The Mork Family Department of
Chemical Engineering and Materials Science
& Department of Chemistry

4TH ANNUAL SOUTHERN CALIFORNIA THEORETICAL CHEMISTRY CONFERENCE

HOSTED BY:
Department of Chemistry
Mork Family Department of Chemical Engineering and Materials Science
University of Southern California

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Amazon Web Services, Department of Chemistry,
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Talks: SGM123
Lunch and posters: Viterbi E-Quad

USC Dornsife
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College of Letters, Arts and Sciences

USC Viterbi
School of Engineering

Schedule

08:00 – 08:30 am	*Coffee (SGM Lobby)*
08:30 – 09:00 am	Robert Cave, Harvey Mudd College **"Quantum Chemical Alchemy: Dynamical Gold from Born-Oppenheimer Lead"**
09:00 – 09:30 am	Joan-Emma Shae, UC Santa Barbara **"Effect of surfaces and osmolytes in modulating peptide assembly"**
09:30 -10:00 am	Philippe Sautet, UC Los Angeles **"Dynamic nature of heterogeneous catalysts"**
10:00 -10:30 am	*Coffee (SGM Lobby)*
10:30 -11:00 am	Vojtech Vlcek, UC Santa Barbara **"Accurate electronic excitations with stochastic many-body methods"**
11:00 -11:30 am	Tsu-Pei Chiu, U of Southern California **"Modeling of protein-DNA binding with a multi-module deep learning framework"**
11:30 – 02:00 pm	*Lunch + Poster session (E-Quad)*
02:00 – 02:30 pm	Philip Shushkov, California Institute of Technology **"Dynamics of O2 formation in hyperthermal collisions of CO2 with Au surfaces"**
02:30 – 03:00 pm	Michael Galperin, UC San Diego **"Green function methods for optoelectronics and molecular dynamics"**
03:00 – 03:30 pm	Enrico Tapavicza, CSU Long Beach **"Computational chemistry meets photochemistry Applications from photobiology to atmospheric chemistry"**
03:30 – 04:00 pm	*Coffee (SGM Lobby)*
04:00 – 04:30 pm	Garnet Chan, California Institute of Technology **"Condensed phase quantum chemistry"**
04:30 – 05:00 pm	Chiho Mak, U of Southern California **"Understanding the Structure of Structureless Regions in the Genome and the Transcriptome"**
05:00 – 05:05 pm	*Poster prizes*

