10:30 COLL **493.** Analysis of interactions at fluid-solid interface: Exploring the complete slip boundary condition. **S.L. Nania**, S.K. Shaw

10:50 COLL **494.** Multilayered metallic nanostructures with an embedded internal standard as surface enhanced Raman substrates. **E.R. Butcher**, D.D. Evanoff

11:10 COLL **495.** X-ray photoelectron spectroscopy at the liquid-nanoparticle interface: Opportunities for colloidal science. **M.A. Brown**

11:30 COLL **496.** Interfacial liquids, Most soft surfactants probed by AFM. **H. Onishi**

11:50 COLL **497.** Selenium: The better anchor group for self-assembled monolayers (SAMs) on gold? **A. Terfort**, M. Zharnikov, P. Cyganik

12:10 COLL **498.** Withdrawn.

Section F

Marriott City Center Denver
Colorado H

Basic Research in Colloids, Surfactants & Nanomaterials

Basic Research on Colloids

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

8:30 COLL **499.** Dynamic adhesion forces between microparticles and substrates in water. **Q. Xu**, Z. Xia, M. Li, L. Zhang, J. Niu

8:50 COLL **500.** Formation of luminescent inorganic precipitation tubes. P.J. Fryfogle, E.J. Nelson, **J.J. Pagano**

9:10 COLL **501.** Incorporation of nanoparticles into tunable, highly-ordered, porous silica films. **Y. Vasquez**, M. Kolle, L.A. Mishchenko, B.D. Hatton, J. Aizenberg

9:30 COLL **502.** Ionic and molecular modifiers of calcium oxalate crystallization: Tailoring interfacial interactions. **B.G. Alamani**, J. Chung, J.D. Rimer

9:50 COLL **503.** Colloidal particle dispersions for the synthesis of full color electrophoretic inks. **K. Belsey**, C. Topping, L. Farrand, S.J. Holder

10:10 COLL **504.** Selecting the swimming mechanisms of colloidal particles: Bubble propulsion vs. self-diffusiophoresis. **S. Wang**, N. Wu

10:30 COLL **505.** Characterization and dispersion behavior of quaternary ammonium encapsulated polyoxometalates in polyurethane. **J. Lundin**, S.L. Giles, P. Fulmer, R.F. Cozzens, J.H. Wynne

10:50 COLL **506.** Janus particles for probing and manipulating immune functions. **Y. Yu**, Y. Gao, L. Sanchez, Y. Jia

11:10 COLL **507.** Intra-phase mixing in binary drops translating through corrugated microchannels. **T. Ward**

11:30 COLL **508.** Molecular dynamics simulations of colloidal nanoparticles solvation. **S. Sen**, P. Kral

11:50 COLL **509.** Theoretical description of architectures of nanoparticles. **N. Almora Barrios**, N. Lopez

THURSDAY AFTERNOON

Section A

Marriott City Center Denver
Colorado A

Natural Resource Capture, Storage & Energy Conversion

Biofuels, Fuel Cells, Membranes, Electrolytes, & Batteries (BFCMEB)

J. Liu, *Organizer*
S. Bashir, *Organizer, Presiding*
X. Wang, *Presiding*

2:00 COLL **510.** Understanding abiotic:biotic interface: Molecular-level insights into the behavior of enzymes covalently immobilized on surfaces. T. Ogorzalek, Y. Liu, S. Wei, C.L. Brooks, Z. Chen, **N. Marsh**

2:30 COLL **511.** Direct synthesis of single layer layered double hydroxide nanosheets. **J. Yu**, B.R. Martin, J.E. Sims, L. Sun

2:55 COLL **512.** Silyl electrolytes for lithium-ion battery applications. **L.J. Lyons**

3:20 COLL **513.** Withdrawn.

3:45 COLL **514.** Creation of natural dye sensitized solar cell by using nanostructured titanium oxide. **J. Uddin**, S.S. Jenny, A. Ahmed, S. Yadav, M. Jiru

4:10 COLL **515.** Amphiphilic functionalization of cathode catalyst to advance electrochemical reactivity of fuel cells. **D. Gaona**, S. Bashir, J.L. Liu

Section B

Marriott City Center Denver
Colorado I/J

Interfacial Biomolecular Recognition

Cosponsored by BIOL‡

Financially supported by Avanti Polar Lipids, Inc.

J. Ross, *Organizer*
B. E. Bowler, M. Kastantin, *Organizers, Presiding*

2:00 COLL **516.** Aiding developments of single-molecule force spectroscopy for biosensing via molecular simulation. **Z.E. Hughes**, K.L. Drew, T. Walsh

2:25 COLL **517.** Use of surface-specific spectroscopy techniques to unravel molecular recognition in biosensing. **O.N. Oliveira**

2:50 COLL **518.** New roles for antifreeze proteins in recognizing non-ice surfaces. **X. Wen**

3:15 Intermission.

3:30 COLL **519.** Studying receptor-mediated liposome fusion kinetics at aqueous/liquid crystal interfaces. **K. Macri**, P. Noonan, D.K. Schwartz

3:55 COLL **520.** Effect of nanoparticle surface chemistry and salt concentration on binding to RNA and DNA. **J.A. Nash**, A. Singh, N.K. Li, Y.G. Yingling

4:20 COLL **521.** Ultrasound biosensing techniques based on biomolecule-induced aggregation of nanodroplets. **R. Chattaraj**, P. Mohan, J.D. Besmer, C.M. Livingston, A.P. Goodwin

4:45 COLL **522.** Impedimetric biosensors for detecting VEGF based on PEDOT carboxylic acid/PEDOT copolymer. **M. Kim**, R. Iezzi, D.C. Martin

Section C

Marriott City Center Denver
Colorado C/D

Basic Research in Colloids, Surfactants & Nanomaterials

Carbon and Organic Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **310.** Artificial light harvesting system composed of organic dyes and clay minerals. **S. Takagi**, Y. Ishida, T. Shimada

2:20 COLL **523.** SiC porous materials derived from apple for high-performance electromagnetic interference shielding. **Z. Wang**, C. Liu, Y. Xu

2:40 COLL **524.** Modeling fullerene aggregation in electrolyte solutions: A combined deterministic-stochastic framework. S. Mortuza, **S. Banerjee**

3:00 COLL **525.** Synthesis of carbon-based nanoscale composite particles for imaging applications. **M.J. Meziani**, **M.A. Mottaleb**, B. Yoo, Y. Sun

3:20 COLL **526.** Label-free two photon imaging of live cells using graphene dots. **P.C. Ray**

3:40 COLL **527.** Developing carbenes as surface modifiers. **M. Macleod**, J.A. Johnson

4:00 COLL **528.** Carbon dots preparation and effect on protein fibrillation. **S. Li**, R.M. Leblanc

4:20 COLL **529.** Conductance and rectification through asymmetric biphenyl molecule systems. **J.E. Meany**, S.A. Woski

4:40 COLL **530.** Electron transfer and molecular binding to nanostructured carbon for supercapacitor materials. D. Banks, J. Mitchell, I. Shcherbakov, **J.C. Poler**

Section D

Marriott City Center Denver
Denver III

Basic Research in Colloids, Surfactants & Nanomaterials

Functionalized Nanoparticles

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **531.** Withdrawn.

2:20 COLL **532.** Withdrawn.

2:40 COLL **533.** Phase transport of citrate stabilized gold nanoparticles using nonspecifically adsorbed polymers. **L.B. Thompson**, A.M. Alkilany, A. Caravana

3:00 COLL **534.** Highly efficient poly-lysine functionalization of gold surfaces by dual click reactions utilizing dithiol adsorbates. **A. Shakiba**, A.C. Jamison, T. Lee

3:20 COLL **535.** Toward understanding electronic and optical properties of colloidal germanium nanocrystals as a function of size and surface ligand. **A.L. Holmes**, J. Hütges, A. Reckmann, E. Muthuswamy, K. Meerholz, S. Kauzlarich

3:40 COLL **536.** Withdrawn.

4:00 COLL **537.** Orthogonal functionalization of patchy particles. **X. Zheng**, Y. Wang, Y. Wang, D. Pine, M. Weck

4:20 COLL **538.** Strong hydrophobizer: Laterally chemisorbed low-molecular-weight polydimethylsiloxane. **T. Lee**, S. Chae

4:40 COLL **539.** Elucidating structure/property relationships of peptide-decorated Au nanoparticles using advanced molecular simulations. **Z.E. Hughes**, T. Walsh

Section E

Marriott City Center Denver
Colorado G

Basic Research in Colloids, Surfactants & Nanomaterials

Semiconductor Materials

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **540.** Optical signatures of crystal phase in semiconductor nanocrystals. **S. Lim**, A. Schleife, A. Smith

2:20 COLL **541.** Shape controlled narrow-gap tin chalocogenide nanostructures. **S. Guo**

2:40 COLL **542.** Colloidal synthesis and photocatalytic properties of orthorhombic $AgGaS_2$ nanocrystals. **C. Fan**, M. Regulacio, M. Han, A. Xu

3:00 COLL **543.** Careful control of confinement potential and interfacial lattice strain in colloidal quantum dots to improve radiative recombination and fluorescence blinking. **C.D. Heyes**

3:20 COLL **544.** Size characterization and alternative synthesis of monolayer-protected quantum dots. A.E. Conner, L.R. Tinoco, W.L. Wright, S.C. Francone, E.V. Aguilar, F.E. Acosta, **D.T. Miles**

3:40 COLL **545.** Excited state dynamics in doped quantum dots. **C. Tuinenga**, P.V. Kamat

4:00 COLL **546.** Withdrawn.

4:20 COLL **547.** Characterization of the transformation of collodial CdSe quantum dots into ferroelectric particles. **T. Wrenn**, J. McBride, J. Mares

4:40 COLL **548.** Formation of 1D-nanostructures using surface-directed vapor-liquid-solid growth process. **B. Nikoobakht**, A. Herzing

Section F

Marriott City Center Denver
Colorado H

Basic Research in Colloids, Surfactants & Nanomaterials

Colloidal Assembly and Gels

Cosponsored by PRES

R. Nagarajan, *Organizer, Presiding*

2:00 COLL **549.** Electric field-directed nanowire assembly. **S.J. Boehm**, L. Lin, C.D. Keating, T.S. Mayer

2:20 COLL **550.** Designing a super-assembly using mixed biological and synthetic nanostructures. **J. Reyes**, R. Balaraman, N.D. Becerra-Mora, J.B. Fiske, P. Kohli

2:40 COLL **551.** Bifurcation in the equilibrium height of colloidal particles near an electrode in oscillatory electric fields. **T. Woehl**, B. Chen, K. Heatley, N. Talken, C. Dutcher, S. Bukosky, W. Ristenpart

3:00 COLL **552.** Self-assembly of colloidal nanoparticles into chiral ribbons and hollow capsules. **P. Kral**

3:20 COLL **553.** Self-assembly of nanometer scaled macroions in dilute solution. **J. Zhou**, T. Liu

3:40 COLL **554.** Direct nanoscale visualization of the kinetics of colloidal gold nanoparticle chain assembly. **T. Woehl**, T. Prozorov

4:00 COLL **555.** Withdrawn.

