9:30 COLL 859. Selective electropolymerization of aniline on an ITO electrode using magnetic nanoparticles and a varying magnetic field. **D. Wirth**

9:50 COLL 860. Morphology, structure, and optical properties of 2D SnS nanoplates synthesized via a hot-injection method. **N. Trejo**, A. Hunter, M. Nguyen, C. Wrasman, J. Dwyer, E.S. Aydil

10:10 COLL 861. Synthesizing and screening high mobility nanoparticles. **D. Garcia-Rojas**, G. Escalera, A. Mendoza-Garcia, C. Masterson, V. Colvin

10:30 COLL 862. Surfactant-induced shape changes in oil droplets caged in deformable polymer shells as templates for the synthesis of anisotropic polymer particles. **X. Guo**, N.L. Abbott, D.M. Lynn

10:50 COLL 863. Synthesis and chemical transformation of nickel nanoparticles embedded in silica. **B.B. Lynch**, B.D. Anderson, W.J. Kennedy, J.B. Tracy

11:10 COLL 864. Carboxylate decomposition: A critical step in high temperature synthesis of metal oxide nanocrystals. **C. Masterson**, A. Mendoza-Garcia, V. Colvin

11:30 COLL 865. Synthesis and characterization of metal-doped synthetic melanin nanoparticles. **Z. Wang**, Y. Li, Y. Huang, N.C. Gianneschi

11:50 COLL 866. Effect of solution composition on Pu oxide nanoparticle morphology. **T. Parsons-Moss**, J. Shusterman, D. Olive, Z. Dai, M. Zavarin, A. Kersting

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms: Metals

Sponsored by CATL, Cosponsored by COLL and ENVR

Oxides

Sponsored by CATL, Cosponsored by COLL and ENVR

Functional Lignocellulosics & Nanotechnology

Responsive Materials & Biosensors

Sponsored by CELL, Cosponsored by CARB and COLL

THURSDAY AFTERNOON

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Elucidation of Mechanisms & Kinetics on Surfaces

Oxidation Reactions

Sponsored by CATL, Cosponsored by COLL and ENVR

Beyond Hydrocarbons

Sponsored by CATL, Cosponsored by COLL and ENVR

Functional Lignocellulosics & Nanotechnology

(nano)Paper: From Fundamentals to Applications/Antimicrobial, Functional Materials

Sponsored by CELL, Cosponsored by CARB and COLL

COMP

Division of Computers in Chemistry

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

BUSINESS MEETINGS:
Business Meeting, 3:00 PM: Sat

SOCIAL EVENTS:
Social Hour, 7:00 PM: Sat

SUNDAY MORNING

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Allosteric Regulation & Mechanisms

Cosponsored by PHYS

C. Chang, *Organizer*

G. Verkhivker, *Organizer, Presiding*

8:30 Introductory Remarks.

8:45 COMP 1. Allosteric mechanisms in receptor function and modulation: Toward a new pharmacology. **J. Changeux**

9:30 COMP 2. Allosteric functional mechanisms of molecular machines in the cell membrane. **H. Weinstein**, M.V. LeVine, G. Khelashvili, M.A. Cuendet, A. Razavi

10:00 COMP 3. Allostery driven by metal ions: Getting transition metal ions around cells safely. **K.M. Merz**

10:30 Intermission.

10:50 COMP 4. Dissecting and controlling protein allostery. **N. Dokholyan**

11:20 COMP 5. Entangled relationships: Protein flexibility, allostery, and mutation. **D. Livesay**

11:50 COMP 6. Toward rational allosteric engineering of molecular motor and switch protein function. **B. Grant**

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG[‡] and PHYS

K. Honkala, B. Liu, *Organizers*

B. Liu, *Presiding*

8:30 COMP 7. Advances in density functional theory for molecules and materials. N. Mardirossian, **M.P. Head-Gordon**

9:05 COMP 8. New discovery tools for transition metal catalyst design. T.Z. Gani, J.P. Janet, E. Ioannidis, **H.J. Kulik**

9:40 COMP 9. Automated surface structure determination and reaction path identification. **B. Hammer**

10:15 Intermission.

10:35 COMP 10. Formation and structure of black anatase TiO_2: A combined force field and first principles study. S. Selcuk, X. Zhao, **A. Selloni**

11:10 COMP 11. Discovery of new polymer photocatalysts for water splitting: The role of computational chemistry. P. Guiglion, A. Monti, **M.A. Zwijnenburg**

11:45 COMP 12. Theoretical water splitting mechanisms on manganese oxide clusters. **C.M. Aikens**, A. Fernando, M. Just, K. Skinner, A.Z. Clayborne, T.N. Haddock

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

G. Gidofalvi, E. Hohenstein, *Organizers*

A. E. DePrince, *Organizer, Presiding*

8:30 COMP 13. On-the-fly CASPT2 nonadiabatic dynamics. **T. Shiozaki**

9:10 COMP 14. Reaching towards FeMoCo. Z. Li, S. Guo, A. Sokolov, **G.K. Chan**

9:50 COMP 15. Reduced-order formulation of multi-reference perturbation theory via tensor hyper-contraction. **C. Song**, T.J. Martinez

10:15 Intermission.

10:30 COMP 16. Coupled cluster theory for hundreds of atoms. **F. Neese**

11:10 COMP 17. Generalized active space method for affordable multi-reference calculations. **L. Gagliardi**

11:50 COMP 18. Construction of R12 geminal-projected particle-hole creation operators for many-electron systems using diagrammatic factorization approach. M.G. Bayne, **A. Chakraborty**

Section D

InterContinental San Francisco

Cathedral Hill

Computational Studies of Water

D. J. Sindhikara, *Organizer*

V. Mouchlis, *Presiding*

8:30 COMP 19. Thermodynamic characterization of water in biomolecular recognition. R. Abel, S. Mondal, C. Masse, J. Greenwood, G. Harriman, M. Ashwell, S. Bhat, **T. Beuming**, R. Wester, L. Frye, R. Kapeller, R. Friesner

9:10 COMP 20. Protein hydration free energies in explicit vs implicit solvent - a direct comparison. **P. Setny**

9:40 COMP 21. Testing a desolvation term in molecular docking on a model cavity. **T.E. Balius**, M. Fischer, R.M. Stein, T.B. Adler, C.N. Nguyen, A. Cruz, M.K. Gilson, T.P. Kurtzman, B. Shoichet

10:10 Intermission.

10:25 COMP 22. Conserved H_2O in protein-ligand complexes: An evaluation of water prediction tools. **E. Nittinger**, P.A. Gibbons, V. Tsui, M. Rarey, D.F. Ortwine

10:50 COMP 23. Water prediction validated by x-ray crystallography in the B1 domain of neuropilin-1. **A. Chan**

11:15 COMP 24. Comparing water dynamics in cryo-EM and x-ray derived molecular models. **F. Tofoleanu**, F.C. Pickard, S. Subramaniam, B. Brooks

11:40 COMP 25. Toward a force-field validation engine: Attach-Pull-Release calculations of host-guest binding thermodynamics. **J. Yin**, M.K. Gilson

Section E

InterContinental San Francisco

Laurel Hill

Computer-Aided Peptide Design

In-Silico Peptide Modeling

Cosponsored by CINF

Q. Deng, S. N. Ha, *Organizers*, *Presiding*

8:30 COMP 26. BRIKARD: A kinematics-based algorithm for the conformational sampling and design of macrocycles. **E. Coutsias**

9:00 COMP 27. Computational modeling of cyclic peptides. S. McHugh, D. Slough, H. Yu, J. Rogers, **Y. Lin**

9:30 COMP 28. Fragment-centric topographical mapping of protein-peptide interaction interfaces. **Y. Zhang**

10:00 Intermission.

10:15 COMP 29. Relative binding free energies from flexible peptide binding simulations. **A. Perez**, J.A. Morrone, Q. Deng, S.N. Ha, K. Dill

10:45 COMP 30. Recent advances in structure-based prediction of protein-peptide binding affinities. **T. Beuming**, H. Li, E. Feyfant

11:15 COMP 31. Stapled peptides: Specific reagents, potential therapeutics. **C. Verma**

Section F

InterContinental San Francisco

Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, J. M. Blaney, *Organizers*

E. Metwally, V. Shanmugasundaram, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 COMP 32. Computational & data sciences in the cloud – To be or not to be. **R.K. Kondru**

9:05 COMP 33. Lessons learned in using Cloud BigCompute to transform computational chemistry research. **J. Stowe**

9:35 COMP 34. Getting our heads into the cloud: GSK experiences using cloud computing for structure based drug design. **A.P. Graves**

10:05 Intermission.

10:20 COMP 35. Practical lessons learned on a long and winding road to The Cloud. **N.P. Labello**, G.A. Bakken

10:50 COMP 36. Design anywhere: A mobile app for drug design. **H. Zhang**, J. Lajiness, J. Hughes, M. Lajiness, J. Wang

‡ Cooperative Cosponsorship

11:20 COMP **37.** Accelerating discovery in the cloud: A cohesive workflow for the virtual screening and refinement of computationally-intensive libraries. **E. Metwally**

Materials Informatics & Computational Modeling

Sponsored by CINF, Cosponsored by COMP and POLY

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Simulating Electrons on Large Scale

Sponsored by PHYS, Cosponsored by COMP

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

SUNDAY AFTERNOON

Section A

InterContinental San Francisco
Twin Peaks

Undergraduate Research & National Meeting Roundtable

E. C. Sherer, *Organizer*

M. C. Nagan, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 COMP **38.** Introduction to quantum chemistry. **A.E. DePrince**

2:25 COMP **39.** Molecular mechanics in computational chemistry: An overview for undergraduates. **C.L. Simmerling**

3:15 Discussion.

4:05 Intermission.

4:20 Panel Discussion.

5:10 Concluding Remarks.

Section B

InterContinental San Francisco
Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

B. Liu, *Organizer*

K. Honkala, *Organizer, Presiding*

1:30 COMP **40.** Insight into catalyst activity and selectivity drawn from molecular modeling. **A.T. Bell**

2:05 COMP **41.** First-principles based multiscale multiparadigm methods with applications to complex material. **W.A. Goddard**

2:40 COMP **42.** First principles kinetic modeling of methane oxidation over Pd and PdO. M. Jorgensen, M. Van den Bossche, **H. Gronbeck**

3:15 Intermission.

3:35 COMP **43.** Mechanism of CO and CO_2 hydrogenation over copper-based catalysts. **F. Studt**

4:10 COMP **44.** Crystal phase effect on CO activation for Fischer-Tropsch synthesis. J. Liu, **W. Li**

4:45 COMP **45.** Gold particle size effect for CO oxidation: A first-principles study. **J. Liu**, E. Hensen, I. Filot

Section C

InterContinental San Francisco
Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, G. Gidofalvi, *Organizers*

E. Hohenstein, *Organizer, Presiding*

1:30 COMP **46.** Accurate nonadiabatic dynamics. **D.R. Yarkony**

2:10 COMP **47.** Painless modeling of dynamics near conical intersections. **B.G. Levine**, G.A. Meek

2:50 COMP **48.** Energy dissipation at metal surfaces: The surprisingly high non-adiabaticity of Na diffusion on Cu(111). **S.P. Rittmeyer**, K.U. Reuter

3:15 Intermission.

3:30 COMP **49.** Dynamics of electron transfer near a metals surface. **J.E. Subotnik**, W. Dou, W. Ouyang

4:10 COMP **50.** Single-reference dynamics of strongly correlated systems: How far can we go? **M. Barbatti**

4:50 COMP **51.** New theoretical approaches to simulate photoinduced proton-coupled electron transfer reactions. **P. Huo**

Section D

InterContinental San Francisco
Cathedral Hill

Computational Studies of Water

Binding & Biology

D. J. Sindhikara, *Organizer*

F. L. Kearns, *Presiding*

1:30 COMP **52.** Methods and models for condensed phase simulation of water. **T.L. Head-Gordon**

2:00 COMP **53.** Capturing dynamics, along with thermodynamics, in the Implicit Solvent using the SuperPosition Approximation (IS-SPA) model. **P.T. Lake**, M. McCullagh

2:30 COMP **54.** Good from far, far from good: Comparing quantum and classical hydration of model ions. **R.C. Remsing**

3:00 Intermission.

3:15 COMP **55.** Modeling radical interactions with water. **J. Arey**, P. Tentscher

3:35 COMP **56.** New dissociative water model. **O. Akin-Ojo**

3:55 COMP **57.** Rate theory in two-dimensional reaction coordinate space: Applications to ion-pairing. **S. Roy**, M.D. Baer, C.J. Mundy, G.K. Schenter

4:15 COMP **58.** Enhanced modeling of water in two-dimensions with rose potentials. **C.J. Fennell**

4:35 COMP **59.** How to model chemical reactions in electrolytes? **S. Ringe**, H. Oberhofer, K.U. Reuter

Section E

InterContinental San Francisco
Laurel Hill

Computer-Aided Peptide Design

Computational Approaches to Peptide ADME

Cosponsored by CINF

Q. Deng, S. N. Ha, *Organizers*, *Presiding*

1:30 COMP **60.** ADME analysis of therapeutic peptides: Preserving product value. **J.H. Hochman**

2:00 COMP **61.** Factors for governing cell permeability and oral bioavailability in macrocycles. **S. Lokey**

2:30 COMP **62.** High throughput method for the indirect detection of intramolecular hydrogen bonding. **S. Sciabola**

3:00 Intermission.

3:15 COMP **63.** Property trends among permeable cyclic peptides. **A. Mathiowetz**

3:45 COMP **64.** Mechanism-based ADME/PK prediction, with applications to macrocycles. **M.P. Jacobson**

4:15 COMP **65.** Design of technology-compatible cyclic peptide scaffolds with oral bioavailability. **A. Golosov**

4:45 COMP **66.** PepSee — A new tool for peptide analysis & design. **M. Gastreich**, M. Skovgaard

Section F

InterContinental San Francisco
Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, E. Metwally, *Organizers*

J. M. Blaney, V. Shanmugasundaram, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 COMP **67.** Cloud first strategy that accelerates informatics and computations in drug discovery. **J. Feng**

2:05 COMP **68.** High performance and/or cloud computing for free energy prediction using molecular dynamics simulations? S. Wan, D.W. Wright, S.J. Zasada, A.P. Bhati, **P.V. Coveney**

2:35 COMP **69.** Lessons learned in developing and delivering a secure, multi-tenant environment for drug discovery R&D informatics. **W.W. Smith**, B.A. Bunin

3:05 Intermission.

