List of Posters

Monday Poster Session

1. Adamska, Lyundmyla
   Electronic and Optical Properties of Borophene, a Two-dimensional Transparent Metal
2. Ajala, Adeayo
   Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies
3. Al-Saadon, Rachael
   An examination of thermally activated delayed fluorescence using the particle-particle random phase approximation
4. Allen, Caley
   Mechanical unfolding of single- and multi- motif proteins
5. Allen, Thomas
   Proton Transfer Rates from Quantum-Classical Path Integral Simulations
6. Alt, Eric
   Dynamic Polymer Networks
7. Avila, Thomas
   Characterization of electrostatic relaxation dynamics in water
8. Bajaj, Akash
   Recovering the flat plane condition in semi-local density functional theory
9. Balasubramani, Sreeganesh
   Second order molecular properties from the random phase approximation (RPA)
10. Bandara, Asanga
    Protein Co-localization in Membrane Domain Interface and Mediation of Interface Line Tension
11. Baral, Minati
    Efficient Hydroxyquinoline based C3-Symetric Tripodal Chemosensor: Density Functional Studies
12. Becker, Andrea
    Effect of Electrode Surface Structure on Electron Transport in Molecular Junctions
13. Bellonzi, Nicole
    Recent Developments in Ab Initio Tools for Spin Nonadiabatic Systems
14. Bendavid Isseroff, Leah
    Interfacial Properties of Two-dimensional CdS/Graphene Nanocomposites
15. Bennett, Doran
    Multiscale principles of photosynthetic light harvesting
16. Bernales, Verinia
    Multiconfiguration Quantum Embedding Methods
17. Bose, Amartya
    Quantum Mechanical Rate Calculations in Condensed Phase Reactions
18. Bricker, William
    Cyanine Dye Aggregation Behavior on Scaffolded DNA Origami
19. Brown, Sandra
    Monitoring water clusters “melt” through vibrational spectroscopy
20. Charest, Nathaniel
    Low-Resolution Methods For Simulation Of Amyloid Formation
21. Chatterjee, Sambarta
    Quantum – Classical Path Integral with Langevin friction

List of Posters

22. Chaudhuri, Subhajyoti
    Electron Transfer Assisted by Vibronic Coupling from Multiple Modes
23. Chen, Hsing-Ta
    Inchworm Monte Carlo for exact non-adiabatic dynamics
24. Chen, Renai
    Electron-transfer-induced heat transport in molecular environments
25. Chen, Xing
    Understanding of solvent effects on surface-enhanced Raman scattering: insight from atomistic description of electrodynamics combined with classical molecular dynamics
26. Chen, Zehua
    Multireference density functional theory with generalized auxiliary systems
27. Chong, Gene
    Adsorption dynamics and structure of ligands on gold nanoparticles
28. Cotton, Stephen
    Classical Molecular Dynamics Simulation of Electronically Non-Adiabatic
29. Culpitt, Tanner
    Multicomponent and Electronic Density Functional Theory Embedding
30. Daly, Clyde
    Temperature Studies of the Solvation Environment of CO2 in Ionic Liquids
31. Dannenhoffer-Lafage, Thomas
    Reactive Coarse-grained Molecular Dynamics
32. DeLyser, Michael
    Extending Pressure Matching to Interfacial Systems
33. Derricotte, Wallace
    Localized Intrinsic Valence Virtual Orbitals for Automated Classification of Core Excited States
34. Ding, Feizhi
    Embedded Mean-Field Theory for High-Efficiency Electronic Structure
35. Ding, Wendu
    Plasmon-Coupled Resonance Energy Transfer
36. Dunn, Ian
    Toward Energy-Conserving, Linear-Scaling, Real Space Ab Initio Molecular Dynamics
37. Durumeric, Alesander
    Ultra-Coarse-Graining: Detecting and Optimizing Coarse-Grained Representations
38. Dwelle, Kaitlyn
    An electrochemically active, coarse-grained model of transport through an ion conducting polymer electrolyte
39. Fernando, Amendra
    Rational Design of Triblock peptide-linker-lipid Targeting Family B GPCRs
40. Ford, Jason
    Multiple time step integrators for accelerating *ab initio* molecular dynamics
41. Gani, Terry Zhi Hao
    New Computational Tools for High-Throughput Discovery in Transition Metal Catalysis
42. Gebhardt, Julian
    Adding to the perovskite universe - inverse hybrid perovskites
43. Geva, Nadav
    Atomistic Simulation of Energy Transfer Between Nanocrystalline Semiconductors and Organic Semiconductors