4:20 COLL **556.** Magnetoactive hydrogels for dynamic modulation of pro-angiogenic signaling from mesenchymal stem cells. **K.A. Kilian**, A. Abdeen

4:40 COLL **557.** Monodisperse polymeric ionic liquid microgels by post modifications and their versatile biomedical applications. **N. Sahiner**, A.O. Yasar, S. Yildiz, S. Demirci, **N. Aktas**

5:00 COLL **558.** Supercooled water in nanoconfinement: Molecular simulation study of single-molecule and collective dynamics. N.J. Kuon, **A.A. Milischuk**, B.M. Ladanyi

5:20 COLL **559.** Ionic liquids and water: the surprising connection. **M.A. Gebbie**, H.A. Dobbs, M. Valtiner, J.N. Israelachvili

COMP

Division of Computers in Chemistry

E. Esposito and S. Wildman, *Program Chairs*

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

SUNDAY MORNING

Section B

Colorado Convention Center
Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

M. Halls, *Organizer*
G. B. Fitzgerald, *Organizer, Presiding*

8:30 COMP **1.** Using Gaussian to aid in π-conjugated semiconducting polymer design for organic photovoltaics. **C.K. Luscombe**

9:00 COMP **2.** Computational description of donor-acceptor pi-conjugated materials for organic photovoltaics applications. **J.E. Bredas**

9:30 Intermission.

9:45 COMP **3.** High-throughput computational design of semiconducting polymers: Predictions and rational guidance from DFT calculations. **B.M. Wong**

10:15 COMP **4.** Application of density functional theory in the design of organic molecules for intramolecular singlet fission. Q. Wu, **E. Busby**, J. Xia, J. Low, R. Song, J.R. Miller, X. Zhu, L.M. Campos, M. Sfeir

10:45 COMP **5.** Atomistic simulations of donor-acceptor polymer morphologies for high-efficiency organic photovoltaic. **T.W. Kemper**, R.E. Larsen, D.C. Olson

Section C

Colorado Convention Center

Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Dynamics

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

8:30 COMP **6.** Nonadiabatic molecular dynamics of singlet fission and charge separation. **O.V. Prezhdo**

9:00 COMP **7.** First principles ultrafast charge transfer dynamics in solution: A time-domain TDDFT approach coupled with dielectric relaxation. **F. Ding**, D. Lingerfelt, B. Mennucci, X. Li

9:30 COMP **8.** Modeling inter-domain electron tunneling in copper monooxygenases. **A. Migliore**, D.N. Beratan

10:00 Intermission.

10:15 COMP **9.** Time-dependent two-component electronic structure methods for modeling spin dynamics. **X. Li**, F. Ding, J. Goings

10:45 COMP **10.** Pseudopotential approach to electronic structure of anionic species on metallic surfaces. **A.F. Izmaylov**

Section D

Colorado Convention Center

Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **11.** Structural informatics modeling of Daclatasvir and analogs reveals asymmetric binding to HCV-NS5A: Dual mechanisms responsible for picomolar activity and acquired resistance. **J.H. Nettles**, R. Stanton, J. Broyde, F. Amblard, H. Zhang, L. Zhou, J. Shi, T. McBrayer, T. Whitaker, S.J. Coats, J.J. Kohler, R.F. Schinazi

9:00 COMP **12.** Structure-based discovery and de novo design of HIV fusion inhibitors. **W.J. Allen**, R.C. Rizzo

9:30 COMP **13.** Dual layer QM/MM binding study of antimicrobial oligomer-viral capsid complexes. **T. Martin**, E.H. Hill, D.G. Whitten, E.Y. Chi, D.G. Evans

10:00 Intermission.

10:00 COMP **14.** Fungicides and exploration of chemical spaces: Homology modeling of lanosterol 14-alpha-demethylase. **L. Nitsch** Velasquez

10:30 COMP **15.** Identification and characterization of allosteric site(s) for dihydrogambogic acid (DHGA) and trans-β-caryophyllene (TBC) as cannabinoid CB_2 allosteric modulators. **P. Pandey**, K.K. Roy, R.J. Doerksen

11:00 COMP **16.** Molecular docking screens for the discovery of novel A_2A adenosine receptor agonists: Are there any in chemical libraries? **D. Rodriguez**, Z. Gao, S.M. Moss, K.A. Jacobson, J. Carlsson

Section E

Colorado Convention Center

Mile High Ballroom 4F

Molecular Mechanics

Proteins

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **17.** Computational approach to enzyme design. S. Sirin, **W. Sherman**

9:00 COMP **18.** Molecular dynamics simulations on the periplasmic-open state lactose permease. **X. Zhuang**, J.B. Klauda

9:30 COMP **19.** Investigating the structure and dynamics of the PIK3CA wild-type and H1047R oncogenic mutant for potential allosteric modulation. P. Gkeka, A. Papafotika, S. Christoforidis, **Z. Cournia**

10:00 Intermission.

10:15 COMP **20.** Structural insight into ROS1/ALK kinase conformational dynamics. **N.A. Vellore**, J. Wagner, C.A. Edie, M.W. Deininger, B.J. Druker, T. O'Hare, M.A. Davare

10:45 COMP **21.** Computational study of pH-dependent conformational changes in proteins. **N. Di Russo**, A.E. Roitberg

11:15 COMP **22.** cAMP modulation of the hyperpolarization-activated cyclic nucleotide-gated 2 ion channels. **F. Tofoleanu**, B. Brooks

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Accurate Energies for Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid β: Structures and Molecular Interactions

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Advances in Simulation Methodology

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Sponsored by PHYS, Cosponsored by COMP

SUNDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Ballroom 1D

Molecular Mechanics

Methodology

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **23.** Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. **G. Koenig**, B. Brooks

2:00 COMP **24.** Importance of sugar pucker correction to QM/MM simulation of RNA systems. **M. Huang**, D.M. York

2:30 COMP **25.** Improving efficiency in SMD simulations through a hybrid differential relaxation algorithm. **C.L. Ramirez**, A. Zeida, G.E. Jara, A.E. Roitberg, M.A. Marti

3:00 Intermission.

3:15 COMP **26.** Enhancing constant-pH simulation in explicit solvent with a two-dimensional replica exchange method. **J. Lee**, B. Miller, A. Damjanovic, B. Brooks

3:45 COMP **27.** Toward a virtual chemist: Application to asymmetric catalyst discovery. **J. Pottel**, M. Bezanson, N. Moitessier

4:15 COMP **28.** Computer-aided molecular design of neutral lanthanide extractants. **B.W. McCann**

Section B

Colorado Convention Center

Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

G. B. Fitzgerald, *Organizer*

M. Halls, *Organizer, Presiding*

1:30 COMP **29.** Finding polymorphs of organic semiconductors. **P. Clancy**, K.M. Lenn, P. Frazier

2:00 COMP **30.** Coarse-grained simulations of benzodithiophene-thienopyrrolodione copolymer film structure for organic photovoltaics. **E. Jankowski**, D.C. Olson

2:30 COMP **31.** Molecular dynamics of prototypical organic photovoltaic materials. S. Yerusu, **V.K. Kuppa**

3:00 Intermission.

3:15 COMP **32.** High throughput computational approaches to materials discovery and development for organic electronics. **M.E. Thompson**, P. Saris, P.I. Djurovich, L. Martin

3:45 COMP **33.** Efficient knowledge discovery of optoelectronic materials using evolutionary strategies. **T.F. Hughes**, Y. Cao, J. Gavartin, D.J. Giesen, A. Goldberg, M.D. Halls, S. Kwak

4:15 COMP **34.** Charge percolation in noncrystalline molecular materials. **N. Jackson**, L.X. Chen, M.A. Ratner

Section C

Colorado Convention Center

Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Embedding: QM/QM and QM/MM

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

1:30 COMP **36.** Embedded descriptions of condensed phases. **G.K. Chan**

2:00 COMP **35.** Embedding from multiscale chemical problems to crystal energetics. **F.R. Manby**

2:30 COMP **37.** Embedded correlated wavefunction theory: Advances and applications. **E.A. Carter**

3:00 Intermission.

3:15 COMP **38.** Molecular fragments as a tool for electronic structure. **T.A. Van Voorhis**

3:45 COMP **39.** High-level QM/MM free energy simulations at affordable computational costs. P.S. Hudson, G. Koenig, F.L. Kearns, S. Boresch, **H.L. Woodcock**

4:15 COMP **40.** MoD-QM/MM structural refinement method: Characterization of hydrogen bonding in the Oxytricha nova G-quadruplex. J. Ho, C.M. Ragain, J. Gascon, E.R. Batista, J. Loria, **V.S. Batista**

Section D

Colorado Convention Center

Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **41.** Structure-focused modeling approach to identify family-specific kinase inhibitors. S. Ravichandran, B.T. Luke, J.R. Collins

2:00 COMP **42.** Computational analysis of the binding specificity of DMH1 to Alk2, Alk5, and VEGFR2 kinases. A. Alsamarah, J. Hao, Y.L. Luo

2:30 COMP **43.** Chemical fragments positively interact with protein side chains: An analysis of PDB and CSDB database. **M. Tu**

3:00 Intermission.

3:15 COMP **44.** Knowledge based conformation sampling algorithms and its application in Foldit drug design game. S.K. Kothiwale, J. Mendenhall, S. Combs, J. Meiler

3:45 COMP **45.** X-ray fragment screening for allosteric sites. M. Verdonk

4:15 COMP **46.** Withdrawn.

Section E

Colorado Convention Center

Mile High Ballroom 4F

Quantum Chemistry

Methodology

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **47.** Fast calculation of two-electron integrals. A numerical approach. **P.E. Lopes**

2:00 COMP **48.** Advances in local RI methods for SCF calculations. S. Manzer, E. Epifanovsky, M.P. Head-Gordon

2:30 COMP **49.** Exploiting sparsity to enable petascale applications in material science and quantum chemistry. **M. Keceli**, H. Zhang, P. Zapol, D.A. Dixon, A.F. Wagner

3:00 Intermission.

