WEST COAST THEORETICAL CHEMISTRY SYMPOSIUM: POSTERS

Stanford University, Sapp Center, 28th March 2018

Organizers: Martin Head-Gordon, Tom Markland, Eran Rabani and Joe Subotnik

1. Aaron Virshup, Arzeda Corporation, "*Computational chemistry at scale: building modeling pipelines for enzyme design*"
2. Addison Schile, UC Berkeley, "*Understanding Quantum Dynamical Regimes with Stochastic Unraveling of Quantum Master Equations*"
3. Aleksandr O. Lykhin, University of Nevada, Reno, "*Intersystem Crossing in the Tunneling Regime: A Case of Thiophosgene*"
4. Ali Abou Taka, UC Merced, "*An Examination of Factors Affecting the Accuracy of Quantum Chemical Frequency Calculations for First-Row Transition Metal Compounds*"
5. Amael Obliger, UC Berkeley, "*Large intrinsic anion interdiffusion in lead halides perovskites*"
6. Amikam Levy, UC Berkeley, "*Noise resistant quantum control using dynamical invariants*"
7. Andres Montoya-Castillo, Stanford University, "*On the exact continuous mapping of fermions*"
8. Ardavan Farahvash, UC Davis, "*A multifaceted computational analysis of water sparsity in cytochrome coxidase*"
9. B. Scott Fales, Stanford University, "*Large Scale Electron Correlation Calculations: Rank-Reduced Full Configuration*"
10. Benoit Mignolet, University of Liege, "*Probing the high-excited states dynamics in the methyl azide molecule: a joint experimental-theoretical study*"
11. Boris Fain, InterX Inc., "*On the importance of accounting for Nuclear Quantum Effects in Ab Initio Calibrated Force Fields.*"
12. David Sanchez, Stanford University, "*Ultrafast Dynamics: A study of photoinduced ring-opening in 1,3-cyclohexadiene and derivatives*"
13. Deniz Tuna, Stanford University, "*Excited States, Photochemical Reaction Paths and Multiple-Spawning Photodynamics of Urocanic Acid and Orange Carotenoid Protein*"
14. Diptarka Hait, UC Berkeley, "*How accurate is density functional theory at predicting dipole moments?*"
15. Edgar J Landinez, Lawrence Livermore National Laboratory, "*Improving the Accuracy of AFQMC with Non-Orthogonal Multi-Determinant Wave Functions*"
16. Erum Mansoor, UC Berkeley, "*Understanding Adsorption and Catalysis in Zeolites using Long-range corrected DFT models*"
17. Evan Antoniuk, Stanford University, "*New Assembly-Free Bulk Layered Heterostructures: Electronic, Mechanical, and Optical Properties*"
18. Fang Liu, MIT, "*Exploiting Graphical Processing Units to Enable Accurate Excited State Potential Energy Surface Calculation for Large Molecules*"
19. Feng Wu, UC Santa Cruz, "*Charged Defects in Two Dimensional Materials from Many Body Perturbation Theory*"
20. Grace Johnson, Stanford University, "*Elucidating excitation energy transport in LHCII using a GPU-accelerated ab initio exciton model*"
21. Haochuan Wei, UC Berkeley, "*Reduced-Scaling Fock-space Variational Monte Carlo*"
22. Hassan Harb, UC Merced, "*Structure and Bonding of Lanthanide Hydroxides Ln-OH (Ln=La-Lu)*"
23. Hayley Weir, Stanford University, "*Nonadiabatic simulation of cis-stilbene with FOMO-CASCI in the 400 femtosecond regime*"
24. Hyesu Jang, UC Davis, "*Quantum chemical studies of redox properties and conformational changes of a four-center iron CO2 reduction electrocatalyst*"
25. Jacqueline Shea, UC Berkeley, "*Enforcing Size-Consistency in an Excited State Variational Principle*"
26. Jason Ford, Stanford University, "*Fragment-Based Multiple Time Step Integration for Ab Initio Molecular Dynamics in Covalently Linked Systems*"
27. Jerome F. Gonthier, UC Berkeley, "*Insight into 2-body and 3-body Dispersion Interactions*"
28. Jimmy Yu, Stanford University, "*Fractional Occupation Molecular Orbital-Complete Active Space Configuration Interaction with Corrections from Density Functional Theory*"
29. Joe Napoli, Stanford University, "*Decoding the spectroscopic features and timescales of aqueous proton defects*"
30. John J. Karnes, UC Santa Cruz, "*Mixing oil and water: The thermodynamics and mechanism of water transferring into oil*"

