequences in the design and analysis of sequence-specific minor groove complexes. **W. Wilson**, A. Paul, N. Harika, P. Guo, A. Kumar, D.W. Boykin

SECTION B
Omni San Diego Hotel
Gallery 3A

Drug Design

Free Energy Methods

M. R. Landon, Y. Tseng, *Organizers*
V. D. Cruzeiro, *Presiding*

8:30 **419.** No one-size-fits-all: Evaluation of free energy methods for drug discovery campaigns. **K. Armacost**, X. Yan, Z. Guo, E. Metwally, H. Gunaydin, B. Sherborne

8:55 **420.** Rigorous free energy perturbation approach to estimating relative binding affinities between ligands with multiple protonation and tautomeric states. **C. de Oliveira**, H. Yu, W. Chen, R. Abel, L. Wang

9:20 **421.** Assessing the role and impact of force field and charge model selection on free energy calculations using the movable type (MT) method. **O. Borbulevych**, Z. Zheng, L. Westerhoff

9:45 **422.** Computational design of a binding mode flip for the validation of a novel class of potent tri-vector cyclophilin inhibitors. A. De Simone, C. Georgiou, H. Ioannidis, A. Gupta, J. Juarez-Jimenez, D. Doughty-Shenton, E.A. Blackburn, M. Wear, J.P. Richards, P. Barlow, N. Carragher, M. Walkinshaw, A. Hulme, **J. Michel**

10:10 Intermission.

10:25 **423.** Exploring protein–ligand interactions using multilayer molecules-in-molecules (MIM) fragmentation-based approach. B. Thapa, **K. Raghavachari**

10:50 **424.** Free energy calculations with thermodynamic integration in MOE using AMBER. **M. Ebert**

11:15 **425.** Exploring combinatorial chemical spaces with a discrete-Gibbs sampler-based -dynamics approach. **J.Z. Vilseck**, X. Ding, R. Hayes, C.L. Brooks

11:40 **426.** Development and validation of a relative Free Energy Perturbation (FEP) workflow. **P. Raman**

SECTION C
Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, N. Mayhall, *Organizers*
H. P. Hratchian, *Organizer, Presiding*

8:30 **427.** Addressing limitations of density functional theory for transition metal chemistry. **S. Mallikarjun Sharada**

9:05 **428.** Transition metal catalysts with complex electronic properties. **P.M. Zimmerman**

9:40 **429.** Automated generation of benchmark sets guided by a Bayesian decision maker. **C.J. Stein**, J. Proppe, T. Gaudin, R.J. Hickman, M.P. Head-Gordon, A. Aspuru-Guzik

10:05 Intermission.

10:25 **430.** Automated selectivity predictions for transition metal catalyzed reactions. **S.E. Wheeler**, V.M. Ingman, A.J. Schaefer

11:00 **431.** *In-situ* automated analysis and control of transition metal chemistry simulation. **F. Liu**, C. Duan, H.J. Kulik

11:35 **432.** Effect of localized states on exciton transfer in colloidal quantum dots. **T.G. Goldzak**, A.R. McIsaac, T.A. Van Voorhis

SECTION D
Omni San Diego Hotel
Gaslamp 2

Molecular Mechanics

J. Shen, *Organizer*
E. Pecora de Barros, *Presiding*

8:30 **433.** Importance of data selection for machine learning-based atomistic potentials. **J.S. Smith**, B.T. Nebgen, N. Lubbers, S. Tretiak, K. Barros

9:00 **434.** Machine learning coarse-grained model for water. **H. Chan**, M. Cherukara, B. Narayanan, T. Loeffler, C. Benmore, S.K. Gray, S. Sankaranarayanan

9:20 **435.** Dynamic modes of ignition phenomena: Learning chemistry from data. **C. Brown**, R. Mohr, M. Alaghemandi, J. Green, I. Mezic

9:40 **436.** Topological coarse-graining: Building ultra efficient computer models of aggregation using network Hamiltonians. **G. Grazioli**, Y. Yu, M. Unhelkar, R.W. Martin, C.T. Butts

10:00 **437.** Automated protein coarse-grained force field optimisation using free energy simulations. **J. Caceres-Delpiano**, L. Wang, J.W. Essex

10:15 Intermission.