List of Posters

44. Ghosh, Soumen
    Modeling Electronic Dynamics in Large Systems Using Semiempirical Effective Hamiltonians
45. Gieseking, Rebecca Lynn
    Semiempirical Modeling of Plasmonic Ag Nanoclusters and the Chemical Mechanism in Surface-Enhanced Raman Scattering
46. Goldsmith, Zachary
    Nonadiabatic Proton-Coupled Electron Transfer at Electrochemical Interfaces: Hydrogen Evolution on Gold in Non-Aqueous Media
47. Goyal, Puja
    Role of Active Site Conformational Changes in Photocycle Activation of the AppA BLUF Photoreceptor
48. Greene, Samuel
    The TT-SOFT Method: An Efficient Approach to High-Dimensional Quantum Dynamics Simulations Based on the Tensor-Train Decomposition
49. Gu, Bing
    Stark control of electrons
50. Guerrero, Ruben
    A novel approach to the implementation of the J-engine on GPGPUs
51. Guo, Ziwei
    Gibbs Ensemble Monte Carlo with Solvent Repacking: Phase Coexistence of Size-asymmetrical Binary Lennard-Jones Mixtures
52. Harshan, Aparna
    Electronic Structure Calculations of NiFe Oxyhydroxide Electrocatalysts: Characterization and Spectroelectrochemical Analysis
53. Hase, Florian
    Designing artificial neural networks for high-throughput calculations on exciton energy transport properties
54. Heavey, Thomas
    Testing and Proposing Organic Catalysts with in silico Chemistry
55. Hino, Alexander
    Characterizing Chromophore-Chromophore and Chromophore-Environment Interactions Through Computational Methods
56. Ho, Phay
    Large-scale Monte-Carlo/ Molecular-Dynamics Calculations of Clusters in Intense X-Ray Pulses
57. Hocky, Glen
    Coarse-grained directed simulations via adaptive linear biases
58. Huang, Kai
    Design of multi-functional nanogate in response to multiple external stimuli using amphiphilic diblock copolymer
59. Huynh, Mioy
    Tuning Electron-Proton Transfer Mediators for Molecular Electrocatalysis
60. Jain, Amber
    Vibrational energy relaxation – application of quantum-classical methods
61. Janet, Jon Paul
    Training neural networks for transition metal complex screening and design

List of Posters

62. Jiang, Chenwei
    "Watching" the Dark State in Ultrafast Nonadiabatic Photoisomerization Process of a Light-Driven Molecular Rotary Motor
63. Jin, Jaehyeok
    Extending the Range and Physical Accuracy of Coarse-Grained Models with Ultra-Coarse Graining
64. Jin, Ye
    Excitation energies from particle-particle random phase approximation with accurate optimized effective potentials
65. Jin, Yifan
    Ionization Potential Optimized Consistent Global Hybrid Exchange-correlation Functional
66. Jung, Kenneth
    Extending Imaginary Time Path Integral Techniques to Evaluate Multi-time Correlation Functions
67. Kanungo, B K
    Theoretical Prediction of Formation Constants of Some Bio-relevant Mixed Chelates of Divalent Copper Containing Bipyridyl and N-N, N-O and O-O Donor Ligands
68. Karnaukh, Elizabeth
    Electronic structure and redox chemistry of heme centers in protein environments: a case study of bacterial cytochrome c peroxidases
69. Kilgour, Michael
    Advancing Path Integral Techniques for Simulations of Quantum Dissipation and Transport
70. Kim, Jeong
    Designing quantum dot precursors with new first-Principles inorganic discovery tools
71. Kohn, Alexander
    Quantum yields made easy: Towards an evaluation of non-radiative rates
72. Kumar, Manav
    Calculating spectral densities for perylene-3,4,9,10-tetracarboxylic diimides (PTCDI)
73. Lam, Yan
    Modeling the Volmer Reaction on Metal Electrodes with Nonadiabatic Proton-Coupled Electron Transfer Theory and Gouy-Chapman-Stern Model of the Electrochemical Double Layer
74. Lebold, Kathryn
    The state point dependence of coarse-grained potentials for liquids
75. Lee, MiKyung
    First-principles Study of Energy Transfer Processes of the Open and Closed Quaternary Structures of Light-Harvesting Complexes in Cryptophyte Algae
76. Lee, Sebastian
    Towards Black Box Projection-based Embedding
77. Lewis, Kirk
    Many-body perturbation theory analysis of GaN defects
78. Li, Chenyang
    Driven Similarity Renormalization Group Multireference Perturbation Theory
79. Li, Pengfei
    Modeling of Proton-Coupled Electron Transfer in Soybean Lipoxygenase: QM/MM Free Energy Surfaces and Nonadiabatic Rate Constants