3:20 COMP **70.** What's with all this GPU-accelerated cloud computing stuff? **M.E. Berger**

3:50 COMP **71.** Cloud is the only place for computational chemistry: Why this is a once-in-a-lifetime opportunity for the field to leap forward. **P.C. Hawkins**, A.G. Skillman, R. Tolbert, J. LaFon, C. Bruce, A. Nicholls

4:20 COMP **72.** Enhancing internal computational capabilities with the cloud. **J. Duca**, D. Chin, C. Hajdin, S. Litster

Materials Informatics & Computational Modeling

Sponsored by CINF, Cosponsored by COMP and POLY

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Simulating Quantum Nuclei on Large Scale

Sponsored by PHYS, Cosponsored by COMP

Computations for CO_2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY MORNING

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

Z. Luthey-Schulten, *Presiding*

8:30 COMP **73.** Energy landscape theory: From folding to function in genetic networking. **P.G. Wolynes**

9:00 COMP **74.** Touring the protein folding landscape: The view depends on how and where you look. **S. Marqusee**

9:30 COMP **75.** Exploring allostery from protein folding to function using coarse-grained models. **C.L. Brooks**

10:00 Intermission.

10:20 COMP **76.** Exploring protein function: The convergence of structure based models and co-evolutionary information. **J.N. Onuchic**

10:50 COMP **77.** Significance of neuronal structural complexity and spatial heterogeneity in modulating dopamine reuptake dynamics. C. Kaya, M.H. Cheng, E. Block, T. Bartol, T. Sejnowski, A. Sorkin, J.R. Faeder, **I. Bahar**

11:20 COMP **78.** Exploring fitness and free energy landscapes of proteins for allostery and binding. **R.M. Levy**

Section B

InterContinental San Francisco
Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, *Organizer*

B. Liu, *Organizer, Presiding*

8:30 COMP **79.** First-principles modeling and design of catalytic materials. **P. Sautet**

9:05 COMP **80.** Electroreduction of CO_2 to hydrocarbons and alcohols. **E. Skulason**, J. Hussain, H. Jonsson

9:40 COMP **81.** Engineering metal/SnOx interfaces for electrochemical CO_2 reduction. **H. Xin**, S. Wang

10:15 Intermission.

10:35 COMP **82.** Structure, stability, and reactivity of nano-structured oxides supported on metals. **A. Vojvodic**

11:10 COMP **83.** Toward modeling practical catalysis from first principles. W. An, Y. Liang, H. Kim, S. Liu, **P. Liu**

11:45 COMP **84.** Electrochemical reduction of nitric oxide on Pt-surfaces: A combined DFT and kMC approach. H. Chun, V. Apaja, **A.Z. Clayborne**, J.P. Greeley, K. Honkala

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, E. Hohenstein, *Organizers*

G. Gidofalvi, *Organizer, Presiding*

8:30 COMP **85.** DMRG: Orbital selection, dynamic correlation, and nuclear gradients. **M. Reiher**

9:10 COMP **86.** Wavefunction forms based on identities from combinatorics. **P. Ayers**

9:50 COMP **87.** Coupled-Cluster Valence Bond Singles and Doubles (CCVB-SD): Block-tensor based implementation and application to polyacenes. **J. Lee**, D. Small, M.P. Head-Gordon

10:15 Intermission.

10:30 COMP **88.** New vistas on the strong correlation problem. **G.E. Scuseria**

11:10 COMP **89.** Perturbative multireference similarity renormalization group approaches for ground and excited states. C. Li, K.P. Hannon, **F.A. Evangelista**

11:50 COMP **90.** GPU-accelerated state-averaged complete active space self-consistent field and derivative methods enable accurate, large-scale nonadiabatic dynamics simulations. **J.W. Snyder**, E. Hohenstein, B. Curchod, B. Fales, R.M. Parrish, T.J. Martinez

Section D

InterContinental San Francisco

Cathedral Hill

Computational Studies of Water

Phenomena & Properties

D. J. Sindhikara, *Organizer*

T. E. Balius, *Presiding*

8:30 COMP **91.** Water structuring above planar hydrophobic surfaces. **U. Schnupf**, J. Brady

8:55 COMP **92.** Monte Carlo simulations probing the liquid/vapor interface of water/hexane mixtures. **M.S. Minkara**, D.J. Stein, C.J. Peters, J. Siepmann

9:20 COMP **93.** Surface potential of water with *ab initio* molecular dynamics. **T.T. Duignan**, M.D. Baer, G.K. Schenter, C. Mundy

9:45 COMP **94.** Deviation of the surface tension of water suggests the possible emergence of a new form of liquid upon supercooling. **F. Wang**

10:10 Intermission.

10:25 COMP **95.** Modelling the refractive index of the air-water interface. **F. Longford**, J.W. Essex, C. Skylaris, J.G. Frey

10:45 COMP **96.** Understanding the sensitivity of nucleation free energies to the molecular model in water and ion/water systems. **S.J. Keasler**, M.A. Olson, J. Schlecht, S. Pavlenko, J. Siepmann

11:05 COMP **97.** Hydrophobic polymer collapse: Unravelling molecular mechanisms for osmolyte protection and denaturation. **N. van der Vegt**

11:25 COMP **98.** Fluctuation phenomena and structure of revPBE water at ambient and high pressure (up to 360 MPa). **M. Galib**, G.K. Schenter, J. Fulton, C.J. Mundy

11:45 COMP **99.** Predictive description of electronic properties in aqueous solutions. **T. Pham**, M. Govoni, R. Seidel, S.E. Bradforth, E. Schwegler, G.A. Galli

Section E

InterContinental San Francisco

Laurel Hill

Drug Design

Docking & Protein-Ligand Interaction Analysis

M. R. Landon, Y. Tseng, *Organizers*

T. Abramyan, *Presiding*

8:30 COMP **100.** Protein-ligand scoring with convolutional neural networks. **D. Koes**, M. Ragoza, E. Idrobo, J. Hochuli, J. Sunseri

8:55 COMP **101.** Predicting hot and warm spots on proteins for fragment binding. **P. Rathi**, F. Ludlow, R.J. Hall, C. Murray, P. Mortenson, M. Verdonk

9:20 COMP **102.** PlayMolecule DeepSite: Protein binding site detector using 3D convolutional neural networks. **G. De Fabritiis**

9:45 Intermission.

10:05 COMP **103.** Understanding protein-ligand binding at the molecular level: Using swap-based methods to visualise binding free energy components. **C.J. Woods**, M. Malaisree

10:30 COMP **104.** Docking - old hat or hats off. **C. Lemmen**, C. Detering, M. Gastreich

10:55 COMP **105.** Interrogating protein ligand interactions– Knowledge base from PDB/CSD and energy decomposition methods. **J.H. Voigt**, U. Schmitz

11:20 COMP **106.** Development of a novel CHARMM-based flexible receptor-flexible ligand docking procedure. S.K. Vankayala, J.D. Larkin, **H.L. Woodcock**

Section F

InterContinental San Francisco

Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, V. Shanmugasundaram, *Organizers*

J. M. Blaney, E. Metwally, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 COMP **107.** Steps to getting science in the cloud at Merck. **R. Pete**, S.A. Johnson, B. Sherborne

9:05 COMP **108.** Deploying large-scale binding-affinity calculations to the cloud. **B.T. Hannigan**

9:35 COMP **109.** Xcellerate informatics: A cloud-based solution for clinical data integration and real-time monitoring of clinical trials. **D.K. Agrafiotis**

10:05 Intermission.

10:20 COMP **110.** Cyrus's journey to the cloud: How we got there and what we've learned. **L. Nivon**

10:50 COMP **111.** Distributed computing resources, from grid to cloud: Welcome to the HPC world! **E. Arnoult**

11:20 COMP **112.** Druggability assessment of the structural proteome with inclusion of light protein flexibility. **A.C. Cheng**, F. Boulnois, K. Loving, A. Lin

Advances in High-Throughput Screening

Sponsored by CINF, Cosponsored by COMP and MEDI

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Ab Initio & DFT

Sponsored by PHYS, Cosponsored by COMP

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

I. Bahar, *Presiding*

1:30 COMP **113.** Allosteric effects of weak transient protein-protein interactions: Crowding in cells and evolutionary consequences. **E. Shakhnovich**, S. Bhattacharyya, S. Bershtein

2:00 COMP **114.** Ribosome biogenesis in replicating cells: Integration of experiment and theory. **Z. Luthey-Schulten**

2:30 COMP **115.** Systematic perturbation of a fundamental biological switch. **T. Kortemme**

3:00 Intermission.

3:20 COMP **116.** Role of electrostatics in allosteric regulation. **M.P. Jacobson**

3:50 COMP **117.** Molecular principles for optimizing protein-DNA interactions. **K. Levy**

4:20 COMP **118.** Mediation of allosteric communication by inter-domain bridges. J. Guo, C. Guo, **H. Zhou**

4:50 COMP **119.** Phospholipase A2: A unique paradigm of allosteric regulation by membranes. **V. Mouchlis**, J. McCammon, E.A. Dennis

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, B. Liu, *Organizers*

A. Z. Clayborne, *Presiding*

1:30 COMP **120.** Catalyst design on the computer. **J.K. Norskov**

2:05 COMP **121.** Static or dynamic? A first-principles multiscale modeling perspective on the nature of the surface of operating catalysts. **K.U. Reuter**

2:40 COMP **122.** First principles analysis of reactivity trends at the interface between metal nanoparticles and doped oxide supports. **J. Greeley**, T.S. Choksi, P. Majumdar, Z. Zhao, Y. Cui, W.F. Schneider, F. Ribeiro

3:15 Intermission.

3:35 COMP **123.** Catalysis of ice formation. **A. Michaelides**

4:10 COMP **124.** First-principles insights to the CO oxidation on oxidized Rh. **A. Hellman**

4:30 COMP **125.** Group additivity for adsorbed polyols at a Pt(111) surface under aqueous conditions. **B. Schweitzer**, G. Gu, S. Steinmann, C. Michel, P. Sautet, D.G. Vlachos

4:50 COMP **126.** General structure-activity relationships for transition metal oxides. **V. Fung**, F. Tao, D. Jiang

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, G. Gidofalvi, *Organizers*

E. Hohenstein, *Organizer, Presiding*

1:30 COMP **127.** Nonadiabatic dynamics of photoinduced proton-coupled electron transfer processes. **S. Hammes-Schiffer**

2:10 COMP **128.** Nonadiabatic molecular dynamics for spin-forbidden processes. D. Fedorov, R. Zaari, **S.A. Varganov**

2:50 COMP **129.** Can quantized vibrational effects be obtained from Ehrenfest mixed quantum-classical dynamics? **J.J. Goings**, D.B. Lingerfelt, X. Li

3:15 Intermission.

3:30 COMP **130.** Charge transfer dynamics, excited state energetics, and organic photovoltaics. **N. Ananth**

4:10 COMP **131.** Optomechanical control of photochemical quantum yields in a biological chromophore model. **M. Olivucci**, L. Frutos, A. Valentini

‡ *Cooperative Cosponsorship*

4:50 COMP **132.** Quantum dynamics in CS^+ collision with H using time dependent wave packet dynamics. **R. Kaur**, D. Thogluva

Section D

InterContinental San Francisco
Cathedral Hill

Data Science Challenges in Computational Chemistry

Cosponsored by CINF

M. Feig, *Organizer*

C. L. Simmerling, G. Vacek, *Organizers*, *Presiding*

1:30 COMP **133.** Meaningful state space discretization at the macro-cluster level. H. Liu, M. Li, J. Fan, **S. Huo**

2:00 COMP **134.** Building Markov state models of diffusion processes in many-particle systems from generic order parameters. **J.F. Rudzinski**, M. Radu, K. Kremer, T. Bereau

2:30 COMP **135.** Understanding and applying multistate reweighting in a broad molecular simulation context. **M.R. Shirts**

3:00 Intermission.

3:15 COMP **136.** Cluster analysis of molecular simulation trajectories for systems where both conformation and orientation of the sampled states are important. **T. Abramyan**, J. Snyder, A.A. Thyparambil, S. Stuart, R.A. Latour

3:45 COMP **137.** HTMD: High-throughput molecular dynamics for molecular discovery. **G. De Fabritiis**

4:15 COMP **138.** Geometric searching in large collections of protein-ligand interfaces. T. Inhester, E. Nittinger, **M. Rarey**

4:45 COMP **139.** Proper data extraction and curation in an era of linked open data – Are we there yet? **B. Zdrazil**, G.F. Ecker

Section E

InterContinental San Francisco
Laurel Hill

Drug Design

Computational Methods & Approaches

M. R. Landon, Y. Tseng, *Organizers*

J. L. Paulsen, *Presiding*

1:30 COMP **140.** Common hits approach: Combining pharmacophore modeling and molecular dynamics simulations. **M. Wieder**, A. Garon, U. Perricone, T. Seidel, S. Boresch, T. Langer

1:55 COMP **141.** Protein binding sites dynamics in drug discovery. **D. Janezic**, J. Konc

2:20 COMP **142.** New approaches for binding site and ligand prediction and their use in drug discovery. **J. Konc**, D. Janezic

2:45 Intermission.

3:05 COMP **143.** pmemdGT: An efficient and accurate GPU-accelerated thermodynamics integration simulation package. **T. Lee**, D.M. York

3:30 COMP **144.** Efficient free energy perturbation Hamiltonian replica exchange molecular dynamics method for absolute binding affinity predictions. **W. Jiang**

3:55 COMP **145.** Calculating the absolute binding free energies for octa-acids and guests. **F. Tofoleanu**, J. Lee, F.C. Pickard, G. Koenig, J. Huang, M. Baek, C. Seok, B. Brooks

4:20 COMP **146.** Hybrid quantum and classical free energies: Separating the wheat from the chaff with configuration space overlaps. **C. Cave-Ayland**, C. Skylaris, J.W. Essex

Section F

InterContinental San Francisco
Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, E. Metwally, *Organizers*

J. M. Blaney, V. Shanmugasundaram, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 COMP **147.** Using the cloud for massive scale-up of computationally intensive physics-based simulations. **V. Eyrich**, J. Watney, Y. Zhao, L. Wang, S. Mondal, S. Bhat, R. Abel

2:05 COMP **148.** CHARMM interface and graphics: A flexible web-user interface for education and application of molecular simulation and multi-scale modeling. J. Smock, V. Schalk, Y. Pevzner, B.T. Miller, **H.L. Woodcock**

2:35 COMP **149.** AceCloud: Molecular dynamics simulations in the cloud. M. Harvey, **G. De Fabritiis**

3:05 Intermission.