3:15 COMP **50.** Accurate and efficient propagator methods for calculating electron binding energies of large molecules: Applications to fullerenes and other large acceptors. **J.V. Ortiz**

3:45 COMP **51.** Learning non-local kinetic energy functionals for hydrocarbons with computers. **J. Parkhill**, K. Yao

4:15 COMP **52.** Simulating plasmon-molecule interactions in the time domain. **A.E. DePrince**

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Gas-phase Kinetics and Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Amyloid Precursor Protein, Origin of Amyloid β

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Classical and Quantum Descriptions of Protein Function

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Complex Materials and Molecules

Sponsored by PHYS, Cosponsored by COMP

MONDAY MORNING

Section A

Colorado Convention Center

Mile High Ballroom 1D

Molecular Mechanics

Force Field Development

Cosponsored by PHYS

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **53.** Multistate reweighting as an effective tool for force field parameterization. **M.R. Shirts**, L. Naden, B. Zimmerman, H. Paliwal

9:00 COMP **54.** Wolf$_2$Pack: A scientific workflow and molecular database for force-field optimization. **K.N. Kirschner**, O. Krämer-Fuhrmann, M. Hülsmann, D. Reith

9:30 COMP **55.** Residue-specific force fields based on protein coil library and their applications. **F. Jiang**, C. Zhou, S. Xun, Y. Wu

Technical program information known at press time.
The official technical program for the 249th ACS National Meeting is available at:
www.acs.org/denver2015

‡ *Cooperative Cosponsorship*

10:00 COMP **56.** Development of a tuned interfacial force field for the simulation of protein adsorption to poly(methyl methacrylate). **J.A. Yancey**, T.M. Abramyan, J.A. Snyder, S.J. Stuart, R.A. Latour

10:30 Intermission.

10:45 COMP **57.** Accurate parameterization of ionic surfactants at high concentration. **G.B. Goh**, D.M. Eike, B.P. Murch, C.L. Brooks III

11:15 COMP **58.** Development of an accurate multipolar-polarizable force field for ionic liquids. **H. Torabifard**, G.A. Cisneros

11:45 COMP **59.** Concentration effect on the hydrogen-bond strength between small molecules at the oil/water interface. **V.K. Yadav**

Section B

Colorado Convention Center
Mile High Ballroom 1E

Computational Design, Discovery and Optimization of Organic Semiconductor Materials

Cosponsored by PHYS

G. B. Fitzgerald, M. Halls, *Organizers*
M. Thompson, *Presiding*

8:30 COMP **60.** Modeling of organic light emitting diodes: From molecular to device properties. P. Kordt, J. van der Holst, M. Al Helwi, W. Kowalsky, F. May, A.B. Badinksi, C. Lennartz, **D. Andrienko**

9:00 COMP **61.** Theoretical investigation of organic light-emitting diode materials. **O. Kwon**

9:30 COMP **62.** Molecular design for high efficiency thermally activated delayed fluorescence aimed for OLED application. K. Shizu, **Q. Zhang**, S. Huang, H. Kaji, **C. Adachi**

10:00 Intermission.

10:15 COMP **63.** Computational screening of organic light-emitting diodes. **A. Aspuru-Guzik**

10:45 COMP **64.** Quantum chemical view on OLEDs: designing charge transport materials and phosphorescent emitters. **C. Lennartz**, F. May, D. Andrienko

11:15 COMP **65.** Tunable charge transport in donor-acceptor charge transfer complexes. K.P. Goetz, **O.D. Jurchescu**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Correlation Methods & DFT

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

8:30 COMP **67.** Many-body dispersion interactions in molecular crystals. **N. Marom**

9:00 COMP **68.** Electronic structure of pi-conjugated materials for organic electronics applications. **J.E. Bredas**

9:30 COMP **69.** Systematically Improvable multi-scale methods for correlated electron systems. **D. Zgid**

10:00 Intermission.

10:15 COMP **66.** Scaling coupled-cluster theory to nanoclusters using molecular cluster perturbation theory. **J.N. Byrd**, N. Jindal, B. Sanders, R.J. Bartlett

10:45 COMP **70.** Improving electronic excitation energies and couplings. **J.E. Subotnik**, E.C. Alguire, X. Liu, Q. Ou

11:15 COMP **71.** Ab initio characterization of the electrochemical stability and solvation properties of condensed-phase ethylene carbonate and dimethyl carbonate mixtures. T. Barnes, J. Kaminski, O. Borodin, **T.F. Miller**

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Cosponsored by MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **72.** Fragment-based free energy perturbation. T. Steinbrecher, **W. Sherman**

9:00 COMP **73.** Binding specificity of bone morphogenetic protein (BMP) receptors: Insight from free energy simulations. **Y.L. Luo**, A. Alsamarah, W. Jiang, J. Hao

9:30 COMP **74.** Quantifying key determinants of molecular recognition: Significance of pi interactions and charged hydrogen bonds in protein-ligand binding. **B.K. Rai**, G.A. Bakken

10:00 Intermission.

10:15 COMP **75.** Design of peptides for improved binding to radiation-inducible targets in cancer therapy. **S.A. Wildman**

10:45 COMP **76.** Toward structure prediction of cyclic peptides. H. Yu, **Y. Lin**

11:15 COMP **77.** Benchmark of ensemble docking against crystal docking for use in kinases drug discovery projects. **T.L. Claiborne**, R.V. Swift, R.E. Amaro

Section E

Colorado Convention Center
Mile High Ballroom 4F

Molecular Mechanics

Proteins

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **78.** Structural and energetic insight into the cross-seeding amyloid assemblies of human IAPP and rat IAPP. **M. Zhang**, R. Hu, H. Chen, Q. Wang, C. Zhao, J. Zheng

9:00 COMP **79.** NS3 helicase translocation along ssRNA. **A. Perez-Villa**, M. Darvas, G. Bussi

9:30 COMP **80.** Binding studies of a *Saccharomyces cerevisiae* peripheral protein Osh4. **V. Monje-Galvan**, J.B. Klauda

10:00 Intermission.

10:15 COMP **81.** Stabilization effects of disulfide bonds and dimerization on CXCL7. **C. Singer**, C. Herring, E. Ermakova, D.J. Jacobs, I. Nesmelova

10:45 COMP **82.** All-atom simulation of the folding and binding of an intrinsically disordered protein. **R.E. Ithuralde**, A.E. Roitberg, A.G. Turjanski

11:15 COMP **83.** Possible mechanism for redox control of human neuroglobin activity revealed by crystallography and simulation. **D.C. Chatfield**, O. Morozov, J.P. Roach

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Enzyme Kinetics and Dynamics

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

α-Synuclein, the Parkinson's Protein

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Membrane Proteins

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Excited States in Biology

Sponsored by PHYS, Cosponsored by COMP

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Cosponsored by PHYS

K. Merz, A. E. Roitberg, *Organizers*
D. M. York, *Organizer, Presiding*

1:30 COMP **84.** Proteins are the easy part: Chemical diversity in the PDB archive. **H.M. Berman**

2:00 COMP **85.** Origins of Species: The evolutionary biology of computer agents. **I. Kuntz**

2:30 COMP **86.** How well can a force field match the Born-Oppenheimer surface? The water dimer as an example. **T. Darden**

3:00 Intermission.

3:15 COMP **87.** Collagen triple helix interactions with the integrin receptor: Highlighting the role of conformational fluctuations. **J. Baum**

3:45 COMP **88.** Structure of disorder. **J. Holton**, P. Janowski, D.A. Case, D.S. Cerutti

4:15 COMP **89.** Simulation of pH-dependent unfolding and target-inhibitor interactions. **D. Bashford**

Section B

Colorado Convention Center
Mile High Ballroom 1E

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C. Shields

G. C. Shields, *Organizer*
E. C. Sherer, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 COMP **90.** Concertedness and synchronicity—from arynes to electrochemistry. **C.J. Cramer**

2:10 COMP **91.** Molecular simulations in conjunction with experimental studies illustrate internal protein logic controlled by conformation and dynamic structural change. **T.E. Morrell**, I.U. Rafalska-Metcalf, J. Chu, H. Yang

2:30 COMP **92.** Predicting permeability and target binding of complex macrocycles. **K.W. Lexa**, M.P. Jacobson

3:00 Intermission.

3:20 COMP **93.** Molecular studies of halogen bonding, protein folding and combustion. **C.A. Parish**

3:50 COMP **94.** Anharmonic effects in vibrational spectra of protonated water clusters. **K.A. Archer**, T. Odbadrakh, J.A. Fournier, M.A. Johnson, K.D. Jordan

4:10 COMP **95.** Insight Into hydrazone-based dye fluorescence from density functional theory. **M.D. Liptak**, E.H. Horak

4:40 COMP **96.** Recent developments in high accuracy nonbonded interactions in the CHARMM simulation package. **F.C. Pickard**, A.C. Simmonett, B. Brooks

5:10 COMP **97.** Examining the interface: Simulations exploring the effect of solid substrates on thin liquid films. **K.E. Anderson**, S. Wenzel, H.M. Nemec, J. Lee, S. Watkins, T. Stoneham, J.I. Siepmann

Section C

Colorado Convention Center
Mile High Ballroom 1F

Electronic Structure Methods for Highly Polarizable Systems

Excitons

Cosponsored by PHYS

D. Lambrecht, J. Parkhill, *Organizers, Presiding*

1:30 COMP **98.** Toward new materials for singlet fission. J. Wen, M. Jovanovic, Z. Havlas, **J. Michl**

2:00 COMP **99.** Exciton delocalization in disordered conjugated polymer films. **A. Willard**

2:30 COMP **100.** Numerical simulations of the optical response and energy transfer coupled exciton-plasmon systems. M. Sukharev, **A. Nitzan**

3:00 Intermission.