10:25 **438.** NAMD 2.13 and beyond: New features, larger systems, and faster GPU simulations. **J. Maia**, D. Hardy, B. Radak, J. Ribeiro, J. Stone, E. Tajkhorshid

10:45 **439.** Knowledge-based statistical scoring function for protein-DNA interactions with enhanced generalization for structural variation. **L. Qiu**

11:05 **440.** Rapid graph-based determination of mechanical coupling in proteins. **L.E. Johnson**, Q. Huang, B. Ginovska, A. Fenton, S. Raugei

11:25 **441.** Physical validity in molecular simulations. **P.T. Merz**, M.R. Shirts

11:45 **442.** Benchmarking quantum chemistry methods for accurate fixed-charge electrostatic models. A. Zhou, M. Schauperl, L. Wang, **P.S. Nerenberg**

12:05 **443.** Accessible molecular modeling environment with VMD and NAMD. **J. Ribeiro**, E. Tajkhorshid

SECTION E
Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics: Molecular Simulations for Materials Design

C. M. Aikens, J. Shen, *Organizers*
S. J. Dampf, *Presiding*

8:30 **444.** From quantum to continuum: Multi-scale modelling of nanocomposites. **P.V. Coveney**

9:00 **445.** Charge transport networks in amorphous organic semiconductors. **M. Matta**, R.J. Gowers, C.T. Chapman, G.C. Schatz

9:20 **446.** Solid-state electrolytes: Li-metal interfaces. **J.M. Seminario**, D.E. Galvez-Aranda

9:40 **447.** Metashooting: Tool for Investigating mechanisms of material conversion. **S. Leoni**

10:00 Intermission.

10:20 **448.** Advances in atomistic methods for materials chemistry. **S.B. Sinnott**

10:50 **449.** Withdrawn

11:10 **450.** Modeling variations in the composition of ionic liquid-solvent mixtures confined inside nanopores. **A. Fang**, A. Smolyanitsky

11:30 **451.** Molecular modeling of ionic liquid-based electrolytes. S. Schweizer, **D. Firaha**, M. Neumann, J. Hill

11:50 **452.** Influence of electronic polarization on the structure of ionic liquids. **J.G. McDaniel**

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

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Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

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WEDNESDAY AFTERNOON – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Computational Studies of Water

T. P. Kurtzman, D. J. Sindhikara, *Organizers*
K. M. Hunter, *Presiding*

1:30 **453.** Empirical models of water at interfaces and around solutes. **T. Ichiye**

2:00 **454.** Role of the hydrogen bond network on the anomalies of water. **F. Martelli**

2:25 **455.** Role of entropy in connecting protein solvent shell structure and hydration dynamics. **J.N. Dahanayake**, K.R. Mitchell-Koch

2:45 **456.** Understanding the structure and dynamics of water confined inside metal-organic frameworks. **K.M. Hunter**, F. Paesani

3:00 **457.** Structural and thermodynamic information content of the three-body angle distribution of liquid water. **J. Monroe**, M. Shell

3:15 Intermission.

3:30 **458.** Polarizability, infrared, and Raman spectra of water from first-principles simulations using the SCAN exchange-correlation functional. M. LaCount, **F. Gygi**

4:00 **459.** Useful relationships between localized vibrational modes and anharmonic entropy. **S. Lu**, P.M. Zimmerman

4:20 **460.** Proton transport through carbon nanotubes: Multi-level quantum mechanics/molecular mechanics simulations with NAMD. **M. Spivak**, N. Aluru, E. Tajkhorshid

4:35 **461.** Solvation free energy calculations with quantum mechanics/molecular mechanics and machine learning models. **P. Zhang**, L. Shen, W. Yang

SECTION B
Omni San Diego Hotel
Gallery 3A

Drug Design

Applications of Machine Learning

M. R. Landon, Y. Tseng, *Organizers*
S. Lenka, *Presiding*

1:30 **462.** Mathematical deep learning for drug discovery. **G. Wei**

1:55 **463.** Combining structure-based convolutional neural networks and ligand-based methods to address kinase selectivity. **A. Rossi**, J. Sorenson, I. Wallach

2:20 **464.** High-throughput drug design and lead optimization with PlayMolecule. **F. Chevalier**, G. De Fabritiis

2:45 Intermission.