List of Posters

80. Li, Xin
    An *Ab Initio* Exciton Model Including Single and Double Excitations: Energies, Gradients, Couplings, and Dynamics
81. Li, Zhendong
    Towards Understanding the Electronic Structures of Iron-Molybdenum Cofactor in Nitrogenase with ab initio DMRG and Spin Projections
82. Li, Zhi
    Atomistic Modeling of Electromechanical Spectroscopies in Molecular Junctions
83. Lin, Zhou
    Triplet Tuning – A New “Black-Box” Construction Scheme for System-Dependent Density Functionals
84. Liu, Fang
    Derivation and Implementation of Analytical Derivatives of the Individual State Energies in the SA-REKS Method
85. Liu, Pengchong
    Single-Molecule Imaging Using Atomistic Near-Field Tip-Enhanced Raman Spectroscopy
86. Lotshaw, Philip
    Quantum Thermodynamic Entropy and the Second Law
87. Ma, Boran
    Electrostatic effects on ionomer nano-structures
88. Magana-Fuentes, Miguel
    Approximate EOM-CCSD model for electron attached and ionized states
89. Mahala, Benjamin
    Multiscale and structured interactions affect diffusion dynamics
90. Mallory, Joel
    Probing the Structural Properties of Small Clusters using the Diffusion Monte Carlo Method
91. Mao, Yuezhi
    On the characterization of charge-transfer effects in non-covalently bound molecular complexes
92. Mattingly, Brendan
    Titanium nitride as a potential material for plasmonic assisted photocatalysis
93. Matula, Adam
    Prediction of Optoelectronic Traits of Dyes for Photoelectrochemical Purposes

List of Posters

Tuesday Poster Session

1. Mayes, Maricris
   Towards Understanding the Interactions of Aromatic Dipeptide Nanotubes
2. Mehmood, Rimsha
   Revealing Substrate Positioning Dynamics in Aliphatic Halogenase SyrB2 through Spectroscopically-Guided Simulation
3. Migliore, Agostino
   Significant enhancement of polyene light absorption induced by electrostatic fields
4. Moberg, Daniel
   Molecular-Level Spectroscopic Studies of Ice Using a Many-Body Potential
5. Mohammadyani, Dariush
   Protein assembly in solution and on the membrane using CG-Metadynamics: a case study of LSP1 homodimerization
6. Monhanam, Luke
   Perturbative Approach to Ultrafast in Nonadiabatic Molecular Dynamics
7. Montemore, Matthew
   Electronic excitations in thermal heterogeneous catalysis
8. Montoya Castillo, Andreas
   Unifying quantum master equations and quantum-classical trajectories for photochemistry and electrode processes
9. Morawietz, Tobias
   Structural origin of the temperature-dependent Raman and infrared spectra of liquid water
10. Mukazhanova, Aliya
    The electronic structure of biologically-inspired perylene diimide arrays from first-principles
11. Nagahata, Yutaka
    Reaction rate constants of noisy systems obtained on the transition state trajectory
12. Napoli, Joe
    Decoding spectroscopic features and time-scales of aqueous proton defects
13. Nguyen, Duong
    The effect of channel shape, size, and functionality on directed hydrogen bonding networks
14. Ochoa, Maicol
    Plasmon-exciton energy transfer in nanoparticle-molecule aggregates
15. Palafox Hernandez, Jesus Pablo
    Crystal orientation dependence of heterogeneous nucleation at the Cu-Pb solid- liquid interface
16. Pantelopulos, George
    Role of cholesterol in ternary lipid membrane phase separation observed via coarse-grained simulations
17. Parrish, Robert
    Lightspeed: A Simple, Flexible, and Highly-Optimized Library for the Rapid Development of Production-Level Electronic Structure Theory
18. Patel, Lara
    Sodium chloride cluster formation in methanol and water