3:20 COMP **150.** Virtual screening in the cloud with Pharmit. **D. Koes**

3:50 COMP **151.** Research informatics: Get ready for the cloud! **M. Van Daelen**

4:20 Discussion.

4:40 Concluding Remarks.

Advances in High-Throughput Screening

Sponsored by CINF, Cosponsored by COMP and MEDI

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Semiempirical & DFTB

Sponsored by PHYS, Cosponsored by COMP

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

H. L. Woodcock, *Organizer*

8:00 - 10:00

236, 240-247, 261, 267, 277, 283-284, 286, 290, 305-306, 310-312, 331, 341, 345, 347, 349, 353-357, 360, 362, 365, 368, 375, 377, 383, 389-391, 396-398, 402-403, 406, 410, 416-417, 419, 421, 424, 426. See subsequent listings.

TUESDAY MORNING

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

H. Weinstein, *Presiding*

8:30 COMP **152.** Structural mechanisms of the allosteric regulation of Ras. **J. Kuriyan**

9:00 COMP **153.** Ancient origins of allosteric activation–Exploitation for novel cancer drugs. **D. Kern**

9:30 COMP **154.** Fractal nature of protein interior and its implications for allostery. **A. Kornev**, S.S. Taylor

10:00 Intermission.

10:20 COMP **155.** How EGF and insulin activate their receptors. **D. Leahy**, J. Kavran, P. Byrne

10:50 COMP **156.** Genetically tunable frustration controls allostery in an intrinsically disordered transcription factor. **V.J. Hilser**

11:20 COMP **157.** Role of intrinsically disordered proteins in allosteric regulation of cellular signaling. **P.E. Wright**

Section B

InterContinental San Francisco
Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

B. Liu, *Organizer*

K. Honkala, *Organizer, Presiding*

1:30 COMP **158.** Computational catalysis: Rigor and relevance. **J. Sauer**

2:05 COMP **159.** Diesel oxidation catalysts with improved low temperature activity identified from computational screening. Y. Song, J.S. Arevalo, W. Epling, **L. Grabow**

2:40 COMP **160.** Operando catalysis: Computing the state of a zeolite catalyst at reaction conditions. **W.F. Schneider**, C. Paolucci, H. Li, S. Li

3:15 Intermission.

3:35 COMP **161.** Complete catalytic cycle for fast and standard NH_3-SCR reaction. **H. Falsig**

4:10 COMP **162.** Understanding diffusion during catalytic fast pyrolysis of biomass over H-ZSM-5 by multiscale modeling. L. Bu, B. Knott, P.N. Ciesielski, M.R. Nimlos, D. Robichaud, **S. Kim**

4:30 COMP **163.** Adsorption and activation of water on cuboctahedral rhodium and platinum nanoparticles. **A.S. Bazhenov**, L. Lefferts, K. Honkala

4:50 COMP **164.** Structural study of the Ziegler-Natta catalyst. **V. D'Anna**, P. Sautet

Section C

InterContinental San Francisco
Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, E. Hohenstein, *Organizers*

G. Gidofalvi, *Organizer, Presiding*

8:30 COMP **165.** Direct patching exchange-correlation potential in density functional theory. **C. Huang**

9:10 COMP **166.** Unpaired densities in singlet polyradicals: Local electron correlation treatment in extended multi-reference approaches in comparison with quasi correlated tight binding. **H. Lischka**

9:50 COMP **167.** Derivative coupling vectors from a Davidson approach. **J.A. Kammeraad**, P.M. Zimmerman

10:15 Intermission.

10:30 COMP **168.** Time-dependent two-component relativistic spin dynamics. **X. Li**

11:10 COMP **169.** Excited-state dynamics of mPlum flourecent protein. **S. Faraji**, A. Krylov

11:50 COMP **170.** Nonadiabatic couplings and the choice of density functional: Exchange cannot be neglected. **A.V. Akimov**

Section D

InterContinental San Francisco
Cathedral Hill

Molecular Mechanics

Sampling Long Time Scales

M. Feig, *Organizer*

J. V. Vermaas, *Presiding*

8:30 COMP **171.** Enhancing conformational sampling by modifying the underlying velocity distribution: Digitally filtered hybrid Monte Carlo. **C.S. Pervane**, J.W. Essex

8:55 COMP **172.** Novel enhanced sampling approach for cryptic site discovery on protein targets. **F. Gervasio**

9:25 COMP **173.** Rapid protocol for free energy calculations via multi-dimensional expanded ensemble simulations. **B. Radak**, B. Roux

9:55 Intermission.

10:10 COMP **174.** MS-Fold: Protein structure prediction guided by covalent labeling mass spectrometry data. M. Marlett, S.H. Hinckley, V.H. Wysocki, **S. Lindert**

10:40 COMP **175.** Fast free energy calculations from proximal distribution functions. **S. Ou**, B.M. Pettitt

TECHNICAL PROGRAM

11:10 COMP **176.** Unraveling the mechanistic basis of the CRISPR-Cas9 system via molecular simulations. **G. Palermo**, Y. Miao, R. Walker, M. Jinek, J. McCammon

11:40 COMP **177.** pH-dependent conformational change and its impact on *E.coli* glycinamide ribonucleotide transformylase catalytic activity. **P. Gupta**, A.E. Roitberg

Section E

InterContinental San Francisco

Laurel Hill

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Cosponsored by BIOL, MEDI and WCC

D. J. Kempf, Y. C. Martin, *Organizers*

T. R. Stouch, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 COMP **178.** QSAR: How my success relied on pillars built by Yvonne Connolly Martin. **G. McGaughey**

9:05 COMP **179.** Big data, small data: Pharmacology-based similarity measures and statistically-derived amino acid weightings to inform kinome selectivity. **M. Torrent**

9:30 COMP **180.** Integrated hit generation: Iterative design of experiments, screening sets, and compounds. **J.M. Jansen**, P.S. Lee, V.R. Polyakov, L. Tian, E.J. Martin

9:55 Intermission.

10:10 COMP **181.** Recent advances in applying computation to (bio) catalyst design. **K.W. Lexa**

10:35 COMP **182.** Innovation/evolution of cheminformatics evergreens. **M. Lee**

11:00 COMP **183.** Impact of quantitative drug design: Mighty oaks from little acorns grow. **M. Holloway**

11:25 Concluding Remarks.

Section F

InterContinental San Francisco

Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG‡

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

8:30 COMP **184.** Multi-scale modeling of nanomaterials: From DFT to molecular dynamics simulations. **F. Martin-Martinez**, Z. Qin, G. Jung, M.J. Buehler

8:55 COMP **185.** Reliable computational design of biological-inorganic materials to the large nanometer scale using INTERFACE-FF. **H. Heinz**

9:20 COMP **186.** Advances in atomic-scale methods for materials chemistry. **S.B. Sinnott**

9:45 COMP **187.** Inference-boosted first-principles molecular dynamics for chemo-mechanical modelling. **A. De Vita**

10:10 Intermission.

10:30 COMP **188.** Modeling the formation of sodium and calcium aluminosilicate gels at the mesoscale using coarse-grained Monte Carlo. **K. Yang**, C. White

10:45 COMP **189.** Simulations of polymer membranes with chain altering and conservative Monte Carlo moves. **A. Bick**, L. Subramanian

11:10 COMP **190.** Solvation and encapsulation of photoactive species: Insights from excited state DFTB. N. Garcia, A. Banducci, Z. Pollard, K. Komoto, **T. Kowalczyk**

11:35 COMP **191.** Recent DFTB extension for improving accuracy and boosting the efficiency for computational applications to nanomaterials. **T. Frauenheim**

12:00 COMP **192.** Entropy sampling for zeolite-catalyzed reactions at operating conditions. **K. De Wispelaere**, T. Bligaard, J.K. Norskov, V. Van Speybroeck

12:15 COMP **193.** Self-adaptive Reactive Force Fields (SERFF): Force matching for molecular dynamics simulation of reactive materials. **N. Goldman**

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Single Crystal Catalysis

Sponsored by CATL, Cosponsored by COMP

Quantum Dynamics in Large Scale Systems

Large-Scale Simulations in Materials Systems

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Material Science

Properties

C. M. Aikens, *Organizer*

R. C. Remsing, *Presiding*

1:30 COMP **194.** Breaking badly: DFT-D2 gives sizeable errors for tensile strengths in bulk solids. **B.M. Wong**, N. Ilawe

2:00 COMP **195.** Simulation of shock-wave properties in fused silica using soft-core potential. **S. Izvekov**, E.F. Byrd, N. Weingarten, B.M. Rice

2:30 COMP **196.** Reactive modeling of silica formation. J. Deetz, **R. Faller**

3:00 Intermission.

3:30 COMP **197.** Nanoscale charge balancing mechanism in alkali substituted C-S-H gels from first-principles calculations. **O. Ozcelik**, C. White

4:00 COMP **198.** Impact of environment on mechanical and physical properties of polyethylene: Comparison between experiments and simulation. **A. Shamloo**, A. Soldera, D. Rodrigue

4:30 COMP **199.** Computational studies of crystallization on the nanoscale. **J. Delhommelle**, C. Desgranges

5:00 COMP **200.** Modeling and simulations of functionalized magnetic nanoparticles as drug delivery systems. K. Karathanou, **Z. Cournia**

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, B. Liu, *Organizers*

A. Z. Clayborne, *Presiding*

8:30 COMP **201.** Catalysis by functionalized nanoparticles. **N. Lopez**

9:05 COMP **202.** Computational design of nanoalloy catalysts from DFT, genetic algorithms and machine learning. **T. Vegge**, P.C. Jennings, T. Bligaard, H.A. Hansen

9:40 COMP **203.** Subnanometer metal clusters as catalysts for energy conversion and storage. **L.A. Curtiss**, C. Liu, P. Zapol, S. Vajda

10:15 Intermission.

10:35 COMP **204.** Alloying supported Pt clusters with boron: Coke antagonist. **A. Alexandrova**, M. Ha, E. Jimenez-Izal

11:10 COMP **205.** Revealing the pathway of CO_2 reduction in a multicenter iron carbonyl catalyst using an *ab initio* nanoreactor. **L. Wang**, M.E. Hutchings, Y. Qiu

11:30 COMP **206.** Ab initio study of the hydrogen-producing mechanisms of cobaloximes in acetonitrile-water mixtures. **J. Chen**, P. Sit

11:50 COMP **207.** Protein-environment effect on catalysis performance in H_2-producing [NiFe] hydrogenases. **S. Qiu**, L.M. Azofra, D.R. MacFarlane, C. Sun

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

G. Gidofalvi, E. Hohenstein, *Organizers*

A. E. DePrince, *Organizer, Presiding*

1:30 COMP **208.** Two-electron reduced density matrices in electronic structure and dynamics. **D.A. Mazziotti**

2:10 COMP **209.** Using single-excitation wavefunctions to compute exciton-binding energies in singlet fission materials. **N. Mayhall**

2:40 COMP **210.** Strong correlation in coupled F-centers. **B.G. Janesko**

3:10 Intermission.

3:25 COMP **211.** Quantum chemistry strategies: Addressing strongly correlated transition metal and heavy element species. C. Plascencia, S. Yuwono, G. Schoendorff, **A.K. Wilson**

4:05 COMP **212.** Recent developments with the multifacet graphically contracted function electronic structure method. **R. Shepard**, S.R. Brozell, G. Gidofalvi

4:45 COMP **213.** Multi-reference electron correlation with large active spaces from time-dependent perturbation theory with density matrix renormalization group. **A. Sokolov**, G. Chan

Section D

InterContinental San Francisco

Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

N. J. Deyonker, *Presiding*

1:30 COMP **214.** Atropisomerization of 8-membered dibenzolactam: Experimental NMR and theoretical DFT study. **A. Buevich**

1:55 COMP **215.** Computational study of the photoelectron spectra of Europium-oxide, -hydride, and -hydroxide. **H. Harb**, L.M. Thompson, H.P. Hratchian

2:20 COMP **216.** Reaction mechanism of group II introns hydrolytic splicing investigated by QM/MM MD simulations. **L. Casalino**, G. Palermo, U. Roethlisberger, A. Magistrato

2:45 COMP **217.** Reactive first principles Monte Carlo simulations of nitrogen/oxygen and hydrogen sulfide/carbon dioxide mixtures. **E. Fetisov**, M. Shah, I.W. Kuo, C. Knight, J. Siepmann

3:10 Intermission.

3:25 COMP **218.** Combining quantum and QSAR methods for prediction of acid dissociation constants. L. Hosseini-Gerami, R. Leth, P. Hunt, **M.D. Segall**

3:50 COMP **219.** Computational investigation of o-aminomethylphenylboronic acid saccharide receptors. **J. Larkin**

4:15 COMP **220.** TINKTEP: Polarizable QM/MM based on linear-scaling DFT and the AMOEBA force field. **J. Dziedzic**, M.P. Head-Gordon, T.L. Head-Gordon, C. Skylaris

4:40 COMP **221.** Solvent/enzyme-perturbed transition state sampling and its applications. **Z. Yang**, Y. Li, J. Park, C. Doubleday, K.N. Houk

Section E

InterContinental San Francisco

Laurel Hill

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Cosponsored by BIOL, MEDI and WCC

D. J. Kempf, T. R. Stouch, *Organizers*

Y. C. Martin, *Organizer, Presiding*

1:30 COMP **222.** Collaborating to bring resources to neglected diseases research. **D.J. Kempf**

2:00 COMP **223.** NTD drug discovery booster: A novel approach for hit to lead chemistry. **B. Perry**

2:30 COMP **224.** Combining strengths of phenotype and target-based approaches to discover novel TB drugs. **J. Sacchettini**

3:00 Intermission.

3:15 COMP **225.** Antitubercular 3-(4- aminophenyl)oxazolidin-2-ones: Progress towards better, safer TB agents. **C.B. Cooper**

3:45 COMP **226.** Tylosin analogs as anti-filarial agents: Medicinal chemistry optimization and candidate selection. **T.W. Von Geldern**, D.J. Kempf, K. Marsh, H.E. Morton, L. Ford, J. Turner, S. Ward, M. Taylor, A. Hoerauf, S. Specht

‡ *Cooperative Cosponsorship*

4:15 COMP 227. Award Address (ACS Award for Computers in Chemical & Pharmaceutical Research sponsored by ACS Division of Computers in Chemistry). CADD and chemoinformatics within an inter-institution collaboration for TB drug discovery. **Y.C. Martin**

Section F

InterContinental San Francisco
Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG²

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

1:30 COMP 228. Recent advances in the quantum simulation of materials. **G.E. Scuseria**

1:55 COMP 229. Making density-functional embedding theory applicable to spin-polarized materials and covalent materials. **C. Huang**, A.B. Munoz, M. Pavone

2:20 COMP 230. Ab-initio materials spectra. J. McClain, T. Berkelbach, Q. Sun, **G. Chan**

2:45 COMP 231. Alchemy, chemical space, and quantum mechanics. **O. von Lilienfeld**

3:10 Intermission.