3:15 COMP **101.** Understanding the coupling between molecular excited states and plasmons. **L. Jensen**

3:45 COMP **373.** Ab initio implementation of the Frenkel-Davydov exciton model. **J. Herbert**, A. Morrison

4:15 COMP **102.** Effect of shape, size, and heterojunction on excitonic interactions in semiconductor nanoparticles. J. Scher, **A. Chakraborty**

4:45 COMP **103.** Chiroptical properties and excitation data with local coupled cluster methods. **H. McAlexander**, T. Crawford

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

ADME & Informatics

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **104.** Methodology for machine learning in chemical design. **S. Chonde**, J. Storer, K.T. Mueller, S. Kumara

2:00 COMP **105.** PubChem and big data. **S. Kim**, G. Fu, L. Han, B. Yu, L. Geer, A. Gindulyte, S. He, P. Thiessen, E.E. Bolton, S.H. Bryant

2:30 COMP **106.** Toward the ubiquitous use of cheminformatics: From the development of reliability boosters for structure-based molecular docking to the analysis and modeling of hyperdimensional HTS data. **D. Fourches**

3:00 Intermission.

3:15 COMP **107.** Evaluating structural toxicity alerts with metabolism and reactivity models. **T. Hughes**, G.P. Miller, S. Swamidass

3:35 COMP **108.** Predicting regioselectivity and lability of cytochrome P450 metabolism using quantum mechanical simulations. M.D. Segall, **J. Tyzack**, P. Hunt

4:15 COMP **109.** In silico approaches to CYP P450 site-of-metabolism (SOM) and microsomal stability prediction. **J.H. Voigt**, U. Schmitz

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Methodology

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **110.** Combining active-space coupled-cluster approaches with moment energy corrections via the CC(*P*;*Q*) methodology: Ground and excited states. **P. Piecuch**, J. Shen, N.P. Bauman

2:00 COMP **111.** Calculation of two-photon absorption cross-sections within EOM-EE-CCSD formalism: Theory and examples. **K. Nanda**, A. Krylov

2:30 COMP **112.** Systematic expansion of active spaces beyond the CASSCF limit: A GASSCF/SplitGAS benchmark study. **K.D. Vogiatzis**, G. Li Manni, S. Stoneburner, D. Ma, L. Gagliardi

3:00 Intermission.

3:15 COMP **113.** Time-dependent projected Hartree-Fock for degenerate excited states. **T. Tsuchimochi**, T.A. Van Voorhis

3:45 COMP **114.** Variational state specific solvent models for excited states from time dependent self-consistent field methods. **J. Bjorgaard**, K. Velizhanin, S. Tretiak

4:15 COMP **115.** Accurate ab initio potential energy curves and spectroscopic properties of C_2 singlet states. **J. Boschen**, D. Theis, K. Ruedenberg, T.L. Windus

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Catalysis

Sponsored by PHYS, Cosponsored by COMP

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Islet Amyloid Polypeptide (IAPP) at the Water/Lipid Interface

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Molecular Machines

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Multiple Chromophores

Sponsored by PHYS, Cosponsored by COMP

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

E. X. Esposito and S. A. Wildman, *Organizers*

8:00 - 10:00
180, 182-183, 222, 235, 259, 261-262, 264, 265, 275, 280, 291. See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1D

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Cosponsored by PHYS

A. E. Roitberg, D. M. York, *Organizers*
K. Merz, *Organizer, Presiding*

8:30 COMP **116.** Molecular understanding of hydrophobic association in ethanol-water mixtures. **T. Ichiye**

9:00 COMP **117.** Quantum mechanical force fields: A breakthrough in multiscale modeling tools. **D.M. York**

9:30 Intermission.

9:45 COMP **118.** Decoding the dynamics properties of protein loops by the combination of NMR and molecular dynamics simulations. Y. Gu, D. Li, **R. Bruschweiler**

10:15 COMP **119.** Reproducibilty and convergence in the assessment, validation and improvement of force fields for RNA. **T.E. Cheatham**

10:45 COMP **120.** Thermodynamic estimates from molecular dynamics. **C.B. Post**

Section B

Colorado Convention Center
Mile High Ballroom 1E

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C. Shields

E. C. Sherer, G. C. Shields, *Organizers, Presiding*

8:30 COMP **121.** Thermodynamic quantities and structural information from a molecular printing press. **K.M. Merz**

9:00 COMP **122.** Addressing problems at the interface of chemistry and medicine: Computational and chemical biology approaches. **K. Alser**, G.C. Shields, D.G. McCafferty

9:20 COMP **123.** From the atmosphere to the interstellar medium: Long-range molecular interactions. **M.A. Allodi**, S. Ioppolo, B.A. McGuire, G.A. Blake

9:40 Intermission.

10:00 COMP **124.** Comparison of diffusion Monte Carlo and CCSD(T) methods on model systems. **K.D. Jordan**, M.J. Deible

10:30 COMP **125.** From the computational chemistry lab to treating cancer: Inspiration for drug development in our time. **K. Larkin**

10:50 COMP **126.** Evolution of methods for modeling hydrogen-bonded systems accurately and efficiently. **B. Temelso**, G.C. Shields

11:20 COMP **127.** Role of water in arginine-rich motif peptide-RNA recognition. L. Michael, B. Miller, S. Bernard, M. Hoffman, W. Hodges, Z. Fallon, **M.C. Nagan**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Materials Science

Quantum Materials

E. X. Esposito, *Organizer, Presiding*

8:30 COMP **128.** Self-consistent projector constrained density functional theory in ONETEP. **G. Teobaldi**, D.D. O'Regan, N.D. Hine, A.A. Mostofi

9:00 COMP **129.** Stopping powers from time-dependent density functional theory. **R.J. Magyar**

9:30 COMP **130.** Hybrid functional study of stability and electronic structure of $Cu_2ZnSn(S,Se)_4$ polytypes. **J. Park**, I. Repins, S. Wei

10:00 Intermission.

10:15 COMP **131.** Enhanced oxygen vacancy formation in cation doped bulk Cr_2O_3. **M. Nolan**, M. Legesse, A. Van Veen

10:45 COMP **132.** CO_2 adsorption in M-IRMOF10 (M=Mg, Ca, Fe, Cu, Zn, Ge, Sr, Cd, Sn, Ba). **J.D. Borycz**, D. Tiana, E. Haldoupis, L. Gagliardi, J.I. Siepmann

11:15 COMP **133.** AIMing toward better prediction of corrosion inhibitor prediction. **R.L. Cook**

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Methodology

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **134.** Flexible CDOCKER: Development and application of a docking method incorporating non-rigid receptors within CHARMM. **J. Gagnon**, S. Law, C.L. Brooks

9:00 COMP **135.** Small molecule design using single step free energy perturbation (SSFEP): Blinded validation against the relative binding affinities of inhibitors of p38 and ACK1 kinases. E. Raman, A.D. Mackerell, **R.A. Denny**

9:30 COMP **136.** Expert system for predicting different local structure-activity relationship environments using the concept of emerging chemical patterns. **V. Namasivayam**, D. Gupta-Ostermann, J. Balfer, J. Bajorath

10:00 Intermission.

10:15 COMP **137.** Scoring doesn't work — or does it? **C. Detering**

10:45 COMP **138.** ProBiS-ligands: A web server for prediction of ligands by examination of protein binding sites. **D. Janezic**, J. Konc

11:15 COMP **139.** Movable type method applied to the biomolecules study. **Z. Zheng**, M. Ucisik, K.M. Merz

Section E

Colorado Convention Center
Mile High Ballroom 4F

Computational Study of Water

D. J. Sindhikara, *Organizer, Presiding*

8:30 COMP **140.** Water's role in compound design for drug discovery. **H. Zhu**

9:00 COMP **141.** Quantitative prediction of water thermodynamics and applications to drug design. **W. Sherman**

9:30 COMP **142.** Insights into hydration propensity from systematic analyses of water in crystal structures. **S. Vyas**, C. Groom, S. Ward, I. Bruno

10:00 Intermission.

10:15 COMP **143.** Water-biomolecule interaction studied by 3D-RISM and X-ray scattering. **H.T. Nguyen**, D.A. Case

10:45 COMP **144.** Water dynamics in aqueous solutions of hydrophilic and amphiphilic peptides: Molecular simulation study of polarizability anisotropy response. **B.M. Ladanyi**, A.A. Milischuk

11:15 COMP **145.** Study of the protonation states of the curcumin molecule and their visible absorption spectra in aqueous solution using M06, SMD, and TDDFT and compared to experiment. **J.D. Alia**, P. Braegelmann, T. Roettgen, H. Goemann

TUESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of David A. Case

Cosponsored by PHYS

K. Merz, D. M. York, *Organizers*
A. E. Roitberg, *Organizer, Presiding*

1:30 COMP **146.** Role of functional disorder in large protein complexes. **H. Dyson**, S. Sue, S. Mukerjee

2:00 COMP **147.** Mechanistic strategies in the HDV ribozyme: Metal ion identity controls the reaction pathway. **S. Hammes-Schiffer**, P.C. Bevilacqua

2:30 COMP **148.** Development of the ff14SB force field and application to protein folding simulations. **C.L. Simmerling**, J. Maier, H. Nguyen

3:00 Intermission.

3:15 COMP **149.** Withdrawn.

3:45 COMP **150. Award Address** (ACS Award for Computers in Chemical and Pharmaceutical Research sponsored by the ACS Division of Computers in Chemistry). Simulating biomolecules with implicit solvent models: GB, PB and 3D-RISM. **D.A. Case**

Section B

Colorado Convention Center
Mile High Ballroom 1E

ACS Award for Research at an Undergraduate Institution: Symposium in Honor of George C. Shields

E. C. Sherer, G. C. Shields, *Organizers, Presiding*

1:30 COMP **151.** On things that move. Protons, electrons, and other beasts in molecular modeling. **A.E. Roitberg**

2:00 COMP **152.** Highlights of a science career that began with undergraduate research. **H. McCuen**

2:20 COMP **153.** Computational chemistry's impact beyond discovery chemistry: Spectroscopy, cheminformatics and application of density functional theory in support of process/analytical chemistry. **E.C. Sherer**

2:50 Intermission.

3:10 COMP **154.** It's all about the fundamentals. **K. Kirschner**

3:40 COMP **155.** Conformation of retinal controls the pKa of protonated Schiff base during rhodopsin activation. **S. Feller**

4:10 COMP **156.** Role of quantum chemistry, PM3 and magic water clusters in unlocking Rodin's "Gates of Hell". **M. Jurema**

4:30 COMP **157. Award Address** (ACS Award for Research at an Undergraduate Institution sponsored by Research Corporation for Science Advancement). Research with undergraduates — a fabulous career. **G.C. Shields**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Materials Science

Application and Movement

E. X. Esposito, *Organizer, Presiding*

1:30 COMP **158.** Low-temperature removal of crystallized fats: Investigation of nanodiamond adsorption on the disruption of the aqueous tristearin interface. **Z.E. Hughes**, T. Walsh

2:00 COMP **159.** Using crystal structures to understand pharmaceutical materials. S. Vyas, **C. Groom**, S. Ward, N. Feeder, I. Bruno

2:30 COMP **160.** Molecular dynamics simulations of biomolecules adsorbed on colloidal nanoparticles. **P. Samanta**, S. Wu, S. Sen, P. Kral

3:00 Intermission.