List of Posters

19. Pazmany, Vivian
    Raman Signatures of Pt-Au Interactions in Quasi-One Dimensional Metal-Organic Nanowires
20. Perera, Duwage
    Quantum Mechanical studies of catalytic effects on water splitting
21. Piskulich, Ezekiel
    Molecular Simulation of Gas-Expanded Liquids: Phase Equilibrium and Structure of CO2 Expanded Ethylene Oxide and Methanol
22. Popov, Alexander
    Multi-scale simulations of a high-temperature diatomic reactive gas
23. Provazza, Justin
    Partial Linearized Density Matrix Dynamics for Nonlinear Electronic Spectroscopy
24. Qi, Helena
    Explaining unexpected interactions in the structurally characterized proteome with large-scale electronic structure modeling
25. Rahnamoun, Ali
    Nano-bio interface between polyelectrolytes and bacterial lipopolysaccharides
26. Rasaiah, Jayendran
    Proton transfer and recombination of the H+ and OH- ions In bulk water and water wires from a dissociating water model
27. Reid, Keon
    Binding, Folding, and Insertion of a β-Hairpin Peptide at a Lipid Bilayer Surface: Insights from Molecular Dynamics Simulations and Experiment
28. Ricke, Nathan
    Bootstrap Embedding: A low-scaling, fragment-based method for strong correlation
29. Romero, Jhonathan
    Generalized coupled-cluster approaches for quantum simulation of strongly correlated system
30. Rontondaro, Matthew
    Nitrous Oxide as a Probe of Aqueous Cation Solvation Environments: Ultrafast Mid-IR Pump-Probe Measurements and Molecular Dynamics Simulations
31. Roy, Saswata
    Quinone photobasicity is mediated by hole injection
32. Ru, Xuyan
    Regimes of electron transfer in Geobacter Sulfurreducens pili
33. Rudshteyn, Benjamin
    Determination of Orientation of Bipyridine Re(I) fac-tricarbonyl Electrocatalysts on Au, on SrTiO3, and on TiO2 Surfaces through Computational and Experimental SFG Spectroscopy
34. Sanchez Lengeling, Benjamin
    Fine tuned generation of Molecules with Objective-Reinforced Generative Adversarial Networks (ORGAN)
36. Sanchez, David
    TDDFT in Regions of Strong and Coupling: A NAMD Study of Cyclohexadiene and 7- Dehydrocholesterol
37. Sawaya, Nicolas
    Designing a single-molecule exciton transistor
38. Sayfutyarova, Elvira
    Building active spaces automatically and systematically from atomic valence orbitals