3:00 **465.** Systematic target deconvolution: Are we there yet?. **G. Zahoranszky-Kohalmi**, R. Guha, M.G. Cyr, C. Danchik, S. Fang, M. Henderson, A. Zakharov

3:25 **466.** Leveraging machine learning and the Free-Wilson approach in lead optimization: Efficient discovery of a new chemical class modulating the $GABA_A$ α_5 receptor. **O. Hucke**, M. Bieler, J. Larsen, T. Dyhring, T.A. Jacobsen, K.S. Nielsen, H. Schauerte, Y. Cui, S. Peters, N. Heine, C. Eickmeier, R. Arban, F. Montel

3:50 **467.** Developing Kernel, a virtual assistant for medicinal chemistry discovery teams at Eli Lilly. **M.P. Baumgartner**, L. Vidler

SECTION C
Omni San Diego Hotel
Gaslamp 1

Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry

C. M. Aikens, H. P. Hratchian, *Organizers*
N. Mayhall, *Organizer, Presiding*

1:30 **468.** Computational studies of the properties of transition metal and metal oxide clusters. **D.A. Dixon**

2:05 **469.** Accurate models of reaction mechanisms to understand activity and selectivity of catalytic organometallic complexes. R.C. Chapleski, S.B. Isbill, **S. Roy**

2:40 **470.** Combined methodological approach for configuration interaction of orthogonal and non-orthogonal SCF solutions. **A.D. Mahler**, L.M. Thompson

3:05 Intermission.

3:25 **471.** Quantum chemistry of strongly correlated transition metal systems with the Adaptive Sampling Configuration Interaction Self Consistent Field (ASCI-SCF) method. **D. Hait**, D.S. Levine, N. Tubman, K.B. Whaley, M.P. Head-Gordon

3:50 **472.** CASPT2 molecular geometries and electronic structures of transition metal complexes. **B. Vlaisavljevich**

4:25 **473.** When should we use relativistic methods for transition metals?. **X. Li**

SECTION D
Omni San Diego Hotel
Gaslamp 2

Material Science

Light-Matter Interaction in Materials: MOFs & Separations

C. M. Aikens, *Organizer*
H. Carson, *Presiding*

1:30 **474.** Design of new thermally activated delayed fluorescence materials for oled applications. R. Ozek, **V. Aviyente**, S. Catak, A. Monari

1:50 **475.** Theoretical insights into the mechanisms of aggregation-induced emission and photo/thermal *E/Z* isomerization of a cyanostilbene derivative. **N. Yamamoto**

2:10 **476.** Finding the right building blocks for molecular optimization: Mining a database of organic semiconductors. **C. Kunkel**, C. Schober, J.T. Margraf, K.U. Reuter, H. Oberhofer

2:30 **477.** Unlocking the electronic genome of functionalized polycyclic aromatic hydrocarbon molecules and crystals. C. Mora, S. Jezowski, K. Pearce, C. Pacheco, A. Cosley, H. Oberhofer, **C.U. Pomona**

2:50 **478.** Charge transfer in metal/organic semiconductor interfaces from quantum chemical calculations. **O. Ozcelik**, F. Paesani

3:10 **479.** Chemistry of remotely separated species hybridized by strong light-matter coupling. **M. Du**, R. Florentino Ribeiro, L.A. Martínez-Martínez, Z. Hu, V.M. Menon, J. Yuen-Zhou

3:30 Intermission.

3:50 **480.** DFT+U within a numeric atom centered orbital framework and its intricacies. **M. Kick**, K.U. Reuter, H. Oberhofer

4:10 **481.** Metal-organic frameworks: From database to supramolecular effects in complexation. **A. Mitrofanov**, V. Korolev, E. Marchenko, N. Eremin, N. Andreadi, P. Matveev, N. Borisova, A. Eliseev, V. Tkachenko

4:30 **482.** Towards computational materials design of metal-organic framework semiconductors. **C.J. Muschielok**, H. Oberhofer

4:50 **483.** Efficient simulation of aerosol filtration. **D.R. Rottach**, Z. Lei

5:10 **484.** Computational modeling of mixing solids as high-performance CO_2 sorbents for capture technology. **Y. Duan**

SECTION E
Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics: Conformational Dynamics of Receptors, Ion Channels & Transporters