3:30 COMP 232. Finite-temperature *ab initio* many-body perturbation and coupled-cluster calculations of condensed matter. **S. Hirata**

3:55 COMP 233. Self-consistent many-body methods for bond-making and breaking. **P. Rinke**

4:20 COMP 234. Fast and accurate quantum Monte Carlo methods for material science. **D. Alfe**, A. Zen, M. Gillan, S. Sorella, A. Michaelides

4:45 COMP 235. Extending the applicability of quantum Monte Carlo methods to large molecules. **C. Filippi**

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Electrocatalysis

Sponsored by CATL, Cosponsored by COMP

Quantum Dynamics in Large Scale Systems

Large-Scale Simulations in Biological Systems

Sponsored by PHYS, Cosponsored by COMP

TUESDAY EVENING

Section A

Moscone Center
West Hall

Chemical Computing Group Graduate Student Travel Awards

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

6:00 - 8:00

COMP 236. QM-NEW: An efficient and accurate QM/MM free energy estimator and its application to pKa predictions. **F.L. Kearns**, P.S. Hudson, S. Boresch, H.L. Woodcock

COMP 237. Automatic and systematic construction of active spaces from the atomic valence orbitals. **E.R. Sayfutyarova**, G. Chan

COMP 238. Controlling coherent electron transfer in bi-nuclear platinum complexes. **P.J. Lestrange**, D.B. Lingerfelt, X. Li, L.X. Chen

COMP 239. Molecular simulations provide crucial insights into the mechanisms of biocatalysis in ionic liquids. **K. Sprenger**, J. Pfaendtner

Section B

Moscone Center
West Hall

COMP Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

COMP 240. Investigating the fluorescence mechanism of boron-nitrogen based glucose chemosensors and non-traditional hydrogen bonding in B_2H_6 -benzene complexes. **F.L. Kearns**, C. Robart, M.T. Kemp, J. Larkin, H.L. Woodcock

COMP 241. New approach for detection and visualization of aggregation-prone regions. **C. Williams**

COMP 242. Microsecond molecular dynamic simulations on the second hydride transfer transition state of *Pseudomonas mevalonii* 3-hydroxy-3-methylglutaryl reductase using Q2MM. **T. Quinn**, B.E. Haines, J. Lei, H. Jiang, X. Huang, P. Helquist, O. Wiest

COMP 243. Benchmarking excited state absorption via LR/RT-TDDFT for a series of organic chromophores. **J. Asher**, D.N. Bowman, N. Govind, C.J. Cramer

COMP 244. Steric effects in the computational modeling of enediynone cyclization reactions. **K. Hoang**, C.Q. Li, B.F. Gherman, J.D. Spence

COMP 245. Hydricity calculation of catalysts using DFT methods. **H. Fallah**, K.R. Brereton, A.J. Miller, T.R. Cundari

COMP 246. Modeling 10000 antibodies in about an hour: Leveraging the power of the Amazon Cloud. **E. Metwally**

COMP 247. Improving drug design by predicting exposed polarity. **F. Ruggiu**, B. Shirley, J.M. Jansen, H.E. Moser

COMP 248. Prediction of API oxidative liability: *In silico* approach towards antioxidant selection, a collaboration of the Medicinal Chemistry, Formulation Sciences and DMPK departments at AbbVie. **H. Geneste**, L. Asmus, G. Backfisch, M. Degenhardt, F. Oellien

COMP 249. Design of novel inhibitors for the aldehyde dehydrogenases. **E. Selner**, **C. Magee**, L.W. Peterson, M.L. Cafiero

COMP 250. DFT analysis of the selectivity of known bioactive ligands in the sulfotransferase and catechol-o-methyltransferase enzymes. **C. Pinckney**, C. Magee, L.W. Peterson, M.L. Cafiero

COMP 251. Towards more accurate models of organic electro-optic materials: Computing the hyperpolarizabilities of dimer and tetramer charge-transfer chromophores. **J. Maat**, C. Isborn, X. Sosa Vazquez

COMP 252. Design and synthesis of novel inhibitors for the tyrosine hydroxylase enzyme. **R. Evans**, L.W. Peterson, M.L. Cafiero

COMP 253. Analysis of random alloy nanoparticles as catalysts for oxidation reduction reactions. **F. Al-Quaiti**, J. Duncan, B. Corona, C. Lee, E. Trevino, G.A. Henkelman

COMP 254. Exponential relationships capturing atomistic short-range repulsion from the Interacting Quantum Atoms (IQA) method. **A. Wilson**, P. Popelier

COMP 255. Withdrawn.

COMP 256. Machine-learning-assisted characterization of chemical transitions: Inhomogeneous mechanisms underlying reactions in homogeneous solution. **J. Zhang**, Z. Zhang, Y. Gao

COMP 257. Computational outlook on ferroelectricity: Transition state optimizations and charge analysis. **M. Romero**, D. Miller, E. Zurek

COMP 258. New approaches to the computational chemistry and computer-assisted application of calculation for steroids. E.J. Parish, G. Ren, Y. Lo, **M. Hsiao**, **H. Honda**, T. Wei

COMP 259. Novel application of mathematical model to the development of biosensor for high blood cholesterol. **G. Ren**, Y. Lo, **H. Honda**, E.J. Parish

COMP 260. Interplay between crystallization and glass transition in bimetallic nanoalloys. **S. Bechelli**, C. Desgranges, J. Delhommelle

COMP 261. Molecular simulation of gas adsorption in metal-organic frameworks. **G. Karuppasamy**, C. Desgranges, J. Delhommelle

COMP 262. Nitrogen-doped graphene nanoflakes: Electronic and optical properties depending on flake sizes and dopant positions. **C. Lin**

COMP 263. Hydrogen placement on potential organic ferroelectric NUBHOH. **M. Ynfante-Corral**

COMP 264. Activity coefficients of sodium chloride (NaCl) at varying concentrations and temperatures calculated using molecular dynamics simulations. **A. Kasinski**, P.B. Moore, R.L. Napoleon

COMP 265. Investigating the hydration of polyamide 6 using theoretical difference infrared spectroscopy. **B. Thomsen**, Y. Sugita, K. Yagi

COMP 266. Simulating the binding pathways of sialic acid and oseltamivir to H274Y neuraminidase with molecular dynamics simulations. **D.F. Dacres**, E.M. Lewis, R. Wenner, A.W. Van Wynsberghe

COMP 267. Polypeptide bonding to surface studied by computational analysis of x-ray photoelectron spectra. **I. Tolbatov**, D. Chipman

COMP 268. Solvation free energies via alchemical free energy calculations: Applications and challenges. **G. Duarte Ramos Matos**, D.Y. Kyud, G. Calabrò, D.L. Mobley

COMP 269. Mechanistic analysis of a palladium-catalyzed enantioselective decarboxylative allylic alkylation reaction. **A. Sargent**, A.T. Morehead

COMP 270. Computing aqueous absorption spectra: Effect of solute polarity and basis set on convergence with respect to the amount of explicit solvent. **J. Milanese**, C. Isborn

COMP 271. Ionization potential optimized hybrid exchange-correlation functional: Improving the accuracy of both core excitation energies and ground state properties. **Y. Jin**, R.J. Bartlett

COMP 272. Localizing frustration in proteins using coevolutionary information. **B. Sirovetz**

COMP 273. Ab initio molecular dynamics simulations, reaction energy profiles and reaction rates constants expressions relevant to Titan's atmosphere: CH + C_2H_2 and H + CH_2CCH_2. **X. Torres-Garcia**, J.M. Lopez-Encarnacion

COMP 274. Divergent mechanistic pathways in a metal-catalyzed hydroacylation reaction. **E. Bolger**, A.T. Morehead, A. Sargent

COMP 275. DFT, CCSD and CASSCF investigations of 1,1 elimination transition state geometries and post-transition state complexes of hydrofluorocarbons. **M. Nestler**, G.L. Heard, B.E. Holmes

COMP 276. Vanddraabe: Identification and statistical analysis of structurally conserved waters via R. **E.X. Esposito**

COMP 277. Plunger method for simulating polymer crystal-melt interfacial tensions. **Q. Chen**, D. Kozuch, S. Milner

COMP 278. Fullerene based materials for cathodic applications in lithium ion battery. **P. Sood**, K. Kim, S.S. Jang

COMP 279. Towards understanding the chemical physics of the spinach fluorogenic RNA aptamer. **K. Range**, I. Bieker, D.M. York

COMP 280. Molecular dynamics simulation study of Normetanephrine (NMN) on amyloid-beta 40 monomer aggregation for treatment of Alzheimer's disease. **K. Shim**, J. Kim, C. Shin, J.R. Kim, S.S. Jang

COMP 281. Analysis of the role of the electronic structure on lithium diffusion in Li10GP2S12 and -Li3PS4 solid electrolytes. **A.T. Hall**, N. Leclerc, N. Adelstein

COMP 282. Novel approaches to the bioinformatics application of spreading factor in the domain identification and functional prediction. Y. Lo, **G. Ren**, H. Shyu, **H. Honda**, T. Wei

COMP 283. Density functional solution for nondynamic and strong correlation. **J. Kong**, E. Proynov, F. Liu

COMP 284. Automating isotope effects computations and analyses. A. Brueckner, S. Cevallos, **O. Ogba**, D.J. O'Leary, P. Cheong

COMP 285. Atomic-scale simulations of self-assembling peptide-conducting polymer hybrid materials. **H. Pan**, Z. Pollard, E. James, A. Murphy, T. Kowalczyk

COMP 286. Color-based illustration of the maximum overlap method. **Z. Pollard**, K. Le, T. Kowalczyk

COMP 287. Accurate estimate of ligand-binding affinity using alchemical free energy calculation via metadynamics. **Y. Tanida**, A. Matsuura

COMP 288. Modeling rhodium-catalyzed hydroacylation of formylstyrene: Competitive formation of indanone and tetralone products. **T. Shoopman**, A.T. Morehead, A. Sargent

COMP 289. Transition state of a 17 minute timescale drug unbinding event. **S. Lotz**, A. Dickson

COMP 290. Visualization of convolutional neural network scoring of protein-ligand binding. **J. Hochuli**, M. Ragoza, D. Koes

COMP 291. Auto generation of Markush structure for maximizing composition patent claim. **P. Wang**, **Y. Tseng**

COMP 292. Putting electrostatics and water at the center of structure-based drug design. **T. Cheeseright**, M.D. Mackey, G. Tedesco, P. Tosco, S. Tomasio

TECHNICAL PROGRAM

COMP **293.** Understanding the behaviour of multifunctional gold nanoparticles (AuNPs). **A. Raman**, C. Jaime, V.F. Puntes

COMP **294.** Effect of ethanol infiltration into dentin collagen fibrils using molecular dynamics simulation. **J. Liu**, **S. Davis**, H. Du, E. Cho, Z. Abrams, M. Lee, J. No, S. Jee, S.S. Jang

COMP **295.** Novel Zn binding moiety for LpxC identified by data mining, virtual screening, and experimental validation. **P.S. Lee**, C. Bellamacina, J. Bojkovic, Z.K. Sweeney, J. Fu, L. Xie, W. Shu, K. Uehara, L. McDowell, A. Lingel

COMP **296.** Impact of sequence homology on DNA microarray hybridization interactions: A Monte Carlo molecular simulation study. K.J. Mei, C. Lucy, M. Pham, **J.M. Stubbs**

COMP **297.** Investigation of rhodium catalysts and reactants for hydroacylation reactions. **E. Schneider**, J. Scanlon

COMP **298.** Sulfur bonds: Exploration of a novel non-covalent intermolecular bond and its role in drug development. **M.R. Koebel**, G. Schmadeke, S. Sirimulla

COMP **299.** Mixed reality visualization application for drug discovery research. **G. Uranga**, S. Sirimulla

COMP **300.** Connectivity-based hierarchy to eliminate systematic errors: Accurate combustion properties of biofuel molecules using DFT. **S. Debnath**

COMP **301.** Molecular dynamics simulation of the behavior of copper atoms in hydrated zeolite Cu-SSZ-13. **D. Clavijo Gutierrez**, A. Chaparro, E. Jaramillo

COMP **302.** Quantum mechanical calculations of UV-VIS spectra of conjugated molecules. **I. Bieker**, B. May

COMP **303.** Synthesis and structure prediction of a novel, potentially electroactive, organic material. **S. Jacinto**, K.R. Cousins, T. Usher

COMP **304.** Ab initio characterization of halogen bonds involving molecular ionic halogen bond donors. K. Tran, **K. Riley**

COMP **305.** CMDnavigator: A tool for interactive analysis and visualization of peptide data. **A.S. Bayden**, D.J. Diller, J.H. Audie, K. Diller

COMP **306.** Spatially extended active sites: Building favorable electrostatic interactions in natural and designed enzymes. T.A. Coulther, P.J. Beuning, **M.J. Ondrechen**

COMP **307.** Mixed lithium indium halides as solid-electrolytes: Computational experiments on drivers of Li^+ diffusion. **T.C. Alves**, A. Zevgolis, **N. Adelstein**

COMP **308.** Identification of promiscuous enzymes for the aza-Morita-Baylis-Hillman reaction. **K. Ozturk**, S. Sayin, N. Celebi-Olcum

COMP **309.** Estimating kinetic rates for β-cyclodextrin. **H. Pratt**, B.R. Jagger, C. Lee, R.E. Amaro

COMP **310.** Conformational dynamics of histone lysine methyltransferases by millisecond-timescale molecular dynamics on Folding@home. **R.P. Wiewiora**, S. Chen, K. Beauchamp, M. Luo, J.D. Chodera

COMP **311.** Multiscale estimation of kinetic rates of trypsin with benzamidine using a hybrid molecular dynamics, brownian dynamics, and milestoning approach. **B.R. Jagger**, L. Votapka, A. Heyneman, R.E. Amaro

COMP **312.** Prediction of pH dependent NMR chemical shifts. **E. Artikis**, C.L. Brooks

COMP **313.** Generic interface streamlines access to results from expertly prepared 3D models. **T. Mansley**, E. Champness, C. Leeding, P. Hunt, N. Foster, M. Segall

COMP **314.** Computational studies of electrochemical initiation of reactions involving nitrogen-radical precursors. **S. Calderon**, H.P. Hratchian