3:15 COMP **161.** Molecular dynamics simulation of CO_2 transport in hydrated Zeolite X. **S. Chakraborty**, S.J. Singer, P.K. Dutta

3:45 COMP **162.** Assessing and predicting flexibility in framework materials with molecular simulation: MOFs, zeolites, and molecular frameworks. A. Ortiz, A. Boutin, **F. Coudert**

4:15 COMP **163.** Zooming in on the solid-to-solid polymorphic transitions in DL-norleucine. **H. Cuppen**, J.A. Van Den Ende, M.M. Smets, D.T. de Jong, S.J. Brugman, H. Meekes

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Methodology

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **164.** Predicting melting points of drug-like molecules using free energy perturbation. **R.A. Denny**, S. Jayaraman, R.J. Unwalla, M.E. Bunnage

2:00 COMP **165.** Biasing potential replica exchange multisite λ-dynamics: Toward scalable and simultaneous free energy calculations of more than 1000 compounds. **G.B. Goh**, K.A. Armacost, C.L. Brooks III

2:30 COMP **166.** Thermodynamics of ligand binding — consequences of local environment for drug optimization. **J. Ulander**

3:00 Intermission.

3:15 COMP **167.** Toward a complete, fully knowledge-driven pseudo force field for protein-ligand interactions. **M. Verdonk**

3:45 COMP **168.** Hierarchy of density functional theory-based benchmarks for a chemical space relevant to drug discovery applications. **A.D. Bochevarov**

4:15 COMP **169.** Rational design of potent factor VIIa inhibitors using quantum chemical methods. **D.L. Cheney**, I. Delucca, P.W. Glunz, W. Jiang, V. Ladziata, B. Parkhurst, Y. Zhang, Y. Zou, J.M. Bozarth, J.M. Luettgen, A.R. Rendina, L. Mueller, A. Wei, J.A. Newitt, J.K. Tamura, D. Seiffert, P.C. Wong, R.R. Wexler, E.S. Priestley

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Applications

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **170.** Theoretical studies of the synchronization of the catalytic cycles in the second half-reaction step of nitric oxide synthase. **I. Shamovsky**, G. Belfield, F. Narjes, L. Ripa, C. Tyrchan, L. Öberg, P. Sjö

2:00 COMP **171.** Insight into the catalytic reaction mechanism of CO oxidation on reducible oxide-supported Au catalysis by AIMD simulation. **Y. Wang**, J. Li, R. Rousseau

2:30 Intermission.

‡ *Cooperative Cosponsorship*

2:45 COMP **172.** Tunable luminescence in CdSe quantum dots doped by Mn impurities. **Y. Dahnovsky**, V. Proshchenbko

3:15 COMP **173.** Highly-reduced corannulene: The influence of alkali metals on the structure and formation of aggregates. **A.Y. Rogachev**

3:45 COMP **174.** Quantum mechanical study of structural and electronic dilution effects in paramagnetic chemical exchange saturation transfer agents. **W.A. Miller**, P.B. Moore

Role of Membrane in Amyloid-Formation & the Pathogenicity of Amyloid Disease

Prions and Beyond

Sponsored by PHYS, Cosponsored by COLL and COMP

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

TUESDAY EVENING

Section A

Colorado Convention Center

Hall B2

NVIDIA GPU Award

M. E. Berger, R. Gomperts, *Organizers*

6:00 - 8:00

COMP **175.** Ligand-specific conformational changes in CCR7 coupled to signaling pathway selection. **Z. Gaieb**, D.D. Lo, D. Morikis

COMP **176.** Theoretical view of the C3d-CR2 binding controversy. **R. Mohan**, R.D. Gorham, D. Morikis

COMP **177.** Entropically driven CK-ASB9 interaction: How GPU-enabled computing provided unique insight into an intrinsically disordered 116 kDa protein complex. **J. Schiffer**, J. Parnell, E.A. Komives, R.E. Amaro

COMP **178.** GPU-enabled real-time electron dynamics of large light-harvesting systems in explicit solvent. **B.M. Wong**, M. Oviedo

COMP **179.** GPU-accelerated implementations of advanced electronic structure methods in Q-Chem. **K. Nanda**, E. Epifanovsky, A. Krylov

Section A

Colorado Convention Center

Hall B2

Poster Session

E. X. Esposito, S. A. Wildman, *Organizers*

6:00 - 8:00

COMP **180.** Possible mechanisms for interconversion of polar forms for the ferroelectric diisopropylammonim halides. **K.R. Cousins**

COMP **181.** Numerical modeling of carbon condensation in detonation products. **C. Mader**

COMP **182.** Identification of a new class of potential antimalaria agents using in-silico methodology. **R. Richardson**

COMP **183.** DFT and MP2 analysis of ligand selectivity in the catechol-O-methyltransferase enzyme. **A.K. Hatstat**, M. Morris, L. Peterson, M.L. Cafiero

COMP **184.** Effects of implicit solvation, relaxed amino acid side chains, and point mutations on the MP2 and DFT calculations of ligand-protein structure and interaction energies of dopaminergic ligands in the SULT1A3 enzyme active site. D. Bigler, L. Peterson, **M.L. Cafiero**

COMP **185.** MP2 and DFT analysis of the ligand selectivity of a sulfotransferase enzyme: SULT 1A. **A.H. Weems**, M.L. Cafiero, L.W. Peterson

COMP **186.** Study of the translocation of chloride ions through *Escherichia coli* transporters using the combined QM/MM method. **C. Davis**, S. Pezeshki, C. Garza, H. Lin

COMP **187.** Weighing energetics against best fit in development of RNA structure prediction models. **D. Bell**, Z. Xia, P. Ren

COMP **188.** Interactions between amino acid and graphene oxide: Experiments and theoretical calculations. **L. Huang**, K.E. Gubbins

COMP **189.** Applying intelligent design to biocatalyst engineering. **J. Pottel**, A. Tomberg, C. Bendell, N. Moitessier

COMP **190.** Interfacial force field parameterization in CHARMM for the accurate representation of peptide adsorption free energy on high-density polyethylene. **T. Abramyan**, J. Snyder, J.A. Yancey, S. Stuart, R.A. Latour

COMP **191.** Anions and computation: A match made in chemical heaven. **R.C. Fortenberry**

COMP **192.** Multiscale approach to decipher enzymatic processing and selectivity of lipids. **L. Riccardi**, J. Arencibia, A. Armirotti, M. Devivo

COMP **193.** In silico discovery of FKBP52 inhibitors as a prospective therapy for prostate cancer. **H. Li**, N. Guy, M.B. Cox, A. Cherkasov

COMP **194.** Withdrawn.

COMP **195.** Identification of 'dynamic hotspots' for lead discovery using MD simulation and spatiotemporal cluster analysis. **A. Arakawa**, O. Ichikawa, K. Yamazaki, K. Fujimoto, M. Okada, A. Yamada, S. Okazaki

COMP **196.** Density-based energy decomposition analysis. **Q. Wu**

COMP **197.** Prioritizing high throughput screening hits using a filtering workflow implemented in KNIME and QSAR models for antimalarial drug discovery. **S. Capuzzi**, D. Fourches, A. Tropsha

COMP **198.** Simulating X-ray, UV, and VIS absorption spectra with orthogonality constrained density functional theory. **F.A. Evangelista**, W.D. Derricotte

COMP **199.** Fast and reliable first principles approaches for the prediction of electro-mechanical properties in organic "smart" materials. K. Werling, B. Albrecht, **D. Lambrecht**

COMP **200.** Towards accurate parameterization for pyrrolidinium-based ionic liquids in lithium-ion batteries. **H. Torabifard**, G.A. Cisneros

COMP **201.** Withdrawn.

COMP **202.** Investigation of the effects of water in the binding site on protein-ligand interaction energy. **H. Sato**, A. Matsuura

COMP **203.** Insights into cobalt oxide water oxidation catalysts: A theoretical perspective from model dimer and cubane complexes. **A. Fernando**, C.M. Aikens

COMP **204.** Molecular modeling of dielectric constant of EC/DMC mixtures. **I. Daniels**, Z. Wang, B. Laird

COMP **205.** Site of reactivity models predict molecular reactivity of diverse chemicals. **T.B. Hughes**, G.P. Miller, S. Swamidass

COMP **206.** Molecular dynamics study of the confinement of alkane guests in an octa-acid dimer. **J. Barnett**, H. Ashbaugh, B.C. Gibb

COMP **207.** Robust and efficient coupled cluster-polarizable solvation methods for electronic molecular properties in the condensed phase. **M. Caricato**

COMP **208.** Pharmacophore-based similarity scoring method for DOCK. **L. Jiang**, R.C. Rizzo

COMP **209.** Mechanistic analysis of water oxidation catalyzed by a mononuclear copper(II) polypeptide in aqueous solutions. **W.C. Isley**, C.J. Cramer

COMP **210.** Development and in silico evaluation of large-scale metabolite identifcation methods using functional group detection for metabolomics. **J.M. Mitchell**, T.W. Fan, A.N. Lane, H.N. Moseley

COMP **211.** Nanoscale structure and dynamics of the liquid ordered phase of lipid bilayers. **E. Lyman**

COMP **212.** Strength, not depth: An exploration of differential membrane binding kinetics of Synaptotagmin-1 and Synaptotagmin-7 C2 domains. **J. Vermaas**, E. Tajkhorshid

COMP **213.** Withdrawn.