J. Shen, *Organizer*
K. H. Burley, *Presiding*

1:30 **485.** Understanding the early stages of rhodopsin activation by combining simulations and experiments. L. Salas Estrada, **A. Grossfield**
2:00 **486.** What molecular dynamics simulations tell us about GPCRs. T.R. Clark, **P. Ibrahim**
2:20 **487.** Allosteric transport in ion channels and receptors. S. Milenkovic, I. Bodrenko, **M. Ceccarelli**
2:40 **488.** Understanding conformational plasticity in GPCR selective pathway activation. **S. Acosta-Gutierrez**, F.L. Gervasio
3:00 Intermission.
3:10 **489.** Inactive state of dopamine D_2 receptor has multiple conformations. **L. Shi**
3:40 **490.** Accelerated molecular dynamics samples slow conformational changes in apo REV-ERBα. **L. Hegazy**
4:00 **491.** Understanding ligand selectivity in bitter taste receptors using multiscale molecular dynamics simulations. F. Fierro, A. Giorgetti, P. Carloni, W. Meyerhof, **M. Alfonso-Prieto**

Computational Quantum Chemistry: From Promise to Prominence: A Symposium in Honor of Henry F. Schaefer

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Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets

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THURSDAY MORNING – COMP

SECTION A
Omni San Diego Hotel
Gallery 2

Computational Studies of Water

T. P. Kurtzman, D. J. Sindhikara, *Organizers*
S. Yue, *Presiding*

8:30 **492.** Role of water in protein-ligand binding: Water locations, network binding free energies, and structure-activity relationships by grand canonical Monte Carlo. **J.W. Essex**, H. Bruce Macdonald, C. Cave-Ayland, G. Ross, M.L. Samways, R. Taylor
9:00 **493.** Development and applications of water-pharmacophore. **A. Cho**, S. Jung, T.P. Kurtzman
9:30 **494.** Equilibration of buried water molecules to enhance protein-ligand binding free energy calculations. **I.Y. Ben-Shalom**, C. Lin, T. Kurtzman, R. Walker, M.K. Gilson
9:50 **495.** Development of a novel water model for molecular dynamics for IDPs: Presenting the CAIPi3P model. **J. de Souza Cunha**, F.S. Zariquiey, A. Bronowska
10:05 Intermission.
10:20 **496.** All-atom molecular dynamics simulation of hygroscopicity in atmospheric aerosols. **D. Roston**
10:40 **497.** New coarse-grained model for water with improved thermodynamic and structural properties: Bottom-up many-body projected water (BUMPer). **J. Jin**, G.A. Voth
10:55 **498.** Direct inversion approach to local permittivity at liquid-liquid interfaces. **D. Egger**, C. Scheurer, K.U. Reuter
11:10 **499.** Dynamic properties of aqueous electrolyte solutions from nonpolarizable, polarizable, and scaled-charge models. **S. Yue**, A. Panagiotopoulos

SECTION B
Omni San Diego Hotel
Gallery 3A

Material Science

2D Materials, Machine Learning, Phase Behavior & Surfaces

C. M. Aikens, *Organizer*
M. Du, *Presiding*

8:30 **500.** Atomic and electronic structure of the edges of bulk and monolayer tin disulfide (SnS_2). **T. Yan**
8:50 **501.** Uncovering the kinetics of sulfurization of molybdenum trioxide by elemental sulfur in the growth of two-dimensional molybdenum disulfide by powder vaporization. **T. Tsafack**, **S.F. Bartolucci**, **J.A. Maurer**
9:10 **502.** Proper first-principles approach on charge-discharge behavior of 2D hetero-structure electrodes. **K. Yim**, C. Lee, R. Tamarany, H. Kim, C. Yoo, H. Yoon, P. Kim
9:30 **503.** Computational study of MXene/epoxy nanocomposite interface and mechanical properties. **Y. Sliozberg**, J. Andzelm, L. Nataraj, C. Hatter, Y. Gogotsi, A. Hall
9:50 **504.** Artificial intelligence guided material design and characterization. **T. Loeffler**, H. Chan, S. Sankaranarayanan

10:10 **505.** Application of machine learning in separation processes using graphene-supported metallic clusters. **J. Zhang**, M. Nguyen, V. Glezakou

10:30 Intermission.