COMP **315.** Bond dissociation enthalpies of halomethanes, haloethanes, haloethenes, and haloacetylene. **K.R. Jorgensen**

COMP **316.** Photocatalytic and electronic implications from first principles characterization of oxygen depletion localized on TiO_2 brookite nanoparticle surfaces. **K.G. Johnson**, E.A. Jarvis

COMP **317.** *Ab initio* characterization of intramolecular and energetic features of the water oxidation mechanism for mononuclear ruthenium and iron catalysts. **K. Hunter**, E.A. Jarvis

COMP **318.** Computational study of how β-loop dynamics regulate HCV polymerase activity in the presence and absence of thumb-site-II inhibitors. **N. Ibrahim**, J. Li, K. Johnson, S. Kirmizialtin

COMP **319.** DFT design of inhibitors of the LpxC enzyme. **C. Dishuck**, R. Roldan, A.J. Dewar, L.W. Peterson, M.L. Cafiero

COMP **320.** DFT study of the selectivity of phenylalanine hydroxylase. **M.C. Perchik**, L.W. Peterson, M.L. Cafiero

COMP **321.** Modeling excited states of the OH radical reaction with cyclopentadiene and the cyclopentadienyl radical. **P.B. Orndorff**, J.B. Foresman

COMP **322.** DFT study of the selectivity of the tyrosinase active site. **D. Wilson**, S. Fields, L.W. Peterson, M.L. Cafiero

COMP **323.** Linkage isomerization In phosphine substitution reactions of $CpRu(PPh_3)_2NCS$. **D. Dang**, R.U. Kirss

COMP **324.** DFT study of the selectivity of monoamine oxidase B (MAOB). **S. Jelinek**, M. Morris, L.W. Peterson, M.L. Cafiero

COMP **325.** Structural insights of a PI3K/mTOR dual inhibitor with the morpholino-triazine scaffold. **T. Takeda**, Y. Wang, S.H. Bryant

COMP **326.** Effect of Gly to Ser mutations at the integrin-binding site on type I collagen. **A. Mekkat**, H. Yu, B. Brodsky, Y. Lin

COMP **327.** Mechanism for the stereoselectivity in metal-salen catalyzed electroreductive cyclization reactions. **L. Bellini**, M.N. Cihak, B.E. Silva, B.F. Gherman, J.A. Miranda

COMP **328.** Withdrawn.

COMP **329.** Approach for analyzing protein pockets using properly interacting probe molecules. **H. Sato**, A. Matsuura

COMP **330.** Elucidating the mechanism of protein unfolding and translocation by the ClpY ATPase during protein degradation. **Y. Shih**, G. Stan

COMP **331.** Quantum mechanical investigation of the inner sphere reduction mechanism of the [(NSNSN)Co(III)Cl^+] and [(NSSSN)Co(III)Cl^+] cations by iron(II). **W. Smith**, T.A. Jackman, O. Sode

COMP **332.** Molecular simulation of transport of DNA grafted nanoparticles. **S. Ciobotarescu**, J. McLaughlin, C. Desgranges, J. Delhommelle

COMP **333.** Molecular simulations of bubble formation in metastable liquids. **B. Gonzalez**, L. Huber, C. Desgranges, J. Delhommelle

COMP **334.** Subset system study of diisopropylammonium bromide: An organic ferroelectric crystal. **C.M. Sanchez**

COMP **335.** Investigation of different binding kinetics among the neuraminidase inhibitors. **G. Kang**, A.W. Van Wynsberghe

COMP **336.** Examining the binding pathways of peramivir to wild-type neuraminidase through molecular dynamics simulations and MM/GBSA analysis. **R. Wenner**, A.W. Abera, B.J. Banman, A.W. Van Wynsberghe

COMP **337.** DFT study of the selectivity of DOPA-decarboxylase. **E. Harrison**, A.R. Ritter, L.W. Peterson, M.L. Cafiero

COMP **338.** Modeling material properties and charge transfer for lithium-ion batteries. **L. Raguette**, R. Jorn

COMP **339.** Analysis of MM/GBSA free energy calculations to investigate the binding pathways of neuraminidase. **E.M. Lewis**, P.F. Marris, L.M. Krause, A.W. Van Wynsberghe

COMP **340.** Novel approaches to the computer assisted informatics of oxysterol and 7-ketocholesteryl benzoate. E.J. Parish, **G. Ren**, Y. Lo, **H. Honda**

COMP **341.** Automated selection of active orbital spaces. **C.J. Stein**, M. Reiher

COMP **342.** Computational studies of the UV/visible absorption spectra of selected merocyanine dyes. **I. Tolbatov**, S. Grimme

COMP **343.** Examining ligand recognition in RNA aptamers via molecular dynamics simulations. **P. Gasper**, A.A. Chen

COMP **344.** Development of a coarse-grained model of polypeptoids for studying self-assembly in solution. **P. Du**, R. Kumar

COMP **345.** Fragment ER: Efficient and accurate binding free energy calculation method for protein-ligand complex. **T. Masuda**, R. Tanimura, N. Matubayasi

COMP **346.** Accurate absorption spectra of aqueous estrogen derivatives via molecular dynamics/EOM-CCSD. **D. Ruuska**, M. Paul, S.N. Eustis

COMP **347.** Visualising the molecular drivers behind drug resistance. **M. Malaisree**, C.J. Woods

COMP **348.** Predicting polythiophene electronic structures: Statistical model screening for the efficient discovery of OPV materials. **M. Cole**, I. Kanal, G. Hutchison

COMP **349.** Molecular simulation study of the 3,4-dihydroxymandelic acid on amyloid beta 40 monomer for treatment of Alzheimer's disease. **E. Tumurbaatar**, J. Kim, C. Shin, S. Jang, J.R. Kim

COMP **350.** Modelling UV-vis spectra for a series of alkenyl substituted pyrroles. **R. Fair**

COMP **351.** Computationally predicted signatures of EGFR exon 20 insertions in non small cell lung cancer and its response to irreversible inhibitors. **B. Su**, D. Huang, P. Wang, O. Lin, **Y. Tseng**

COMP **352.** Longtime simulation of dynamical fractures in vault nanoparticles through multiscale molecular dynamics. **J.M. Espinosa Duran**, A. Abi Mansour, P. Ortoleva

COMP **353.** Molecular modeling of small molecule inhibitors of the Hv1 proton channel. **V.T. Lim**, A.D. Geragotelis, N. Lim, J.A. Freites, D.L. Mobley, D. Tobias

COMP **354.** *In silico* measurements of the ionic current in a K^+ ion channel using weighted ensemble simulations. **S. Capponi**, H. Siddiqi, J. Adelman, J. Rosenberg, M. Grabe

COMP **355.** Ligand- and receptor-based virtual screening for inhibitors of the signal transducer and activator of transcription 5 (STAT5). **E. Gianti**, G. Fiorin, M.L. Klein, R.J. Zauhar

COMP **356.** Incorporating continuum solvent-based receptor desolvation into molecular docking. **R. Stein**, T.E. Balius, B. Shoichet

COMP **357.** Evaluating use of tens to hundreds of active ligands in pharmacophore hypothesis perception. **E.T. Mack**, S.L. Dixon, C.D. Von Bargen, M.P. Repasky

COMP **358.** Density functional theory study of the binding of tyrosine and phenylalanine with graphene. **D.A. Daggag**, J. Lazare, T. Dinadayalane

COMP **359.** Molecular modeling of multicompartment micelle nanoreactors. **C.P. Callaway**, P. Sood, S. Jang

COMP **360.** Identification of ZIKA virus inhibitors using insilico screening. **M. Rivera**, S. Sirimulla

COMP **361.** Non-adiabatic QM/MM: A hybrid approach to doing non-adiabatic excited state dynamics. **D.A. Tracy**, J. Bjorgaard, S. Tretiak, A.E. Roitberg

COMP **362.** Rationalization and visualization of non-bonded interactions using extended Hückel theory. A. Ajamian, C. Williams, P. Labute, **N. Li**

COMP **363.** Simulations of small molecule diffusion in polyelectrolyte solutions. **P.K. Walhout**, Z. He, A.A. McMillan, T.D. Sedlacek

COMP **364.** Python program for solving problems in computer-aided peptide design. **A.S. Bayden**, J.H. Audie, D.J. Diller

COMP **365.** Effects of virion structural changes on binding events related to molecular mechanisms of influenza infections by brownian dynamics simulations. **S.E. Kochanek**, J.D. Durrant, R.E. Amaro

COMP **366.** IKKβ dynamic structure regulates NF-κB pathway in inflammatory response. **T.T. Nguyen**, J. Schiffer, G. Ghosh, R.E. Amaro

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

COMP **367.** Engineering increased activity into a ketosteroid isomerase homologue through predictive computational methods. **G. Levine**, T.A. Coulther, P.J. Beuning, M.J. Ondrechen

COMP **368.** Information-driven fully flexible HADDOCKing: Performance on a benchmark of protein-ligand complexes. **J. Grinstead**, A. Thureau, J.P. Rodrigues, K.R. Reinke, A.F. Ramsing, T.L. Wormwood, A. Bonvin

COMP **369.** Docking studies of camodulin and fulvic acid. **F.C. Zhang**, L. Liu, Y. Wu

COMP **370.** First-principles study of di-substituted donor moieties on NLO properties: Theoretical paradigms of interactive computation. **M. Janjua**

COMP **371.** Study on the interaction between resveratrol and CopC by spectroscopic and docking methods. Z. Song, **F.C. Zhang**

COMP **372.** $C_{59}Pd$: A novel heterogeneous catalytic material for Suzuki-Miyaura reaction. **M.C. Padole**, P. Deshpande

COMP **373.** Withdrawn.

COMP **374.** PYCED: An efficient technique to simulate charge and exciton dynamics coupled with DFT methods for large systems. **P. Ramos**, M. Pavanello

COMP **375.** Theoretical investigation of electron-nuclear dynamics in the $[Au_{25}(SH)_{18}]^{-1}$ thiolate-protected gold nanocluster. **R.D. Senanayake**, A.V. Akimov, C.M. Aikens

COMP **376.** Withdrawn.

COMP **377.** Predicting *N*-methylated cyclic peptide structures to inform force field development. **D. Slough**, H. Yu, S. McHugh, Y. Lin

COMP **378.** ALKBH7 variant related to prostate cancer exhibits altered substrate binding. **A. Walker**, P. Silvestrov, T.A. Müller, R.H. Podolski, G. Dyson, R.P. Hausinger, G.A. Cisneros

COMP **379.** Withdrawn.

COMP **380.** Supramolecular effects in radical chemistry. **G. Gomes**, I. Alabugin

COMP **381.** Withdrawn.

COMP **382.** *In silico* discovery of high performance organic polymers for optical applications. **M. Afzal**, J. Hachmann, C. Cheng

COMP **383.** Linear absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory. **D.R. Nascimento**, A.E. DePrince

COMP **384.** Withdrawn.

COMP **385.** Plasmonic resonances: A systematic analysis of metallic nanoparticles using real-time, time-dependent DFTB. **N. Ilawe**

COMP **386.** Withdrawn.

COMP **387.** Kirkwood Buff derived force field for some biologically important oxo anions. **N. Naleem**, P.E. Smith

COMP **388.** Withdrawn.

COMP **389.** Scaffold repurposing of ring-constrained nucleosides: A molecular modeling perspective. **A. Ciancetta**, D. Tosh, K.A. Jacobson

COMP **390.** Systematic parameterization of lignin for the CHARMM force field. **J.V. Vermaas**, L. Petridis, G. Beckham, M.F. Crowley

COMP **391.** Elucidating the functional roles of spatial organization in cross-membrane signal transduction by a hybrid simulation method. **Y. Wu**

COMP **392.** Insights into the nature of glass formation from ultra-efficient simulations of the supercooled state. **D.S. Simmons**, J. Hung, T.K. Patra, J. Mangalara, V. Meenakshisundaram

COMP **393.** Toward polarizable AMOEBA thermodynamics at fixed charge efficiency using a dual force field approach: Application to peptides and proteins. J.M. Litman, S.D. LuCore, C. O'Connell, **M.J. Schnieders**

COMP **394.** Understand protein functions by comparing the similarity of local structural environments. **Y. Wu**

COMP **395.** Large-scale v2RDM-driven CASSCF methods. **A.E. DePrince**

COMP **396.** Ligand residence times from simulation using loosely coupled parallel trajectories. **A. Dickson**

COMP **397.** Elucidating mechanisms of RNA recognition and processing in the exosome complex via enhanced sampling molecular dynamics simulations. **L. Vukovic**

COMP **398.** Incorporation of sigma hole scoring function in Autodock Vina. **S. Sirimulla**

COMP **399.** Hard-sphere Monte Carlo model of nanomaterial toxicity. **N. Assefa**

COMP **400.** Investigating the structure of PEI-nucleic acid gene delivery complexes using molecular dynamic simulations. **N. Walker**

COMP **401.** Elucidating binding mechanisms of ABA analogues: Activation of PYL5 receptor by pyrabactin and quinabactin. **M. Meigooni**, C. Zhao, D. Shukla

COMP **402.** Binding site protonation and self-correcting occlusion control the Na^+/K^+-pump selectivity. **H. Rui**, P. Artigas, B. Roux

COMP **403.** Towards a rational design of macrolide antibiotics in order to combat the bacterial resistance. **A. Pavlova**, J.M. Parks, A.K. Oyelere, J. Gumbart

COMP **404.** Physiologically relevant transmembrane potential modelling of complex lipid bilayer systems. **X. Lin**, A. Gorfe

COMP **405.** Interaction affinity of biological molecules with 2D materials. **N. Saikia**, K. Waters, U. Saikia, M. Seel, R. Pandey

COMP **406.** Comparative analysis of the structural determinants of endogenous cannabinoids and activity of illicit drugs on cannabinoid receptors. **V.K. Yadav**, K.M. Elokely, M.L. Klein

COMP **407.** Catalytic mechanism of RNase A transphosphorylation. **M. Huang**, D.M. York

COMP **408.** Implementation of analytic gradient for FMO RI-MP2 method. **B.Q. Pham**, M.S. Gordon

COMP **409.** Modeling and simulation of AcrB multi drug transporters functional dynamics. **S. Jamshidi**, M. Sutton, K.M. Rahman

COMP **410.** Through-space and through-bond stabilization of cis alkenyl anions. **H. Villegas**, K.B. Wiberg, B.G. Janesko

COMP **411.** Community participation in the D3R Continuous Evaluation of Ligand Pose Prediction (CELPP) competition. **J. Wagner**, S. Liu, S.M. Gathiaka, R. Malmstrom, M.K. Gilson, R.E. Amaro