COMP **214.** Tolerance-dependent algorithm for core-constrained ligand docking with glide. **I. Tubert-Brohman**, J.L. Banks, M.P. Repasky

COMP **215.** Quartic force fields for electronically excited states: Theoretical ro-vibronic spectra. **W.J. Morgan**, R.C. Fortenberry

COMP **216.** Comparison of local correlation methods applied to chiroptical properties and excited states. **H. McAlexander**, T. Crawford

COMP **217.** Bond length alternation of conjugated oligomers: Performance of recent double-hybrid functionals. **M. Wykes**, N.Q. Su, X. Xu, C. Adamo, J.C. Sancho-García

COMP **218.** Supramolecular engineering via fragment-based design. **B.P. Hay**, B. McCann

COMP **219.** Molecular mechanism of gated ligand binding. **Y. Li**, Z. Dong

COMP **220.** Validation of a tuned interfacial parameter set using dual-force-field CHARMM for the accurate simulation of protein adsorption on a silica glass surface. **J. Snyder**, T. Abramyan, J.A. Yancey, S. Stuart, R.A. Latour

COMP **221.** Implementation of the generalized internal coordinates for molecular geometry, energy gradients, and force constants. **A.V. Marenich**, H.P. Hratchian, J.L. Sonnenberg, M.J. Frisch

COMP **222.** Price of admission: Exploring the transition from straight chain to first cycle in sesquiterpene biosynthesis using quantum chemical calculations. **C.S. Hamann**, M.W. Lodewyk, D.J. Tantillo

COMP **223.** Photoionization of water in gas phase and in bulk: Insight from equation-of-motion coupled-cluster Dyson orbitals. **S. Gozem**, A. Krylov

COMP **224.** Exploring rovibrational states of floppy molecules using diffusion Monte Carlo. **J. Ford**, A.B. McCoy

COMP **225.** Scientific and technological advances in the quantum chemistry package Jaguar. **A.D. Bochevarov**, T.F. Hughes, L.D. Jacobson, D.M. Philipp, M.A. Watson

COMP **226.** DFT study of structural evolution of gold clusters.Au^-_n with n= 40-50. S. Pande, **X.C. Zeng**

COMP **227.** Quantum chemistry for X-ray photoelectron spectroscopy: Computation of XPS chemical shifts in amino acids and simple polypeptides. **I. Tolbatov**, D.M. Chipman

COMP **228.** In silico prediction of charge carrier mobility in organic semiconductors. **S. Kwak**, A. Goldberg, D. Giesen, M. Halls

COMP **229.** Withdrawn.

COMP **230.** Distinguishing the protonation states of the histidine ligands of the Rieske iron-sulfur cluster by ^{15}N isotopic substitution and vibrational frequency shifts. **B.R. Jagger**, A.M. Koval, R.A. Wheeler

COMP **231.** Nucleation mechanisms of γD-crystallin protein aggregates found in cataracts. **S.A. Richards**, R.A. Wheeler

COMP **232.** Computed chemical properties for the functional sorting of the haloacid dehalogenase superfamily. **E.M. Mozur**, M. Touch, M.J. Ondrechen

COMP **233.** Gold nanoparticle-nucleic acid modeling using GPU-accelerated molecular dynamics. **J.A. Nash**, A.L. Kwansa, Y.G. Yingling

COMP **234.** Withdrawn.

COMP **235.** Development of OPLS-AA Force Field Parameters for Ionic Liquids. **S.M. Gathiaka**, B. Li, O. Acevedo

COMP **236.** Accelerating DFT and hybrid DFT in VASP Using GPUs. **P. Fleurat-Lessard**, M. Hutchinson, M. Widom, A. Anciaux-Sedrakian, T. Guignon, D. Stosic, j. Bedorf, S. Tariq

COMP **237.** Simulations of fluorescence solvatochromisms in substituted *p*<-phenylene vinylene oligomer derivatives: Excited state molecular dynamics with implicit solvent. **J. Bjorgaard**, K. Velizhanin, S. Tretiak

COMP **238.** First-principle study of the structural and electronic properties of graphene on Zn(II) phthalocyanine tetrasulfonic acid adsorption. **R. Li**, D. Nicholls, M.R. Hoffmann, N. Oncel

COMP **239.** Quantum mechanical molecular interactions for calculating excitation energy in molecular environments: A first-order interacting space approach. **K. Yanai**, K. Ishimura, J. Hasegawa

COMP **240.** Nitrogen dopants and vacancy defects in graphene nanoflakes: Theoretical study of size-dependent electronic excitation properties. **C. Lin**

COMP **241.** Free energy study of small molecules to RNA with multiple binding poses. **Y. Tanida**, A. Matsuura

COMP **242.** Uncovering topological signatures of instability and metastability. **J. Miorelli**

COMP **243.** Molecular dynamics of metallodiporphyrins. **J. Coda**, W.M. Ames

COMP **244.** Computational insights into intramolecular hydrogen migration via agostic-type interactions. **J. Duchimaza**, K. Yan, A. Ellern, A.D. Sadow, M.S. Gordon

COMP **245.** Predictive methods for CO_2 solubilities in reactive ionic liquids. **Q. Sheridan**, T. Lee, E. Maginn, W.F. Schneider

COMP **246.** Theoretical study of (hetero) aromatic fluorination catalyzed by palladium. P. Fleurat-Lessard, **J. Roger**, C. Testa, J. Hierso

COMP **247.** Computer simulations of forward osmosis for desalination. **O. Lee**

COMP **248.** Withdrawn.

COMP **249.** Computational insight into origins of *Z*-selectivity and enantioselectivity of asymmetric ring-opening/cross-metathesis catalyzed by a stereogenic-at-Ru complex. **J.W. Nelson**, H.D. Pham, X. Wang

COMP **250.** Coordination number and molecular geometry influences on methanethiol binding strength and acidity in $[(Imidazole)_{6-x}Zinc(II)–S(H)CH_3]$ complexes. **D.P. Linder,** K.R. Rodgers

COMP **251.** DFT study of the rate determining steps of carbon chain growth on Co. **D. Petersen**, L. Arnadottir

COMP **252.** Theoretical study on the fluorescent spectrum of enhanced green fluorescent protein. **Y. Uchida**, M. Higashi, S. Hayashi

COMP **253.** Identification of a pKa-regulating motif stabilizing imidazole modified double stranded DNA. **D. Buyst**, V. Gheeraardijn, J. van den Begin, A. Madder, J.C. Martins

COMP **254.** Alpha-hydrogen bonding stereochemical consequences in alpha,beta-unsaturated aldehydes complexed with chiral menthoxyaluminum dichloride Lewis acid catalysts in Diels-Alder reactions. **B. Vernier**, A.N. Ahmed, J. Rohde, J.D. Evanseck

COMP **255.** Calculation of the association trajectories of oseltamivir and sialic acid to wild type and H274Y viral neuraminidase. **R.W. Wenner**, L.M. Krause, J.F. Graziadei, P.F. Marris, A.W. Van Wynsberghe

COMP **256.** Effect of surface defects on the optical properties of silicon quantum dots. **N.K. Dandu**

COMP **257.** Targeted delivery of peptidoglycan immunomodulators using liposomal carriers: MD study of the lipid encapsulation. **K. Feher**

COMP **258.** Semantic web and computational chemistry. **N.S. Ostlund**, B. Wang

COMP **259.** Reparameterization of gold thiolate ReaxFF. **B.M. Barngrover**, E.M. Kinder, T.J. Manges, T.J. Cobb, C.M. Aikens

COMP **260.** Online parameter and property database for the TraPPE force field. **A. Sunnarborg**, A. Bliss, H. Stern, B.L. Eggimann, J.I. Siepmann

COMP **261.** Elucidating a chemical defense mechanism of Antarctic sponges. S.K. Vankayala, **F.L. Kearns**, B.J. Baker, H.L. Woodcock

COMP **262.** Characterization of fullerene structure and electronic properties using DFT and EPR parameters: Charge localization in polymer-fullerene composite solar cells. **J.N. Webb**, J. Niklas, O. Poluektov, K. Mardis

COMP **263.** Quantum chemical studies of gas hydrates. **P. Warrier**, C.A. Koh

COMP **264.** Nature of the β-cyclodextrin-graphene interface: A quantum chemical analysis. **P. Jaiyong**, R.A. Bryce

COMP **265.** Investigation of different binding kinetics among the neuraminidase inhibitors. **G. Kang**, D.J. Mermelstein, R.B. Clayton, A.W. Van Wynsberghe

COMP **266.** Interaction of aqueous ammonium chloride with *Helicobacter pylori* urease. **M. Minkara**, M.N. Weaver, K.M. Merz

COMP **267.** Iron pyridine-2,6-diimine (PDI) scaffolds: A new model with MRMP2. **J. McNeely**, A.Y. Rogachev

COMP **268.** Density functional analysis of donor-acceptor complexes formed between ethers and sulfur trioxide or sulfur dioxide. **G. Van Den Driessche**

COMP **269.** Human pepsin 3A hydrolysis reaction mechanism. **A.N. Mascarenas**, E. Cowles, J.J. Stewart, S.B. Braun-Sand

COMP **270.** Substrate binding of human MTH1 protein. **H.E. Ryan**, M. Carter, J.J. Stewart, S.B. Braun-Sand, P. Stenmark

COMP **271.** Ab initio computations of nuclear quadrupolar coupling constants: Why they don't work, and how to fix them. **G.S. Harbison**

COMP **272.** Characterization of carbene intramolecular reactivity with various substituents through computer modeling. **M. Roth**, W.M. Ames

COMP **273.** Withdrawn.