10:50 **506.** Generating metastable phase diagrams of carbon using machine learning. **S. Srinivasan**, T. Loeffler, H. Chan, J. Wen, D. Luo, S. Sankaranarayanan

11:10 **507.** Anisotropic growth of Pt on Pd nanocubes promotes direct synthesis of hydrogen peroxide. **M. Kim**, G. Han, X. Xiao, J. Song, H. Kim, J. Ahn, S. Han, K. Lee, T. Yu

11:30 **508.** Assessing the structural stabilities of novel uranium materials with DFT and bond valence calculations. **A. Shields**, T.L. Spano, B.B. Anderson, R. Kapsimalis, A. Miskowiec, J.L. Niedziela

11:50 **509.** First-principles guided discovery of novel bimetallic catalysts for direct synthesis of hydrogen peroxide. **S. Han**, B. Yeo, D. Kim

12:10 **510.** Surface charge density and structure for coated gold nanoparticle models. **G. Chong**, E.D. Laudadio, M. Wu, C.J. Murphy, R.J. Hamers, R. Hernandez

SECTION C
Omni San Diego Hotel
Gaslamp 1

Quantum Mechanics

A. E. DePrince, H. P. Hratchian, *Organizers*
S. Bidwell, *Presiding*

8:30 **511.** Advances in electron propagator theory. **H.H. Corzo**, M. Díaz-Tinoco, J.V. Ortiz

9:00 **512.** Designed optically multiadaptive materials. **C.B. Rinderspacher**, R.H. Lambeth

10:00 Intermission.

10:15 **513.** Reformulated analytical gradients for dynamically weighted complete active space self-consistent field. **W.J. Glover**

10:45 **514.** CASPT2 geometries and energies of Fe(II) spin-crossover complexes. **B.A. Finney**, B. Vlaisavljevich

11:15 **515.** Efficient semiempirical excited electronic state methods for photochemical studies of large systems. **C. Bannwarth**, T.J. Martinez

SECTION D
Omni San Diego Hotel
Gaslamp 2

Molecular Mechanics

J. Shen, *Organizer*
B. C. Taylor, *Presiding*

8:30 **516.** Withdrawn

8:50 **517.** Interaction of proteins with polyelectrolytes: Comparison of theory to experiment. **X. Xu**, M.M. Ballauff, J. Dzubiella

9:10 **518.** Progresses in molecular dynamics simulation-directed rational design of intelligent nanoreceptors for chemosensing. X. Sun, L. Riccardi, F. De Biasi, F. Rastrelli, F. Mancin, **M. Devivo**

9:30 **519.** Decryption of the diverse and complex movements in molecular machines. **W. Cai**, H. Fu, X. Shao

9:50 **520.** Simulation of structure/property relationships in block copolymer photoresists for directed self-assembly. A. Peters, B. Nation, C. Breaux, J. Delony, C. Henderson, **P.J. Ludovice**

10:10 Intermission.

10:30 **521.** Effect of tacticity and charge on solubilization free energy of synthetic anionic polyelectrolyte in water by molecular dynamics simulations. R. Chockalingam, **U. Natarajan**

10:50 **522.** Computer led design of functional arylamide foldamers. **Z. Liu**, V. Pophristic, S. Makeneni, S. Houshyar Azar, P. Reagan, R. D'Elia

11:10 **523.** 2D nanomembranes by design using lipid-like peptoids. **M.D. Baer**

11:30 **524.** Nanoscale isolated island polymer brushes: Simulation study. **P.B. Moore**, A. Sidorenko

SECTION E
Omni San Diego Hotel
Gaslamp 3

Molecular Mechanics: Conformational Dynamics of Receptors, Ion Channels & Transporters

J. Shen, *Organizer*
A. Dommer, *Presiding*

8:30 **525.** Molecular mechanisms of ion permeation and gating in ion channels. **R. Pomes**

9:00 **526.** Computational study of changes in conformational dynamics of Piezo1 induced by Yoda 1 agonist binding and membrane tension. **W.M. Botello-Smith**, W. Jiang, Y.C. Lin, H. Zhang, Y.L. Luo, J. Lacroix, A. Ozkan

9:20 **527.** Elucidating molecular mechanisms of anion channelrhodopsins to design new optogenetics tools. **J.M. Paggi**, R.O. Dror

9:40 **528.** Exploring the acid resistance mechanism of electrogenic amino acid antiporters in food-borne pathogens using computational experiments. **M. Prevost**, G. Roos, E. Krammer

10:00 Intermission.

10:10 **529.** Understanding coupled ion exchange in ClC antiporters from the kinetic landscape of Cl-/H+ exchange. **J.M. Swanson**

10:40 **530.** Substrate-induced conformational transitions of the human serotonin transporter. **M. Chan**, B. Selvam, D. Shukla

11:00 **531.** Structure and dynamics of the wild-type and mutant ABC transported CFTR as gleaned from MD simulations. **H. Senderowitz**, N. Khazanov, L. Simchaev, M. Zhenin

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