COMP **412.** Simulation of the interaction between polymer-encapsulated air microbubble and blood cell in the blood vessel. **Z. Wang**

COMP **413.** Unified framework for computer-aided biologics design. **A. Deschenes**

COMP **414.** Challenges in the discovery of macrocyclic cyclophilin inhibitors. **U. Schmitz**, D. Shivakumar

Section C

Moscone Center

West Hall

NVIDIA GPU Award

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

6:00 - 8:00

COMP **415.** Multiscale modeling of poly(ethylene oxide) with ionic liquids: GPU enabled first-principles force fields. **C. Son**, J. McDaniel, J.R. Schmidt, Q. Cui, A. Yethiraj

COMP **416.** GPU implementation of molecular docking with applications to receptor flexibility and energy landscape sampling. **J. Sunseri**, D. Koes

COMP **417.** Calculation of host-guest binding free energies via the AMOEBA polarizable force field. **M.L. Laury**, J.W. Ponder

COMP **418.** ANAKIN-ME: Using deep learning to develop a fully-transferable and chemically accurate GPU-accelerated potential. **J.S. Smith**, O. Isayev, A.E. Roitberg

COMP **419.** GPU-enabled real-time electron dynamics of nitrogen-doped graphene nanoflakes. **S.I. Allec**, B.M. Wong

Section D

Moscone Center

West Hall

OpenEye Outstanding Junior Faculty Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **420.** Multiscale simulations to elucidate enzymatic processing of DNA and RNA. **M. De Vivo**

COMP **421.** Accounting for water in early stage drug discovery and design. **T.P. Kurtzman**

COMP **422.** Accelerating real-time electron dynamics calculations of large plasmonic systems. **B.M. Wong**

COMP **423.** Multireference quantum chemistry and conical intersections at the nanoscale. **B.G. Levine**

COMP **424.** Elucidating heterogeneous ice nucleation mechanisms using large scale rare event simulations. **S. Sarupria**, B. Glatz, R. Defever, W. Hanger, L. Ngo, A. Apon

Section E

Moscone Center

West Hall

Wiley Computers in Chemistry Outstanding Postdoc Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **425.** Electronic transitions in the condensed phase: Real-time and linear-response time-dependent density functional theory. **M. Provorse**, C. Isborn

COMP **426.** Phospholipases A_2 a pharmaceutical target to diminish inflammation. **V. Mouchlis**, J. McCammon, E.A. Dennis

WEDNESDAY MORNING

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Cosponsored by PHYS

G. Verkhivker, *Organizer*

C. Chang, *Organizer, Presiding*

8:30 COMP **427.** Allostery through the lens of a computational microscope. **R.E. Amaro**

9:00 COMP **428.** Discrete molecular dynamics approach to the study of protein conformational changes. **M. Orozco**

9:30 COMP **429.** Molecular simulations of membrane sensing and remodeling dynamics. **G. Hummer**, R. Covino, A. Bahrami, R. Bhaskara, J. Köfinger

10:00 Intermission.

10:20 COMP **430.** ATP hydrolysis as a driver of conformational change, an example of GroEL. J. Liu, K. Kavran, Y. Wang, K. Jia, **R.L. Jernigan**

10:50 COMP **431.** Conformational transition in kinase from explicit solvent simulations and Markov model analysis. **Q. Cui**

11:20 COMP **432.** Surveying key residues for protein allostery using rigid residue scan method. **P. Tao**

Section B

InterContinental San Francisco

Fremont

Material Science

Organic

C. M. Aikens, *Organizer*

A. Abbaspour Tamijani, *Presiding*

8:30 COMP **433.** Functional group dependent conductance of stilbene: A first-principle transport study. **M.R. Neupane**, C. Carlin, C.B. Rinderspacher, J. Andzelm

9:00 COMP **434.** Design principles for organic photovoltaic materials from ab initio simulations. **M.B. Goldey**, D. Reid, J.J. De Pablo, G.A. Galli

9:30 COMP **435.** DFT evidence of unforeseen bending in linearly fused polycyclic rings of hexasilabenzenoids. **A. Gupta**, J. Arora

10:00 Intermission.

10:30 COMP 436. Identification of next-generation materials for organic solar cells via a collaborative theory-experimental approach. **S.A. Lopez**, N.C. Davy, A. Oh, A. Aspuru-Guzik, Y. Loo

11:00 COMP 437. Theory linked with experiment in discovering new functional organic/organometallic materials. **K.R. Cousins**, T. Usher, R. Zhang, D. Miller, D.C. Smith

11:30 COMP 438. Capturing the role of temperature in crystal polymorph stability using molecular modeling. E. Dybeck, N. Abraham, N.P. Schieber, **M.R. Shirts**

12:00 COMP 439. Predicting relative polymorph stability using multistate reweighting methods and Jacobian mapping. **N.P. Schieber**, E. Dybeck, M.R. Shirts

Section C

InterContinental San Francisco

Howard

Drug Design

Structure-Based Approaches

M. R. Landon, Y. Tseng, *Organizers*

C. Dickson, *Presiding*

8:30 COMP 440. Structural insight into sodium-dependent sugar transporters and their inhibition mechanism. **P. Bisignano**, C. Ghezzi, A. Paz, C. Kalyanaraman, M.P. Jacobson, R. Friemann, J. Abramson, E. Wright, M. Grabe

8:55 COMP 441. Structural insight into KRAS A146 mutations from molecular simulations. **T. Abramyan**, K. Rossman, D. Kireev

9:20 COMP 442. Interdependence of inhibitor recognition in HIV-1 protease subsites. **J.L. Paulsen**, F. Leidner, D. Ragland, N. Kurt Yilmaz, C.A. Schiffer

9:45 Intermission.

10:05 COMP 443. Systematic investigation of increased protein flexibility in protein-ligand docking with mixed-resolution Monte Carlo. **J.M. Spiriti**, D.M. Zuckerman

10:30 COMP 444. Computational investigation of the DNA binding domain of p53: A drive towards novel therapeutics. **J.W. Essex**, M.P. Criddle, Z. Ouaray, C. Verma

10:55 COMP 445. Origin of preferential binding of aryl chloride groups in serine protease S1 pockets: An application of Fragment Symmetry-Adapted Perturbation Theory (F-SAPT) to drug protein binding. **D.L. Cheney**, D.F. Sitkoff, R.M. Parrish, C. Sherrill

11:20 COMP 446. Dealing with x-ray data in structure-based design: Estimating and visualizing electron density support. A. Meyder, E. Nittinger, G. Lange, R. Klein, **M. Rarey**

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

Section D

InterContinental San Francisco

Cathedral Hill

Molecular Mechanics

Foldamers, Carbohydrates, Macrocycles & Cyclic Peptides

M. Feig, *Organizer*

J. F. Rudzinski, *Presiding*

8:30 COMP 447. Computational investigations of functional arylamide foldamers. **V. Pophristic**, Z. Liu, A. Abramyan, S. Makeneni

9:00 COMP 448. Mutations tuning the structure and dynamics of amylin fibrils. **F. Tofoleanu**, Y. Yuan, B. Brooks, N. Buchete

9:30 COMP 449. Molecular dynamics modeling of fluorescent rosette nanotubes. **A. Gonzales**, B. Legesse, T. Yamazaki, H. Fenniri

9:55 Intermission.

10:10 COMP 450. Developing enhanced sampling methods for cyclic peptides. **S. McHugh**, J. Rogers, H. Yu, Y. Lin

10:35 COMP 451. Cyclization, docking, and sampling macrocycles with prime. **D.J. Sindhikara**, T. Day, K. Borrelli

11:05 COMP 452. Seeing the invisible: Dynamics of glycans on neuronal NMDA receptors. **A. Sinitskiy**, N. Stanley, V.S. Pande

11:35 COMP 453. Revealing the *T. reesei* Cel6A hydrolysis mechanism via transition path sampling. **H. Mayes**

Section E

InterContinental San Francisco

Laurel Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

D. Nascimento, *Presiding*

8:30 COMP 454. Intersystem crossings kinetics in complex systems: Implementation of minimum energy crossing point search within the fragment molecular orbital method. **D.S. Kaliakin**, Y. Alexeev, D.G. Fedorov, S.A. Varganov

8:55 COMP 455. One- and three-electron bonding in conjugated hydrocarbons. **M. Alkan**, A. Rogachev

9:20 COMP 456. Nonadiabatic molecular dynamics with delta-SCF excited states. **A.V. Akimov**

9:45 COMP 457. Nonadiabatic transition state theory: Application to intersystem crossing in Cl_2CS. **A.O. Lykhin**, S.A. Varganov

10:10 Intermission.

10:25 COMP 458. Electronic structure of single molecule magnets. **B. Vlaisavljevich**, D.E. Freedman, S.T. Liddle, L. Gagliardi, T. Shiozaki

11:00 COMP 459. Computational study of metal-oxo reactive species in porous media with strongly correlated methods. **K.D. Vogiatzis**, L. Gagliardi, E. Pidko

11:35 COMP 460. Modelling the pump-probe spectroscopy of opsin mimics. **B. Demoulin**, G. Cerullo, I. Rivalta, M. Garavelli

Section F

InterContinental San Francisco

Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG‡

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

8:30 COMP 461. Calculations of NMR shifts in metallic and insulating solids. **P. Blaha**

8:55 COMP 462. Computational studies of metal oxide clusters as models for surface defect sites: Modeling electron detachment with efficient electronic structure methods. **H.P. Hratchian**

9:20 COMP 463. Nonlinear properties from TDDFT: Trials and tribulations. **S.M. Parker**, F.U. Furche

9:45 COMP 464. Scalable all-electron theory of real-world molecules and materials - examples: Light harvesting and NMR. **V. Blum**

10:10 Intermission.

10:30 COMP 465. Functional 2D and 3D borides. P.J. Robinson, Z. Cui, **A. Alexandrova**

10:55 COMP 466. Challenges in calculating the bandgap of triazine-based carbon nitride structures. **S.N. Steinmann**, S. Melissen, T. Le Bahers, P. Sautet

11:10 COMP 467. Optical properties of highly absorbing Helquat derivatives: *Ab initio* study. **D. Galaktionova**, E. Muchová, P. Slavicek

11:25 COMP 468. Finding intersystem crossing points between two single-reference potential energy surfaces. **X. Sheng**, L.M. Thompson, H.P. Hratchian

11:40 COMP 469. Describing a strongly correlated model material system with a mean-field method. **J. Kong**, E. Proynov, J. Yu, R. Pachter

12:05 COMP 470. *Ab initio* modeling of charge transport defects in quantum dot arrays. **M.B. Goldey**, N.P. Brawand, M. Voros, G.A. Galli

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Photocatalysis

Sponsored by CATL, Cosponsored by COMP

In situ Characterization Tools

Sponsored by CATL, Cosponsored by COMP

Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

Sponsored by CINF, Cosponsored by COMP

WEDNESDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

R. E. Amaro, *Presiding*

1:30 COMP 471. PROGNOSTIX: A pipeline for personalized diagnostics and drug. **J. Skolnick**

2:00 COMP 472. Investigating allosteric regulation and cryptic pocket formation through enhanced sampling simulations. **F. Gervasio**

2:30 COMP 473. Prediction on allosteric and cryptic sites on ligand-free protein structures. **S. Vajda**, D. Kozakov, D.R. Hall

3:00 Intermission.

3:20 COMP 474. Computational riboswitch detection and design using inverse RNA folding simulations with ligand binding information. M. Drory, I. Kifer, S. Sengupta, Z. Yakhini, **D. Barash**

3:50 COMP 475. Fine-tuned allosteric regulation of neuronal NMDA receptors with potential therapeutic importance. **N. Stanley**, A. Sinitskiy, B.D. Sellers, V.S. Pande

Section B

InterContinental San Francisco

Fremont

Material Science

Electron Transfer & Nanoparticles

C. M. Aikens, *Organizer*

M. Provorse, *Presiding*

1:30 COMP 476. Functional mode hot electron transfer theory. J. Elenewski, J. Cai, W. Jiang, **H. Chen**

2:00 COMP 477. Scaling relationships for nonadiabatic energy relaxation times in warm dense matter: Toward understanding the equation of state. **A.V. Akimov**

2:30 COMP 478. Investigation of many-body correlation in excitonic and biexcitonic systems using electron-hole multicomponent coupled-cluster theory (eh-mcCC). B.H. Ellis, **A. Chakraborty**

3:00 COMP 479. Unraveling excitation energy transfer mechanisms in plasmonic nanoantennas. **N. Ilawe**, M.B. Oviedo, B.M. Wong

3:30 Intermission.

4:00 COMP 480. Luminescence properties of $Au_{38}(SH)_{24}$ and $Au_{22}SH_{18}$ nanoparticles. **K. Weerawardene**, C.M. Aikens

4:30 COMP 481. Theoretical study of the chiroptical activity of BINAP– and DIOP– stabilized undecagold clusters. **N. Karimova**, C.M. Aikens

5:00 COMP 482. Double ring tubular structures of boron clusters stabilized by metal atom doping: M@B_{14} (M = Cr, Fe, and Ni). **P. Saha**, A. Rahane, N. Sukumar, V. Kumar

‡ *Cooperative Cosponsorship*

Section C

InterContinental San Francisco
Howard

Molecular Mechanics

Membrane-Interacting Proteins & Peptides

M. Feig, *Organizer*

S. Lindert, *Presiding*

1:30 COMP **483.** Structure-kinetic relationships of passive membrane permeation from multiscale modeling. **C. Dickson**, V. Hornak, R.A. Pearlstein, J. Duca

2:00 COMP **484.** Modeling permeability through outer-membrane channels in gram-negative pathogens. **S. Acosta-Gutierrez**, I. Bodrenko, S. Susruta, G. Malloci, M. Scorciapino, M. Ceccarelli

2:25 COMP **485.** Studying the substrate specificity and reactivity of MycG: A multifunctional enzyme. **S. Yang**, J.M. Grandner, M. Demars, D.H. Sherman, K.N. Houk

2:50 Intermission.