31. Julia Rogers, UC Berkeley, *"A molecular explanation for how the excited state relaxation dynamics of an artificial photosynthetic system are affected by the chromophore's linker."*
32. Katherine Oosterbaan, UC Berkeley, *"Non-Orthogonal Configuration Interaction Singles for the Calculation of Core-Excited States"*
33. Keiran Thompson, Stanford University, *"A Sparse Adaptive Quantum Propagator"*
34. Layne Frechette, UC Berkeley, *"Exploring the phase behavior of an elastic Ising model for cation exchange"*
35. Lisa Gong, UC Davis, *"Nanoreactor Study of Levulinic Acid Oxidation: Pairing Theory with Experiment"*
36. Luning Zhao, UC Berkeley, *"Variational Principle for Electronic Excitations in Solids"*
37. Marie Humbert-Droz, Stanford PULSE Institute, *"Ab Initio Multiple Spawning Simulation of the Photodynamics and Time-Resolved Photoelectron Spectroscopy (TRPES) of a Photoactive Yellow Protein (PYP) Model Chromophore"*
38. Marshall Hutchings, UC Davis, *"Ab initio bond orders for recording reaction events in reactive ab initio molecular dynamics"*
39. Monika Williams, Stanford University, *"Excited State Intramolecular Proton Transfer of Methyl Salicylate"*
40. Nanhao Chen, UC Davis, *"Molecular dynamics study and kinetic modeling of the fold switching mechanism of a 24hour circadian clock protein"*
41. Nanna Holmgaard List, Stanford University, *"Nonadiabatic electron dynamics with full multiple spawning"*
42. Peter Walters, UC Berkeley, *"Quantum-classical path integral calculations of electron transfer in solution"*
43. Qian Yang, Stanford University, *"Statistical Learning of Reduced Kinetic Monte Carlo Models of Complex Chemistry from Molecular Dynamics Data"*
44. Robert M. Parrish, Stanford University, *"Frameworks for Routine Simulation of Ultrafast Dynamics Experiments"*
45. Romit Chakraborty, UC Berkeley, *"Multi-scale simulations in Chemistry with the Lattice Boltzmann Method"*
46. Ruben Guerrero, Stanford University, *"A heterogeneous approach to the implementation of the J- and K- engines on accelerator cards"*
47. Ruibin Liang, Stanford University, *"Nonadiabatic photodynamics of retinal protonated Schiff base in channelrhodopsin 2"*
48. Sarah Sandholtz, Stanford University, *"Physical Modeling of the Spreading of Epigenetic Modifications through DNA Looping"*
49. Sofia Izmailov, Stanford University, *"Comparing Transition State Theory Rates with Direct Dynamics Simulation"*
50. Stefan Seritan, Stanford University, *"TeraChem in the Cloud: A Framework for Distributed GPU-Accelerated Electronic Structure"*
51. Stephanie Valleau, Stanford University, *"Reaction dynamics of cyanohydrines with hydrogen sulfide in the context of origins of life"*
52. Stephen J Cotton, UC Berkeley, *"Classical Molecular Dynamics Simulation of Electronically Non-Adiabatic Processes via a Symmetrical Quasi-Classical Windowing Model"*
53. Surl-Hee (Shirley) Ahn, Stanford University, *"Investigating the Role of Non-Covalent Interactions in Conformation and Assembly of Triazine-Based Sequence-Defined Polymers"*
54. Tim J. Zuehlsdorff, UC Merced, *"A computationally efficient approach for modeling the absorption lineshape of solvated dyes"*
55. Tobias Morawietz, Stanford University, *"The Interplay of Structure and Dynamics in the Raman Spectrum of Liquid Water over the Full Frequency and Temperature Range"*
56. Trevor Grand Pre, UC Berkeley, *"Current Statistics of Active Brownian Particles"*
57. Tyler Smart, UC Santa Cruz, *"Enhanced Hole Conduction in CuO by Li Doping"*
58. Tyler Takeshita, UC Berkeley, *"Stochastic Formulation of the Resolution of Identity: Application to Second Order Moller-Plesset Perturbation Theory"*
59. Xiaolei Zhu, Stanford University, *"Molten Carbonate Chemistry Revealed by the Ab Initio Nanoreactor"*
60. Chey M. Jones, Stanford University, *"Benchmarking α-CASSCF excited state dynamics simulations for wild-type green fluorescent protein"*
61. Yudong Qiu, UC Davis, *"Polarizable Study for Desalination using Nanoporous Graphene"*
62. Yuezhi Mao, Stanford University, *"Energy Decomposition Analysis in an "Adiabatic" Picture: Theory and Application"*

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