List of Posters

39. Segatta, Francesco
    Modelling Photoinduced Events and Non-Linear Spectroscopy in Complex Multichromophoric Systems
35. Seritan, Stefan
    Ab Initio Interactive Molecular Dynamics: A Hands-On Experience with Quantum Chemistry
40. Shee, James
    Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo
41. Shen, Lin
    Multiscale Quantum Mechanics / Molecular Mechanics Simulations with Neural Networks
42. Shen, Zhe
    Critical Micelle Concentrations and Critical Aggregation Numbers Predicted by a Thermodynamic Model and Molecular Dynamics Simulations
43. Shin, Sucheol
    Three-body molecular interactions mediate the polarization and polarizability of the liquid water-vapor interface
44. Shu, Yinan
    Dual-Functional Tamm-Dancoff Approximation: A Convenient Density Functional Method that Correctly Describes S1/S0 Conical Intersections
45. Schubert, Alexander
    Going beyond the perturbative regime: Post-Marcus methods based on the Generalized Quantum Master Equation
46. Simine, Lena
    eGFP-based motion sensor via electrochemical control of fluorescence
47. Singh, Rakesh
    Stochastic hard collision model for coarse-graining complex solvent dynamics
49. Son, Chang Yun
    Cavity Hydration Dynamics in Cytochrome c Oxidase and Functional Implications
51. Son, Chang Yun
    Multiscale modeling of poly(ethylene oxide) with ionic liquids : GPU enabled first-principles force fields
48. Stelter, David
    Enhanced Sampling of Bilayers, Vesicles, and Lipid-Wrapped Nanoparticles
50. Stevens, David Ryan
    Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase Eta with Quantum Mechanical/Molecular Mechanical Free Energy Simulations
52. Straight, Shelby
    Predictions of the Temperature Dependent Structure of the Air/Water Interface with MB-pol
53. Su, Neil Qiang
    Accurate Quasiparticle Spectra from the T-matrix Self Energy and the Particle-Particle Random Phase Approximation
54. Tabor, Daniel
    High-Throughput Virtual Screening of Flow Battery Electrolytes
55. Tamayo-Mendoza, Teresa
    Automatic differentiation in quantum chemistry

List of Posters

56. Tazhigulov, Ruslan
    Multi-level computational study of Photoinduced Charge Transfer in Cryptochromes
57. Teichen, Paul Thomas
    Self-Assembly of Porous Polymer Gels
58. Teo, Ruijie Darius
    From First Principles: Modulation of Hole Transfer Pathways in the p53 DNA-Binding Domain
59. Thompson, Keiran
    Diffusion Maps Speed Reaction Path Search
60. Valleau, Stephanie
    Dynamics of reactions fundamental to the origins of life
61. Varganov, Sergey
    Predicting Intersystem Crossing Rates: Nonadiabatic Molecular Dynamics vs. Statistical Theory
62. Vassilev-Galindo, Valentin
    Planar hypercoordinate carbon zoo
63. Videla, Pablo
    Quantum Control at a Light-Induced Conical Intersection: Floquet Theory Applied to the Photoisomerization of Rhodopsin
64. Walters, Peter
    Quantum-classical path integral calculations of ferrocene-ferrocenium charge transfer in solution
65. Wang, Hao
    Determining polarizable force fields with electrostatic potentials from quantum mechanical linear response theory
66. Wang, Zhi
    Multiscale Simulation of Proton Transport in the ClC Antiporter
67. Watkins, Laura
    Mechanism of Proton Transport in Influenza A M2 Mutant From Multiscale Simulations
68. Xu, ZiYao
    First-principle time-dependent simulation of organic solar cells
69. Yang, GuanYa
    Size-Independent Machine Learning Based First-Principles Method for Accurate Prediction of the Heat of Formation of Fuels
70. Yang, Jing
    Pseudopotentials for hybrid-density functionals and SCAN
71. Yang, Yang
    Development of a Practical Multicomponent Density Functional for Electron-Proton Correlation to Produce Accurate Proton Densities
72. Yang, Zhongyue
    Environment-Perturbed Transition State Sampling and its Applications in Chemical and Biochemical Reactions in Condensed Media
73. Ye, Hongzhou
    Frankenstein Bootstrap Embedding: A Low-Scaling, Internally Consistent, Hierarchically Improvable Density Matrix Embedding Scheme For Strongly Correlated Systems
74. Yu, Jimmy
    Spurious Rydberg States in the Particle-Particle Tamm-Dancoff Approximation

List of Posters

75. Zhang, Leili
    Structure of Monomeric and Segmented Huntingtin Protein
76. Zhang, Tianyuan
    Recent developments in projector configuration interaction method
77. Zhang, Xiaokun
    Extracting aggregation free energies of mixed clusters from simulations of small systems: application to ionic surfactant micelles
78. Zhao, Qing
    Accurate correction of delocalization error in transition metal catalysis by hybrid functionals and DFT+U
79. Zhu, Tianyu
    Many-Pair Expansion: A Density Functional Hierarchy for both Strongly and Weakly Correlated Systems
80. Zuehlsdorff, Tim
    Modeling vibronic effects in absorption spectra of solvated dyes