3:05 COMP **486.** Graded activation and free energy landscapes of a muscarinic G protein-coupled receptor. **Y. Miao**, J. McCammon

3:35 COMP **487.** Structural insights into conformation and dynamics of the cannabinoid CB2 receptor through an extended MD simulation of CP 55, 940–CB2 complex. **P. Pandey**, K. Roy, R.J. Doerksen

4:05 COMP **488.** Cell-scale computational modeling methodologies for living membranes. **J.V. Vermaas**, E. Tajkhorshid

4:35 COMP **489.** Oncogenic mutations differentially affect bax monomer, dimer, and oligomeric pore formation in the membrane. **M. Zhang**, J. Zheng, R. Nussinov, B. Ma

Section D

InterContinental San Francisco
Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

J. Larkin, *Presiding*

1:30 COMP **490.** QM cluster model examination of constrained biphenyl dihedral rotation within a modified threonyl-tRNA synthetase: A transition state trapped? T.J. Summers, **N.J. Deyonker**

2:05 COMP **491.** High-level characterization of the properties of R-X...π interactions in protein-ligand complexes. **K. Riley**, K. Tran

2:30 COMP **492.** Improved energy decomposition analysis for studying covalent bonds. **D.S. Levine**, M.P. Head-Gordon

2:55 Intermission.

3:10 COMP **493.** Developments in stochastic coupled cluster theory. **A.J. Thom**

3:35 COMP **494.** Electron propagator theory and correlation-bound anions. **J.V. Ortiz**

4:00 COMP **495.** Improving efficiency of semi-direct MP2 through oversubscription. **E. Fought**, V. Sundriyal, M. Sosonkina, T.L. Windus

4:25 COMP **496.** Development of a many-body carbon dioxide potential and its application to clusters up to $(CO_2)_{13}$. **O. Sode**

Section E

InterContinental San Francisco
Laurel Hill

Drug Design

Structure-Activity Relationships & Pharmacophores

M. R. Landon, Y. Tseng, *Organizers*

J. M. Spiriti, *Presiding*

1:30 COMP **497.** Combining protein interaction potentials with water analysis in structure-based design. **T. Cheeseright**, M.D. Mackey, G. Tedesco, S. Tomasio, P. Tosco

1:50 COMP **498.** Optimization of shape fingerprints for protein-ligand systems. **J. Zarnecka**, A.G. Leach, S.J. Enoch

2:10 COMP **499.** Deep learning profile-QSAR 2.0 IC_{50} predictions as accurate as 4-pt IC50s: Applications to polypharmacology. **E.J. Martin**, V. Polyakov, L. Tian

2:30 COMP **500.** Towards in-silica screening of molecule permeation through outer membrane channels in Gram-negative bacteria. I. Bodrenko, S. Acosta Gutierrez, T. D'Agostino, S. Samanta, S. Salis, G. Malloci, M. Scorciapino, **M. Ceccarelli**

2:50 Intermission.

3:10 COMP **501.** Withdrawn.

3:30 COMP **502.** GPCR activation: Principle component analysis as a diagnostic signature correlated with SAR. **D.L. Harris**, J.B. Thomas, Y. Zhang, E. Gay, S. Runyon

3:50 COMP **503.** Molecular simulation of EFdA and related analogs to determine the structural basis of HIV-1 drug resistance. **D. Das**, Y. Takamatsu, S. Kohgo, S. Hattori, H. Hayashi, K. Matsuda, S. Sarafianos, H. Mitsuya, K. Maeda

4:10 COMP **504.** Automated extraction of pharmacophores and toxophores from large-scale *in vitro* pharmacology data. **A. Dossetter**, E.J. Griffen, A.G. Leach, J. Stacey, L. Reid, S. Montague

Section F

InterContinental San Francisco
Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG²

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

1:30 COMP **505.** Towards a chemically accurate description of reactions of molecules with transition metal surfaces. **G. Kroes**

1:55 COMP **506.** Towards accurate and reliable simulations water at interfaces, and more…. **A. Michaelides**

2:20 COMP **507.** Understanding and eliminating delocalization error in transition metal chemistry. T.Z. Gani, Q. Zhao, **H.J. Kulik**

2:45 COMP **508.** Development of a general framework for coupling machine learning and *ab initio* approaches in materials chemistry. **A. Kolpak**

3:10 Intermission.

3:30 COMP **509.** ANAKIN-ME: A general purpose and chemically accurate deep learned potential. J.S. Smith, O. Isayev, **A.E. Roitberg**

3:55 COMP **510.** Efficient parallelization of the calculation of exact exchange for plane-wave DFT. **T.A. Barnes**, J. Deslippe, P. Kent, D. Prendergast

4:10 COMP **511.** Application of ab initio many-body perturbation theory with Gaussian basis sets to the singlet and triplet excitations of organic molecules. **S. Hamed**, T. Rangel, F. Bruneval, J. Neaton

4:25 COMP **512.** QM/MM simulations of TADF materials. **P. de Silva**, T. Zhu, T.A. Van Voorhis

4:50 COMP **513.** Accurate level alignment at molecule-metal interfaces from an optimally-tuned range-separated hybrid functional. **Z. Liu**, D.A. Egger, S. Refaely-Abramson, L. Kronik, J. Neaton

5:05 COMP **514.** Hybrid functional pseudopotentials. **L. Tan**, J. Yang, A.M. Rappe

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Transition Metal & Metal Oxide Catalysis

Sponsored by CATL, Cosponsored by COMP

Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

Sponsored by CINF, Cosponsored by COMP

THURSDAY MORNING

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

M. P. Jacobson, *Presiding*

8:30 COMP **515.** Computer-aided discovery of allosteric modulators for a muscarinic G-protein-coupled receptor. **Y. Miao**, J. McCammon

9:00 COMP **516.** Structure-based design of allosteric K-Ras inhibitors. **A. Gorfe**

9:30 COMP **517.** Kinase allostery atlas. **D. Kozakov**

10:00 Intermission.

10:20 COMP **518.** Mechanisms for allosteric inhibition of protein tyrosine phosphatase 1B. **H.P. Hendrickson**, J. Lipchock, B. Douglas, I. Rivalta, N. Ten, V.S. Batista, J. Loria

10:50 COMP **519.** Order in the disordered polybasic domain of K-Ras. **P.S. Srivastava**, Y. Zhou, H. Liang, K. Cho, J. Hancock, A. Gorfe

11:20 COMP **520.** Exploring the therapeutic landscape of chromatin via integrative computational modeling: An allosteric regulation from transition metal agents. **G. Palermo**, Z. Adhireksan, T. Riedel, Z. Ma, R. Muhammad, U. Roethlisberger, P. Dyson, C. Davey

Section B

InterContinental San Francisco
Fremont

Material Science

Functional Materials & High-Throughput Screening Methods

C. M. Aikens, *Organizer*

N. Saikia, *Presiding*

8:30 COMP **521.** Assessing the potential of $LaCrO_3$ as a *p*-type semiconducting oxide. **A.L. Gavin**, G.W. Watson

9:00 COMP **522.** Interatomic potential for a perovskite electrolyte derived from first principles. **A.K. Lucid**, G.W. Watson

9:30 COMP **523.** High-throughput screening of transparent conducting oxides. **C. Sutton**, R.J. Baldock, L.M. Ghiringhelli, M. Scheffler

10:00 COMP **524.** Gibbs energies of solids through materials informatics. **C. Bartel**, A. Deml, S. Miller, J. Rumptz, A.W. Weimer, S. Lany, C. Musgrave, V. Stevanovic, A. Holder

10:30 Intermission.

11:00 COMP **525.** *In silico* design of 3D covalent organic frameworks for gas adsorption applications. **R. Mercado**, R. Fu, B. Smit

11:30 COMP **526.** Understanding of spectacular gas adsorption/separation phenomena in metal-organic frameworks. R. Pillai, **G. Maurin**, S. Krause, S. Kaskel, J. Yoon, J. Chang

12:00 COMP **527.** Cryptands as cathode materials for batteries. **H. Gokturk**

Section C

InterContinental San Francisco
Howard

Molecular Mechanics

Force Fields

M. Feig, *Organizer*

F. Tofoleanu, *Presiding*

8:30 COMP **528.** Toward more accurate force fields through direct chemical perception. **D.L. Mobley**, C. Bannan, C. Zanette, C.I. Bayly, J.D. Chodera, M.R. Shirts, J. Fass, B. Manubay, P. Eastman, M.K. Gilson

9:00 COMP **529.** Systematic exploration of hydration thermodynamics and kinetics of various approximate polarization schemes. **F.C. Pickard**, A.C. Simmonett, G. Koenig, J. Huang, B. Brooks, J.W. Ponder

9:30 COMP **530.** Consistent integration of experimental and ab initio data into effective molecular force fields. **L. Vlcek**

10:00 Intermission.

10:15 COMP **531.** Refined AMBER force field (FUJI) force field for phospholipids. N. Kamiya, **H. Fujitani**

10:45 COMP **532.** Force field development for water interacting with Pt surfaces. **A.W. Goetz**, R.F. de Morais, B. Schweitzer, P. Fleurat-Lessard, P. Sautet, S. Steinmann, C. Michel

11:15 COMP **533.** Biocompatible force field for thiolated gold nanoclusters in macromolecular environments. **J. Gascon**

11:45 COMP **534.** Thermodynamic calculations of cyclodextrin host-guest binding: A comprehensive evaluation of force field performance. **N.M. Henriksen**, M.K. Gilson

Section D

InterContinental San Francisco
Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

J. J. Foley, *Presiding*

8:30 COMP **535.** Strong-field ionization in molecules using range-separated time-dependent density functional theory. A. Sissay, A. Bruner, P. Abanador, F. Mauger, M. Gaarde, K. Schafer, **K. Lopata**

9:05 COMP **536.** Non-linear conductivity of metals from real-time time-dependent density functional theory. **X. Andrade**, A.A. Correa

9:30 COMP **537.** Excited state absorption from real-time time-dependent density functional theory simulations: Predicting molecular optical response by excited state density propagation. **D.N. Bowman**, J. Asher, S. Fischer, N. Govind, C.J. Cramer

9:55 COMP **538.** Quantum mechanical models with statistical effects and statistical models without quantum effects. **J. Parkhill**

10:30 Intermission.

10:45 COMP **539.** Linear-response, stability and single-particle excited states in noncollinear spin density functional theory. **G. Scalmani**, F. Egidi, M.J. Frisch, X. Li

11:10 COMP **540.** Many-pair expansion: A systematically improvable correction scheme for including strong and long-range correlations in DFT. **P. de Silva**, T. Zhu, T.A. Van Voorhis

11:35 COMP **541.** Unconventional Kohn-Sham theory: Implementation and application of complex-restricted and general orbital density functional theories. **L.W. Bertels**, M.P. Head-Gordon

12:00 COMP **542.** Polarizabilities of π-conjugated chains revisited: Improved results from broken-symmetry, range-separated DFT. **B.M. Wong**, M.B. Oviedo, N. Ilawe

Section E

InterContinental San Francisco
Laurel Hill

Drug Design

Applications

M. R. Landon, Y. Tseng, *Organizers*

M. Korczynska, *Presiding*

8:30 COMP **543.** Molecular simulations disclose a novel mode of one-stranded intercalation in nucleosomes that is DNA topology dependent. **G. Palermo**, Z. Ma, Z. Adhireksan, B. Murray, T. von Erlach, P. Dyson, C. Davey, U. Roethlisberger

8:50 COMP **544.** Withdrawn.

9:10 COMP **545.** Rational bioavailability design: Optimizing bioavailability in lead op with Global Sensitivity Analysis of Physiologically-Based PK (GSA of PBPK). **E.J. Martin**, P. Daga, B. Madej

9:30 COMP **546.** Is alternative binding sapping the strength of current oxime countermeasures? **B.J. Bennion**, T. Carpenter, F.C. Lightstone, T. Nguyen, C.A. Valdez

9:50 Intermission.

10:10 COMP **547.** Rational bioavailability optimization using physiologically-based pharmacokinetics simulations. **B.D. Madej**, E.J. Martin

10:30 COMP **548.** Ligand based drug discovery of novel dengue-2 NS2B-NS3 protease inhibitors. M.M. Nawi, S. Abdul Hamid, M. Hariono, R. Othman, S. Othman, R. Yusuf, N.A. Rahman, **H. Wahab**

10:50 COMP **549.** Virtual fragment screening and linking discovers Jumonji histone demethylase inhibitors. **M. Korczynska**, D.D. Le, M. Siklos, N. Younger, E. Gregori-Puigjané, A. Tumber, T. Krojer, S. Velupillai, C. Gileadi, R. Nowak, E. Iwasa, S.B. Pollock, I. Ortiz Torres, U. Oppermann, B. Shoichet, D.G. Fujimori

11:10 COMP **550.** Molecular drug design targeting a bacterial RNA structure: Atomic resolution mechanistic studies of highly selective unnatural ligand mimic of the *E. coli* FMN riboswitch. **L. Xiao**

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Biomass Catalysis

Sponsored by CATL, Cosponsored by COMP

THURSDAY AFTERNOON

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Mechanisms & Molecular Simulations

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

S. Vajda, *Presiding*

1:30 COMP **551.** Glutamate receptor ion channel activation mechanism revealed by computer experiment. **X. Wu**, B. Brooks

2:00 COMP **552.** CaMKII: A molecular dynamics study of the effects of phosphorylation on its dodecameric form. **I. General**

2:30 COMP **553.** Computational tools for the evaluation of laboratory-engineered biocatalysts. **M. Garcia-Borras**, A. Romero-Rivera, S. Osuna

3:00 Intermission.

3:20 COMP **554.** Constant-pH simulations on capability class computers: First applications. **B. Radak**, J. Phillips, W. Jiang, K. Schulten, B. Roux

3:50 COMP **555.** Directional motion in chiral molecules out of equilibrium. **D. Slochower**, M.K. Gilson

Section B

InterContinental San Francisco
Fremont

Material Science

Surfaces & Catalysts

C. M. Aikens, *Organizer*

A. Shamloo, *Presiding*

1:30 COMP **556.** Growth mechanism of small PdGa bimetallic clusters on MgO (100) surface. **N. Kumar**, D. Chattaraj, I. Kaul, C. Majumder, P. Ghosh

2:00 COMP **557.** Surface characterization of supported catalysts: The interplay between modeling and experiments. **V. D'Anna**, C. Michel, P. Sautet

2:30 COMP **558.** Density-functional study of the $La_2Zr_2O_7$ low-index faces. **Y. Mantz**, Y. Duan

3:00 COMP **559.** Formation and diffusion of oxygen vacancies in complex transition-metal oxides from diffusion quantum Monte Carlo. **J.A. Santana**, J. Krogel, P. Kent, F. Reboredo

3:30 Intermission.