COMP **274.** Using TD-DFT and NTOs to model photocatalysis. **C.M. Midkiff**, A.K. Rappe

COMP **275.** First principle study on optimizing conditions for charge transfer in quantum dots through dye functionalization. **P. Cui**, S. Kilina

COMP **276.** SO2– yet another two-faced ligand. **J. Li**, A.Y. Rogachev

COMP **277.** Impact of substituent size and electronegativity on the band gap of TiO_2 polymorphs. **A.J. Glaid**, M.N. Srnec, J.A. Aitken, J.D. Madura

COMP **278.** Enrichment of computational chemistry data with the semantic web. **B. Wang**, L. Nardozi, S.J. Chalk, M. Sopek, N.S. Ostlund

COMP **279.** HK propagator uniformized along a 1D manifold. **L. Kocia**, E.J. Heller

COMP **280.** Structural determinants of promiscuous and specific binding in protein - protein complexes using component analysis techniques. **A. Sherani**, Y.Y. Zhang, M.L. Radhakrishnan

Technical program information known at press time. The official technical program for the 249th ACS National Meeting is available at: www.acs.org/denver2015

COMP **281.** Q-Chem: An engine for innovation. Z. Gan, E. Epifanovsky, **Y. Shao**

COMP **282.** Adsorption of O_2 on neutral/charged Au_n (n = 1-3) clusters: A comparative study between DFT and coupled cluster calculations. Y. Zhao, **N.S. Khetrapal**, H. Li, Y. Gao, X.C. Zeng

COMP **283.** Exploring the mechanisms of enantioselective organocatalytic reactions: A DFT study. **K.E. Blise**, D.L. Kohen, G.E. Hofmeister, D.G. Alberg, M. Cvitkovic

COMP **284.** Molecular simulations of fluorescent sensors with amyloid-β protein aggregates. **J. Thompson**, E.H. Hill, E.Y. Chi, D.G. Whitten, D.G. Evans

COMP **285.** Constrained heuristic optimization of NLO chromophores. **C.B. Rinderspacher**, J. Elward

COMP **286.** Modeling of a bench-scale biomass pyrolyze: An experimentalist's viewpoint. **R.J. French**

COMP **287.** Modeling some features of the reaction mechanism of chymotrypsin using semiempirical methods. **W.C. Kelly**, S.B. Braun-Sand, J.J. Stewart, **B.M. Guerrero**

COMP **288.** Visualizing the interplay of delocalization and strong correlation in catalysis. **B.G. Janesko**

COMP **289.** Ab initio dynamics of the unfolding and decarboxylation of pseudo-chair carboxyphosphate in aqueous solution. **E. Jesikiewicz**, S. Boesch, S.M. Firestine, J.D. Evanseck

COMP **290.** Carboxyphosphate formation from the reaction of bicarbonate and ATP in ATP-dependent carboxylases. **S.E. Kochanek**, T. Clymer, V. Pakkala, S.M. Firestine, J.D. Evanseck

COMP **291.** Analysis of the components of halogen bonding. **M. Billman**, A.K. Rappe

COMP **292.** GPU-accelerated stochastic evaluation of second-order many-body perturbation energies. **R. Brewster**, S. Willow, S. Hirata

COMP **293.** Molecular modeling of the binding interaction of RGD-functionalized poly(ethylene glycol) hydrogels with lipid bilayer surface. **Y. Lin**, G. Chen, F. Ryvkin

COMP **294.** Ab initio study of halocarbons. **K.R. Jorgensen**

COMP **295.** Computational study of activation energies in 1,3-dipolar cycloadditions. **P. Esempio**, H.A. Trujillo

COMP **296.** Microscale multiphysics simulations of intra-particle transport phenomena and pyrolytic conversion using biomass particle models with realistic morphology and resolved microstructure. **P. Ciesielski**, M.F. Crowley, B. Donohoe, M.R. Nimlos, T. Foust

COMP **297.** Theoretically determined mechanism for the formation of guanine C8 adducts from arylamine derived carcinogens. **A.S. Dutton**, J. Bautista, S. Shrestha

COMP **298.** Feedstocks thermal and compositional effects on pyrolysis yields. **D. Robichaud**

COMP **299.** Theoretical study of criegee biradical molecule in the atmosphere. **S. Alhowity**

COMP **300.** Modeling non-covalent interactions in biomolecules: An ab initio based fragmentation approach. **D. Kosenkov**

COMP **301.** Exploring novel energetic materials: A constrained search approach. **J.M. Elward**, C.B. Rinderspacher

COMP **302.** Withdrawn.

COMP **303.** Chemist view on reaction pathways. N. Chéron, R. Ramozzi, R. Grüber, **P. Fleurat-Lessard**

Section A

Colorado Convention Center
Hall B2

The Chemical Computing Group Excellence Award for Graduate Students

Financially supported by Chemical Computing Group

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **304.** Time-dependent nonequilibrium dynamics in QM/continuum approaches. **F. Ding**, D. Lingerfelt, B. Mennucci, X. Li

COMP **305.** MD-generated volume profiles as a tool for probing transition states of conformational changes. **H. Wiebe**, N. Weinberg

COMP **306.** Theoretical investigations of the fumarate addition reaction: Implications for the biological stability of future fuels and opportunities for bioremediation of hydrocarbon contaminated areas. **V.S. Bharadwaj**, C.M. Maupin, A.M. Dean

COMP **307.** Simulations of the self-assembly of polyelectrolyte block copolymers using dissipative particle dynamics with an implicit solvent ionic strength (ISIS) method. **N.K. Li**, W.H. Fuss, Y.G. Yingling

COMP **308.** Sum frequency generation spectra of the air/water interface from first principles-based models. **G.R. Medders**, F. Paesani

Section A

Colorado Convention Center
Hall B2

The OpenEye Outstanding Junior Faculty Award

Financially supported by OpenEye Scientific Software

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **309.** Physically-motivated first-principles force fields for molecular simulation: Theory and applications. **J.R. Schmidt**, J.G. McDaniel

COMP **310.** RNA design rules through internet-scale social computing and high-throughput chemistry. E. Participants, J. Lee, W. Kladwang, M. Lee, D. Cantu, M. Azizyan, H. Kim, L. Alex, S. Yoon, A. Treuille, **R. Das**

COMP **311.** Development of electron-hole explicitly correlated wave function based method with pseudopotential theory for investigation of optical properties of quantum dot-protein complexes. **A. Chakraborty**

COMP **312.** Benchmarking the adsorption energies on carbon nanotubes. D.G. Smith, **K. Patkowski**

WEDNESDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 1D

Molecular Mechanics

Applications

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **313.** Temperature effects on the spatial distribution of electrolyte mixtures at the aqueous liquid-vapor interface. **B.L. Eggimann**, A. Sunnarborg, J.I. Siepmann

9:00 COMP **314.** Molecular simulation of surface density effects on heterogeneous DNA hybridization. **J.M. Stubbs**, S. Cooper, W. Scamman, M. van den Berg

9:30 COMP **315.** Structural properties of DNA basepair mismatches. A. Kingsland, **L. Maibaum**

10:00 Intermission.

10:15 COMP **316.** Quantam mechanical molecular mechanical calculations using amoeba force fields. **Y. Shao**, A.C. Simmonett, Y. Mao, F.C. Pickard, G. Koenig, B. Brooks, J. Herbert, T.L. Head-Gordon, M.P. Head-Gordon

10:45 COMP **317.** Molecular dynamics by flexible-boundary QM/MM: On-the-fly partial charge transfer between QM and MM subsystems. S. Pezeshki, **H. Lin**

11:15 COMP **318.** Quantum Drude oscillator model for linear scale atomistic simulation – a coarse grained electronic structure allowing for high environmental transferability. **G.J. Martyna**

Section B

Colorado Convention Center
Mile High Ballroom 1E

Quantum Chemistry

Quantum Dynamics & Monte Carlo Simulations

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

8:30 COMP **319.** Second-quantized surface hopping. **A.V. Akimov**, O.V. Prezhdo

9:00 COMP **320.** Systematically improvable models in excited-state dynamics calculations. **A. Molina**, A. Chien, T.G. Goodson, P.M. Zimmerman

9:30 COMP **321.** Real-time electron transport from parity-time symmetric quantum mechanics. J. Elenewski, **H. Chen**

10:00 Intermission.

10:00 COMP **322.** Ring polymer molecular dynamics: New quantum dynamical method for calculating chemical reaction rates. **Y. Suleymanov**

10:30 COMP **323.** Direct dynamics simulations of steroidal ring-closing events. **R.P. Pemberton**, D.J. Tantillo

Section C

Colorado Convention Center
Mile High Ballroom 1F

Computational Pyrolysis & Upgrading of Bio-Oils

Bonding and Kinetics

Cosponsored by MPPG

D. Robichaud, *Organizer*
R. Surendran Assary, R. S. Weber, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COMP **324.** Molecular-level kinetic modeling in biomass thermochemical conversions: Software tools and their applications. **M.T. Klein**

9:20 COMP **325.** Toward automated mechanism generation of lignin pyrolysis models: Development of group additivity parameters for aromatic species. **H.H. Carstensen**, A. Ince, M. Reyniers, G.B. Marin

9:50 COMP **326.** First-principles study of phenol hydrogenation on Pt and Ni catalysts in aqueous phase. **R. Rousseau**, D. Mei, Y. Yoon, R.S. Weber, J.A. Lercher

10:20 Intermission.

10:35 COMP **327.** Charting elementary steps in the cellulose pyrolysis reaction network. **H. Mayes**, X. Zhou, G. Beckham, L.J. Broadbelt

11:05 COMP **328.** In silico zeolite catalyzed carbon-carbon coupling reactions for furan upgrading. **C. Liu**, L. Cheng, R. Surendran Assary, L.A. Curtiss

11:35 COMP **329.** Mechanistic study of furan formation in HZSM-5 using quantum mechanical modeling. **S. Kim**, D. Robichaud, C. Mukarakate, L. Bu, T. Evans, G. Beckham, R.S. Paton, M.R. Nimlos

12:05 Concluding Remarks.

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Ligand-Based

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

8:30 COMP **330.** Halogen bonds in drug design. **S. Sirimulla**

9:00 COMP **331.** Highly visual workflow for designing, selecting and enumerating new compounds for assay. **J.W. Sager**, T.E. Mansley, P. Mounteney

9:30 Intermission.

‡ *Cooperative Cosponsorship*

9:45 COMP **332.** Discovery of new and diverse TLR9 receptor antagonists for regulating innate immune reactions. **A. Goldblum**, A. Burger-Kentischer, A. Mattes, M. Zatsepin

10:15 COMP **333.** In silico design, synthesis, and assays of specific substrates and peptidomimetic inhibitors for proteinase 3. S. Narawane, C. Grauffel, A. Schillinger, B. Haug, **N. Reuter**

10:45 COMP **334.** Ligand based drug design of novel pyrimidine derivatives as Tankyrase inhibitors for the treatment of colorectal cancer. **A.P. Patel**, H.G. Bhatt

Section E

Colorado Convention Center
Mile High Ballroom 4F

Computational Study of Water

D. J. Sindhikara, *Organizer, Presiding*

8:30 COMP **335.** Advanced potential energy surfaces for water simulations. **T.L. Head-Gordon**

9:00 COMP **336.** Development and implementation of an advanced density based potential for water. R.E. Duke, O.N. Starovoytov, J.A. Piquemal, **G.A. Cisneros**

9:30 COMP **337.** Effects of three-body nonadditive exchange and induction forces in liquid water. **O. Akin-Ojo**, K. Szalewicz

10:00 Intermission.

