Northern California Theoretical Chemistry Meeting
Poster Session

#	FIRST	LAST	INSTITUTION	TITLE
1	Christoph	Bannwarth	Stanford University	Combining semiempirical extended tight-binding (xTB) methods with spin-restricted ensemble-referenced Kohn-Sham (REKS) theory
2	Romit	Chakraborty	UC Berkeley/LBNL	Towards In-Silico Design of Metal-Organic Frameworks for Gas Storage
3	Ming	Chen	Lawrence Berkeley National Lab	Overlapped Embedded Fragment Stochastic Density Functional Theory for Covalently Bonded Materials
4	Isabel	Craig	UC Berkeley	A Size Consistent Real Space Geminal Power
5	Avishek	Das	UC Berkeley	Variational Estimation of Large Deviation Functions
6	Scott	Fales	Stanford University	Advances in GPU Accelerated Configuration Interaction for Large-Scale Simulation
7	Katherine Umberto	Ferreras Raucci	Stanford University	Putting Photomechanical Devices to Work: An Ab Initio Multiple Spawning study of Donor Acceptor Stenhouse Adducts
8	Jason	Ford	Stanford University	Building a Hierarchical Kinetic Model of Nitromethane Chemistry
9	Diptarka	Hait	UC Berkeley	What levels of coupled cluster theory are appropriate for transition metal systems?
10	Nanna	Holmgaard List	Stanford	Ab Initio Probing of Photodynamics with Transient X-ray Absorption
11	Dipti	Jasrasaria	UC Berkeley	A stochastic approach to Redfield theory to compute dynamics of large open quantum systems
12	Chey	Jones	Stanford University	Tuning the Photophysics of Chromophore Isomerization in Fluorescent Proteins through Chromophore and Protein Environmental Modifications
13	Aleksey	Kocherzhenko	California State University, East Bay	Unraveling Excitonic Effects for the First Hyperpolarizabilities of Chromophore Aggregates
14	Ruibin	Liang	Stanford University	Nonadiabatic photodynamics of the retinal protonated Schiff base in channelrhodopsin 2
15	Yuezhi	Mao	Stanford University	Accurate prediction of electronic coupling for hole and electron transfer problems using DFT-based approaches
16	Jan	Meisner	Stanford University	A reaction network for methane combustion without experimental parameters constructed with the ab-initio nanoreactor
17	Joe	Napoli	Stanford University	Dynamics of hydrogen bonds and proton defects in the condensed phase.
18	Sam	Niblett	UC Berkeley/LBNL	Interfacial Effects on Ion Pair Dynamics.
19	Leon	Otis	UC Berkeley	Complementary Ansatz Optimization Algorithms in Variational Monte Carlo
20	John	Philbin	UC Berkeley	Electron-Hole Correlations Govern Auger Recombination in Nanostructures
21	Srimukh Prasad	Veccham	UC Berkeley	Polarized Many-Body Expansion
23	Miqdad	Raza	UC Davis	Sodium Ion Conduction in Germanium Phosphide and Germanium Arsenide
24	Julia	Rogers	UC Berkeley	Uncovering a hidden barrier and an accurate reaction coordinate for lipid exchange
25	David	Sanchez	Stanford University	Directly Observing the Photo-induced Ring-Opening of 1,3-Cyclohexadiene via Ultrafast Electron Diffraction and Ab Initio Multiple Spawning
26	Stefan K. Grace	Seritan Johnson	Stanford University	Frameworks for Distributing a GPU-Accelerated *Ab Initio* Exciton Model
27	Jacqueline	Shea	UC Berkeley	Building upon a mean field platform for excited state quantum chemistry

28	Sapana V.	Shedge	UC Merced	The Effect of Ions on the Optical Absorption Spectra of Aqueously Solvated Green Fluorescent Protein(GFP) Chromophore
29	Tim	Stauch	UC Berkeley	Towards an Accurate Calculation of NMR Properties with Wave Function Based Methods
30	Keiran	Thompson	Stanford University	Sparse Adaptive Basis Sets for the Time Dependent Schrodinger Equation
31	Lan	Tran	UC Berkeley	Tracking excited states in state-specific wave function optimization
32	Deniz	Tuna	Stanford University	Multiple-Spawning Nonadiabatic Dynamics Simulations of Photoexcited Urocanic Acid and Orange Carotenoid Protein
33	Brett	Van Der Goetz	UC Berkeley	Tesselations as basis sets in explicitly correlated methods
34	Peter	Walters	UC Berkeley	Electronic energy transfer dynamics in anharmonic environments
35	Hayley	Weir	Stanford University	Elucidating the photochemistry of cis-stilbene with ab initio multiple spawning
36	Monika	Williams	Stanford	Photochemical Dynamics of o-Nitrophenol with Ab Initio Multiple Spawning
37	Junqing	Xu	UC Santa Cruz	Charge and Spin dynamics for Defects in Two-dimensional Materials for Quantum Information
38	Jimmy	Yu	Stanford University	Nonadiabatic photodynamics of the retinal protonated Schiff base in bacteriorhodopsin
39	Luning	Zhao	UC Berkeley	A New Excited State Density Functional Theory For the Correct Modeling of Charge Transfers
40	Yao	Zhao	Stanford University	O(N^5) scaling CCSD(T) and CC3 by Tensor HyperContraction with automatic optimization and implementation