4:00 COMP **560.** Decorating the (110) facet of rutile-type crytallites with CH_4: A first-principles investigation. **A. Abbaspour Tamijani**

4:30 COMP **561.** Dynamics of self-assembled guanine nucleobases on graphene. **N. Saikia**, K. Waters, S.P. Karna, R. Pandey

5:00 COMP **562.** Computational study of the binding of methane and aromatic amino acids with graphene. **T. Dinadayalane**, J. Lazare, D. Daggag

Section C

InterContinental San Francisco
Howard

Molecular Mechanics

Protons & Electrons

M. Feig, *Organizer*

A. Levit, *Presiding*

1:30 COMP **563.** Assessing and optimizing efficiency in nonequilibrium molecular dynamics/Monte Carlo simulations. **B. Radak**, B. Roux

1:55 COMP **564.** High-performance molecular dynamics at constant pH and constant redox potential using AMBER. **V.D. Cruzeiro**, M. Amaral, A.E. Roitberg

2:20 COMP **565.** Unraveling the dynamics of the redox conformational protection of nitrogenase. **F. Feixas**, M. Gimferrer, P. Salvador, M. Garcia-Borras

2:45 COMP **566.** Self-activated mechanism for efficient nucleic acids polymerization. V. Genna, P. Visossich, E. Ippolito, P. Carloni, **M. Devivo**

3:10 Intermission.

3:25 COMP **567.** NH_3 binding to the S_2 state of the O_2-evolving complex of Photosystem II points at H_2O binding during the $S_2 \rightarrow S_3$ transition: Insights from QM/MM, EXAFS, and femtosecond x-ray diffraction. **M. Askerka**, D. Vinyard, J. Wang, G.W. Brudvig, V.S. Batista

3:50 COMP **568.** Thermal isomerization relaxation of azobenzene derivatives studied with QM/MM and transition path sampling. **A. Muzdalo**, P. Saalfrank, **M. Santer**

4:15 COMP **569.** Structural and electronic features of Mg^{2+}-RNA binding motifs: Insights from combined classical molecular dynamics and quantum mechanics simulations. **L. Casalino**, G. Palermo, N. Abdurakhmonova, U. Roethlisberger, A. Magistrato

Section D

InterContinental San Francisco
Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer, Presiding*

1:30 COMP **570.** Large-scale selected configuration interaction based on a Davidson-Liu flow. **R.M. Parrish**, T.J. Martinez

2:05 COMP **571.** Complex basis functions for metastable electronic states: Methodology and applications. **A. White**, C.W. McCurdy, M.P. Head-Gordon

2:30 COMP **572.** Excited states for orbital-optimized second-order perturbation theory. **E. Ramos**, M.P. Head-Gordon

2:55 COMP **573.** Unique electronic dynamics from scattering mediated absorption. **J.J. Foley**

3:30 Intermission.

3:45 COMP **574.** Geminals for dispersion interactions and long-range correlation. **J.F. Gonthier**, M.P. Head-Gordon

4:10 COMP **575.** Hybrid classical/quantum approach for large-scale studies of quantum systems with density matrix embedding theory. **N.C. Rubin**

4:35 COMP **576.** Examining the excited state deactivation pathways of 5-hydroxymethylcytosine. **J. Mato**, K. Keipert, M.S. Gordon

5:00 COMP **577.** Theoretical studies of the catalytic transition metal nanoparticles with flexible structures. **G. Wei**, Z. Liu

Section E

InterContinental San Francisco
Laurel Hill

Drug Design

Applications

M. R. Landon, Y. Tseng, *Organizers*

P. Bisignano, *Presiding*

1:30 COMP **578.** Exploiting water density fluctuations in ion channel drug design. **E. Gianti**, L. Delemotte, M.L. Klein, V. Carnevale

1:55 COMP **579.** Adding pharmacophores to shape and electrostatics - too much of a good thing? **T. Cheeseright**, M.D. Mackey, S. Tomasio

2:20 COMP **580.** Investigation of the molecular electrostatic potentials and the average electron densities of non-classical bioisosteres. **A.A. Arabi**, C.F. Matta

2:45 Intermission.

3:05 COMP **581.** From protons to fragments with XModeScore: How we can use x-ray data coupled with quantum mechanics to explore these elusive species in binding. **L. Westerhoff**, O. Borbulevych

3:30 COMP **582.** Key role of the β5-β6 loop conformation in the substrate specificity of OXA-48–like enzymes: Implications for the β-lactamase-mediated antibiotic resistance. L. Dabos, R. Bonnin, L. Dortet, T. Naas, **B.I. Iorga**

3:55 COMP **583.** *In silico* analysis of Z-77 variants for optimal inhibition of *E. coli* beta-glucuronidase. **K.T. Lane**, H. Gullickson

‡ *Cooperative Cosponsorship*

4:20 COMP **584.** 2A but not 2B: Towards structure-based discovery of new Serotonin receptor modulators. **A. Levit**, D. Wacker, J.D. McCorvy, B.L. Roth, B. Shoichet

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Machine Learning Tools for Catalyst Genome

Sponsored by CATL, Cosponsored by COMP

ENFL

Division of Energy and Fuels

D. J. Heldebrant, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials (see *CATL,* Mon, Tue)

Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy (see *CELL*, Mon)

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis (see *CATL,* Mon, Tue, Wed)

Rising Star Award Symposium (see *WCC, Mon*)

Science for a Sustainable Energy Future: Energy Storage (see *PRES,* Mon)

SOCIAL EVENTS:

Executive Committee Meeting, 4:00 PM: Sun

Dinner, 6:00 PM: Tue

BUSINESS MEETINGS:

Program Meeting, 12:00 PM: Sun

Business Meeting & Social, 12:00 PM: Mon

SUNDAY MORNING

Section A

Grand Hyatt San Francisco

Belvedere

Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain

J. Casey, *Organizer*

J. Nelson, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **1.** Recent improvements of the ICP/MS capabilities of the 8800 for the petroleum industry. **L. Charles-Philippe**, C. Sanchez Rodriguez, F. Chainet, M. Milliand, L. Ayouni, S. Carbonneaux, J. Todoli, A. Desprez

9:20 ENFL **2.** Determination of trace elements in petroleum feedstocks by ICP-MS: From total content towards their distribution. **F.A. Lopez-Linares**, **L. Poirier**, M.M. Boduszynski, C.E. Rechsteiner, M. Moir, D. Leong, C.F. Ovalles, E. Rogel, J. Nelson

9:50 ENFL **3.** Use of GC-ICP-MS for analysis of petroleum and petrochemicals in a service laboratory. **W. Geiger**, B. McElmurry, J. Anguiano

10:20 Intermission.

10:40 ENFL **4.** Using the MS/MS capabilities of the Agilent 8900 ICP-QQQ for ultra-trace analysis of elements in the petroleum value chain. **M. Kelinske**, J. Nelson

50 high to low-abundance minor, trace and ultra-trace elements in crude oils by ICP-OES and QQQ-ICP-MS: New methods of geochemical fingerprinting. **J. Casey**, Y. Gao

11:30 ENFL **6.** Simultaneous measurement of twenty-five trace elements in aviation turbine engine and diesel fuels by inductively coupled plasma tandem mass spectrometry. **G.T. Eldridge**, R.K. Larsen, M.E. Peretich, R.P. Shah, A. Metz

11:55 ENFL **7.** Measurement of copper in aviation turbine engine fuel by inductively coupled plasma tandem mass spectrometry and comparison to graphite furnace atomic absorption spectrometry. **A. Metz**, R.K. Larsen, M.E. Peretich, G.T. Eldridge

Section B

Grand Hyatt San Francisco

Filmore C

C1 Catalysis

Cosponsored by CATL

K. Ding, N. Kumar, *Organizers*

J. J. Spivey, *Organizer, Presiding*

K. Ding, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **8.** Strategies to selectively oxidize methane to methanol. **J.A. Lercher**

9:15 ENFL **9.** Nature of active sites and mechanism of selective methane oxidation by Cu and Fe-modified zeolite catalysts. A. Szecsenyi, G. Li, J. Gascon, E. Hensen, **E. Pidko**

9:35 ENFL **10.** Copper oxide clusters as active catalytic sites of CuMOR zeolite for methane to methanol conversion: Size matters? **D. Palagin**, A.J. Knorpp, A.B. Pinar, M. Ranocchiari, J.A. van Bokhoven

9:55 ENFL **11.** Defining the active sites of low-temperature methane hydroxylation in iron and copper zeolites. **B.E. Snyder**, P. Vanelderen, J. Woertink, B.F. Sels, R.A. Schoonheydt, E.I. Solomon

10:15 Intermission.

10:30 ENFL **12.** Biological methane oxidation. **A.C. Rosenzweig**

11:10 ENFL **13.** Chemical transformation of shale gas components under mild conditions in liquid. **F. Tao**

11:40 ENFL **14.** Direct conversion of methane to methanol and ethanol. C. Okolie, Y. Belhseine, L. Kovarik, E. Stavitski, **C. Sievers**

Section C

Grand Hyatt San Francisco

Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG‡ and PMSE

Y. H. Hu, R. T. Koodali, H. Wang, *Organizers*

Y. Li, Y. Ng, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **15.** Acid treatment enables suppression of electron-hole recombination in hematite for photoelectrochemical water splitting. **Y. Li**

9:15 ENFL **16.** Nanostructured hybrid electrodes for photoelectrochemical CO_2 conversion: Synthetic aspects and structure-property relationships. E. Kecsenovity, A. Kormanyos, B. Endrodi, **C. Janaky**

9:45 ENFL **17.** Vitamin C as a surface modifier for solar hydrogen production. **T. Dramstad**, D. Harts, B. Selvaratnam, R.T. Koodali

10:05 Intermission.

10:15 ENFL **18.** Bismuth-based ternary oxide for photocatalytic and photoelectrochemical water splitting. **Y. Ng**

10:55 ENFL **19.** Engineering nanomaterials for energy conversion. **X. Zheng**

11:25 ENFL **20.** Structure and properties of hydrothermally prepared MoS_2 thin films on gold substrate. **A.S. Ichimura**, R. Sfadia, J. Macias, B. Gunn, A. Newaz, C. Tassone

11:55 ENFL **21.** Photoelectrocatalytic reduction of CO_2 on organic/inorganic nanocomposite photoelectrodes. **A. Kormanyos**, D. Hursan, K. Rajeshwar, C. Janaky

12:15 Concluding Remarks.

Section D

Grand Hyatt San Francisco

Curran

Catalysis for Unconventional Energy Sources

Cosponsored by CATL and MPPG‡

X. Wang, *Organizer*

Y. H. Hu, *Organizer, Presiding*

F. Li, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **22.** Thermochemical studies of catalyst stability and function. **A. Navrotsky**

9:15 ENFL **23.** Mn-containing mixed metal oxides for chemical looping oxidative dehydrogenation of ethane. **F. Li**

9:45 ENFL **24.** Sustainable production of bio-based alcohols, esters, aromatics and polyols from lignin: The art of the right catalyst. **Y. Li**, R. Ma, X. Ma

10:15 Intermission.

10:30 ENFL **25.** Visible light photocatalytic production of H_2. **Y.H. Hu**

11:10 ENFL **26.** Catalyzing energy storage for optimum use of intermittent renewable energy resources. **M. Isaacson**

11:50 ENFL **27.** Light absorbers, interfaces, and catalysts for solar-to-fuel conversion: First-principles calculations. **Y. Ping**

12:20 Concluding Remarks.

Section E

Grand Hyatt San Francisco

Sequoia

Subsurface Technologies for Recovery of Fossil & Geothermal Energy

Cosponsored by CATL and GEOC

C. Fernandez, M. A. Reynolds, *Organizers*

C. Fernandez, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **28.** Results from Newberry volcano EGS demonstration, 2010-2015. **T. Cladouhos**, S. Petty, M.W. Swyer, M. Uddenberg, K. Grasso, Y. Nordin

9:10 ENFL **29.** TOGA: Compositional simulation of three-phase, multi-component, and non-isothermal processes for carbon dioxide utilization and storage in partially depleted oil and gas reservoirs. **C. Oldenburg**, L. Pan

9:35 ENFL **30.** Experiments, simulations, and reduced physics modeling for risk assessment of well integrity at CO_2 storage sites. **N. Huerta**, J. Iyer, V. Vasylkivska, S.A. Carroll, W.L. Du Frane, B. Kutchko, L. Li, H. Mason, P. Roy, S.D. Walsh

10:00 ENFL **31.** Development of an electrochemical sensor for downhole tracer and pH measurements in real-time. **R.F. Hess**, B. Klamm, L. Goldfarb, W.C. Corbin, T.J. Boyle, W.G. Yelton, A.T. Cashion

10:25 Intermission.

10:30 ENFL **32.** Caustic-cracking likely cause of failure in geothermal production casing – well redesign and cementing changes key to replacement well success. **D. Bour**, M. Gao, R. Krishnamurthy, R. Rudolf, R. Hausler

11:05 ENFL **33.** Made-to-order metal-organic frameworks for gas capture and storage. **M. Eddaoudi**, D. Alezi, Y. Belmabkhout

11:30 ENFL **34.** Self-healing polymer-cement composites for geothermal wells and their properties. **M. Childers**, K.A. Rod, M.T. Nguyen, M. Elbakhshwan, S. Gill, W. Um, J. Chun, V. Glezakou, T.J. Roosendaal, T. Wietsma, P.K. Koech, N. Huerta, B. Kutchko, C. Fernandez

11:55 ENFL **35.** Microbial consortia encapsulated with ultralight kaolinite proppant for in-situ microbially enhanced methane recovery. **K. Han**, J. Fuertez, A. Szendrei, V. Nguyen, J. McLennan, T.D. Sparks

12:20 Concluding Remarks.

Section F

Grand Hyatt San Francisco

Cypress

Computations for CO2 Capture, Conversion & Sequestration

Cosponsored by CATL, COMP, GEOC and MPPG‡

V. Glezakou, R. Rousseau, *Organizers*

S. Raugei, *Presiding*

8:30 ENFL **36.** Reaction dynamics of CO_2 in amine solutions from DFT-based simulations. **W. Andreoni**, C. Ma, F. Pietrucci

9:15 ENFL **37.** Understanding the structure and dynamics of CO2-reactive aprotic heterocyclic anion ionic liquids: A molecular simulation study. E. Maginn, **Q. Sheridan**, W.F. Schneider

10:00 Intermission.

10:30 ENFL **38.** March toward task-specific CO_2 capture solvents. **V. Glezakou**, R. Rousseau, D.C. Cantu, D. Malhotra, D.J. Heldebrant, P.K. Koech

11:05 ENFL **39.** Polymorphic transitions of CO_2 molecular crystals: Thermodynamics, kinetics and confinement effects. I. Gimondi, **M. Salvalaglio**

Cellulose Structure & Biosynthesis In the Plant Cell Wall

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Electrocatalysis for Energy Generation & Storage