10:15 COMP **338.** Microscopic structure, equilibrium density, and local environment in liquid water: A highly accurate ab initio path-integral molecular dynamics study. **R.A. Distasio**, B. Santra, H. Ko, F. Martelli, M. Ceriotti, R. Car

10:45 COMP **339.** Ice nucleation on graphene surface supports the classical theory of heterogeneous nucleation. **R. Cabriolu**, T. Li

11:15 COMP **340.** Direct calculation of the rate of homogeneous nucleation of ice for TIP4P/ICE from massively parallel molecular simulations. **A. Haji-Akbari**, P.G. Debenedetti

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Properties and Processes in Solvated Systems

Sponsored by PHYS, Cosponsored by COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Modeling of Macromolecular Structure and Function

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Ballroom 1D

Symposium Organizer Selections

SOS

E. X. Esposito, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **341.** Multi-scale computational investigations of the cAMP activation-mechanism of Protein Kinase A RI_α using Brownian Dynamics and Molecular Dynamics simulations. **S.P. Hirakis**, R. Malmstrom, R.E. Amaro

2:00 COMP **342.** Water dynamics at protein-protein interfaces: A molecular dynamics study of virus-host receptor complexes. **P. Dutta**, M. Botlani, S. Varma

2:30 COMP **343.** Homology modeling and molecular dynamics study of ALKBH1 enzyme. **P. Silvestrov**, T. Müller, K. Clark, R. Hausinger, G.A. Cisneros

3:00 Intermission.

3:15 COMP **344.** Partitioning of nitroaromatic compounds through lipid bilayer. **A. Golius**, O. Isayev, L. Gorb, F. Hill, J.R. Leszczynski

3:45 COMP **345.** Bondalyzer: A tool for the discovery of charge density property relationships. **T.R. Wilson**, M. Eberhart, T. Jones

4:15 COMP **346.** Field-dependent peak shift in real-time time-dependent density functional theory. **M. Provorse**, B. Habenicht, C. Isborn

Section B

Colorado Convention Center
Mile High Ballroom 1E

Membranes

S. A. Wildman, *Organizer, Presiding*

1:30 COMP **347.** Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage. **P.A. Oroskar**, S. Murad, C. Jameson

2:00 COMP **348.** Investigating the forces governing the peripheral membrane association and dissociation of a bacterial phospholipase C (*Bt*PI-PLC). H.M. Khan, C. Grauffel, B. Yang, T. He, R. Mary, A. Gershenson, **N. Reuter**

2:30 COMP **349.** Partitioning of anionic nanoparticles in cholesterol-containing membranes occurs via local disordering and cholesterol depletion. P. Gkeka, P. Angelikopoulos, L. Sarkisov, **Z. Cournia**

3:00 Intermission.

3:15 COMP **350.** Lateral organization and transverse coupling in asymmetric biomembranes. **X. Cheng**, J. Nickels, F. Heberle, J. Katsaras

3:45 COMP **351.** Investigating lipid phase changes from liquid crystalline to ripple to gel phases with all-atom molecular dynamics simulations. **P. Khakbaz**, J.B. Klauda

4:15 COMP **352.** Spatial organization of cellular membranes. K. Sapp, S. He, **L. Maibaum**

Section C

Colorado Convention Center
Mile High Ballroom 1F

Computational Pyrolysis & Upgrading of Bio-Oils

Reaction Engineering

Cosponsored by ENFL‡ and MPPG

R. S. Weber, *Organizer*
D. Robichaud, R. Surendran Assary, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 COMP **353.** Impact of H_2 addition on formation of PAH during anisole pyrolysis. **Y. Koirala**, S. Villano, A.M. Dean, H.H. Carstensen, M. Reyniers, G.B. Marin

2:20 COMP **354.** Insights into the hydrodeoxygenation mechanisms for lignin upgrade. **D.G. Vlachos**

2:50 COMP **355.** Role of solid, liquid, and gaseous phases during pyrolysis of biomass. **R.C. Brown**

3:20 Intermission.

3:35 COMP **356.** Strike a happy medium: Identifying appropriate reaction conditions for upgrading bio-oil. **M.R. Nimlos**, R.S. Weber

4:05 COMP **357.** Reactor simulations for catalytic upgrading of pyrolysis vapors. **J. Ziegler**, S. Pannala, T. Foust, M.R. Nimlos, D. Robichaud

4:35 COMP **358.** Multiscale/multiphysics modeling of biomass fast pyrolysis and vapor phase upgrading reactors. S. Pannala, E. Ramirez, J. Ziegler, D. Robichaud, M.R. Nimlos, T. Foust, C. Daw

5:05 Panel Discussion: What is Needed to Advance the State of the Art in Biomass Conversion and Upgrading?

5:35 COMP **359.** Thermal properties of pine, poplar, and fir blocks from room temperature to 500°C. **D.M. Stevens**, T.L. Westover, C.L. Williams

6:05 Concluding Remarks.

Section D

Colorado Convention Center
Mile High Ballroom 4E

Drug Discovery

Ligand-Based

Cosponsored by CINF and MEDI

Y. Tseng, S. A. Wildman, *Organizers, Presiding*

1:30 COMP **360.** Small molecule crystal structures in drug discovery and development. **C. Groom**, S. Ward, S. Vyas, I. Bruno

2:00 COMP **361.** QSAR modeling independent of input tautomers. M. Waldman, **R. Fraczkiewicz**, R. Clark

2:30 COMP **362.** General applicability of template CoMFA to prospective bioactivity prediction. R.D. Cramer

3:00 COMP **363.** Exploring conformational search protocols for ligand-based virtual screening and 3D QSAR modeling. D. Cappel, S. Dixon, **W. Sherman**, J. Duan

3:30 Intermission.

3:45 COMP **364.** Experimentally derived interaction fields as a basis for ligand-based virtual screening. **C. Groom**, J. Cole, I. Giangreco, O. Korb, S. Gothe, I. Bruno

4:15 COMP **365.** Alignment of diverse ligands for a protein: a solved problem? **T. Cheeseright**, P. Tosco, M. Mackey

4:45 COMP **366.** Exhaustive pairwise overlays: the gold standard for molecular alignment? **P.C. Hawkins**, R.W. Tolbert

Section E

Colorado Convention Center
Mile High Ballroom 4F

Quantum Chemistry

Applications

Cosponsored by PHYS

E. V. Patterson, *Organizer, Presiding*

1:30 COMP **367.** Importance of a nonlocal description of electron–electron interactions in modeling the dissociative adsorption of H_2 on Cu(100). **F. Goeltl**, C. Houriez, M. Guitou, G. Chambaud, P. Sautet

2:00 COMP **368.** Density functional investigation of 2-alkyl-anthraquinone hydrogenation on a palladium cluster. **E. Yuan**, L. Wang, F. Ren

2:30 COMP **369.** Theoretical prediction of the effects of substitution on the efficacies of ruthenium water oxidation catalysts. **A.B. League**, M. Ertem, P. Miro Ramirez, C.J. Cramer

3:00 Intermission.

3:15 COMP **370.** DFT study of dehydrogenation of ethanol on alkaline earth metal oxides. **Y. Izumi**, H. Kamata, H. Ushiyama

3:45 COMP **371.** Stereospecific zirconium catalyzed cycloamination of 4-penteneamine. **W.C. Everett**, T.L. Windus, A.D. Sadow

4:15 COMP **372.** Reversible olefin binding to nickel dithiolenes and a variety of related complexes. **E.N. Brothers**, M.B. Hall

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems: A Symposium in Honor of Donald Truhlar

Nonadiabatic Dynamics

Sponsored by PHYS, Cosponsored by COMP

Modeling Complex Biomolecules: From Structure to Dynamics & Function

Folding and Aggregation

Sponsored by PHYS, Cosponsored by COMP

Modeling Excited States of Complex Systems

Electronic Structure

Sponsored by PHYS, Cosponsored by COMP

ENFL

Division of Energy and Fuels

A. Park, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Computational Pyrolysis and Upgrading of Bio-Oils *(see COMP, Wed)*

Catalytic Materials and Technologies for Upgrading of COx and Natural Gas Oxidation *(see CATL, Tue, Wed, Thu)*

SOCIAL EVENTS:

Dinner, 7:30 PM: Tue

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Ballroom 4A

Nanomaterials for Solar Energy Conversion & Storage

Cosponsored by MPPG‡

R. T. Koodali, Y. H. Ng, N. Wu, *Organizers*
Y. H. Hu, Y. Wu, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **1.** Nanocarbons for optoelectronic applications. **D. Guldi**

8:45 ENFL **2.** Plasmonic metal-semiconductor nanostructures for solar fuel generation. **N. Wu**

9:15 ENFL **3.** Uniform doping of metal oxide nanowires using solid state diffusion for photoelectrochemical water oxidation. **J. Resasco**, N.P. Dasgupta, J. Roque-Rosell, J. Guo, P. Yang

9:35 ENFL **4.** Impact of humidity in the preparation of $CoTiO_3$ perovskites: Effective ABO_3 type catalysts for O_2 evolution. **S. Rasalingam**, R.T. Koodali

9:55 Intermission.

10:00 ENFL **5.** Chalcogenide nanostructured precursors in fabrication of polycrystalline absorber layers in thin-film photovoltaics. **D.R. Radu**

10:30 ENFL **6.** Light management in extremely thin photoelectrode architectures. **I. Thomann**

11:00 ENFL **7.** Sustainable inorganic nanocrystals for solar energy conversion and storage applications. **K. Ramasamy**, R. Gupta, H. Sims, S. Ivanov, A. Gupta

11:20 ENFL **8.** Tailoring zinc oxide nanostructures for solar cell applications. K. Sakar, E.V. Braden, L. Song, M. Rawolle, S.V. Roth, **P. Mueller-Buschbaum**

11:40 ENFL **9.** Structural studies of solution-grown iron pyrite (FeS_2) nanoparticles via synchrotron and neutron diffraction. **R.C. Miller**, D. Agocs, S. Fredrick, J.R. Neilson, A.L. Prieto

Section B

Colorado Convention Center
Mile High Ballroom 4B

Materials & Interfaces in Lithium Batteries & Beyond

New Materials/Systems

A. A. Gewirth, A. Manivannan, *Organizers*
Y. Shao, D. Wang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENFL **10.** From nanomaterials to energy storage systems. **J. Liu**

8:35 ENFL **11.** Flexible high-energy Li-ion batteries with fast-charging capability. **J. Cho**

9:05 ENFL **12.** Enable high energy-density lithium-ion battery conversion cathodes based on iron fluorides using integrated in situ experimental and computational approaches. **S. Jin**, L. Li