Poster Session: Presenters and Titles

Poster	Name	Title
1	Adam Bruner	Computation of Optical Pump X-ray Probe Spectroscopy with RT-TDDFT
2	Arthur Pyuskulyan	
3	Borna Zandkarimi	Surface-supported cluster catalysis: Fluxionality and the importance of ensemble representation
4	Brian Nguyen	Divergence of Perturbation Theory in Noncovalent Interactions
5	Bridgett Kohno	
6	Chang Yun Son	Polarization induced ion adsorption on aqueous interfaces: Solvent effect on image charge interactions
7	Colin Egan	Many-Body Effects in Protonated and Deprotonated Water Clusters
8	Daeheum Cho	Probing the Conical Intersections by the Time-Resolved Ultrafast Single-Molecule X-ray Diffraction
9	Danielle Torres	Computational Analysis of the Radical Cation Cyclization of Oxime Ethers Containing Built-In Thiophene or Furan Groups
10	David Reilley	Novel Dynamic Coupling Resolves the Ambiguous Mechanism of Phenylalanine Hydroxylase Oxygen Binding
11	Debbie Zhuang	Many-Body Effects Determine the Hydration Structure of Alkali Ions in Solution
12	Dennis Svatunek	Distortion controlled reactivity of 2-Pyridyl-1,2,4,5-tetrazines
13	Ethan Phan	
14	Francisca Sagredo	Accurate double excitations from ensemble density functional calculations
15	Gianmarc Grazioli	Network Hamiltonians for Modeling Amyloid Fibril Formation
16	Hari Pandey	Computing all free energy barriers in drug designing: A milestoning enabled methodology and its application to P38-MAP Kinase-SB2 system.
17	Henrik R. Larsson	Combining Selected Configuration Interaction with the Density Matrix Renormalization Group
18	Ioan-Bogdan Magdău	THz-THz-Raman Simulations in Bromoform
19	Daniel Jacobson	Aggregation of Brownian Particles at a Reactive Boundary
20	Jared Jetter	Nitrogen-Doped Graphene Catalyst Simulation with Grand Canonical Potential Kinetics
21	Jason Yu	A Functional Self-Consistent Approach to Post-KS methods
22	Jeongmin Kim	Lithium-Ion Solvation and Electroreduction at Metal/Polymer Interfaces for Lithium Metal Batteries: An Atomistic Molecular Dynamics Study
23	Jianan Sun	Examining ligand-HIV protease dissociation: pathway, energy, flexibility, and comparison with association processes
24	Jorge A. Campos-Gonzalez-Angulo	Autocatalytic effects of vibrational polaritons in electron transfer.
25	Jorge Rosa	Path-accelerated molecular dynamics: A parallel-in-time method for long-timescale dynamics based on path integrals
26	Joshua S. Kretchmer	Non-equilibrium electron dynamics during atomic scattering off surfaces
27	Kartik Lakshmi Rallapalli	Rational Engineering of CRISPR-Based Genome Editors Using Computational Methods
28	Katherine Bay	Evaluation of DFT Methods and Implicit Solvation Models for Anion-Binding Host-Guest Systems
29	Kelly Hunter	
30	Kimberly Zhang	Core Electron Binding Energies of Solvated Carboxylic Acid

Poster Session: Presenters and Titles

Poster	Name	Title
31	Kingsley Y. Wu	Computer-Aided Enzyme Design for Enhancing the Catalytic Rate of Tryptophan Synthase Alpha-subunit (TrpA)
32	Lixue Cheng	Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis
33	Luis A. Martínez-Martínez	Triplet harvesting in the polaritonic regime: a variational polaron approach
34	Luke N. Mohanam	libkrylov, a Modular Open-Source Software Library for Extremely Large Eigenvalue and Linear Problems
35	Lyuzhou Ye	Probing molecular chirality by orbital angular momentum carrying X-ray pulses
36	Mario Motta	Quantum imaginary-time evolution, quantum Lanczos and quantum thermal averaging
37	Matthew Du	Chemistry of remotely separated species hybridized by strong light-matter coupling
38	Matthew Zimmer	Force transduction creates long-ranged coupling in SecM-stalled ribosomes
39	Mohammad R. Momeni	Accurate modeling of dynamical properties of water in confined nanopores of metal organic frameworks
40	Pavel Pokhilko	Implementation of spin-orbit couplings for equation-of-motion coupled-cluster methods
41	Phillip Helms	Dynamical phase appearance in the current fluctuations of a driven diffusive model via tensor networks
42	Raphael F. Ribeiro	Enhanced optical nonlinearities under infrared strong coupling
43	Rongpeng Li	
44	Sandra E. Brown	Development of accurate potential energy functions by way of the many-body expansion
45	Sebastian J. R. Lee	Analytical Nuclear Gradients for Projection-based Wavefunction-in-DFT Embedding
46	Shahaf Asban	Quantum phase-sensitive diffraction and imaging using entangled photons
47	Shane M. Parker	Modeling excited state chemistry with TDDFT
48	Si-Han Chen	Structure-kinetics relationship study of CDK8 inhibitors with milestoning
49	Song Wang	
50	Sree Ganesh Balasubramani	Static polarizabilities within GKS-spRPA
51	Stefano M. Cavaletto	Resonant x-ray sum-frequency-generation spectroscopy for imaging ultrafast electron dynamics
52	Ted Yu	DFT simulation of Edge Halogenated Nanosheets as an ORR catalyst in Fuel Cells
53	Tim Cholko	Dynamics and Intermolecular Interactions of ssDNA in Nucleic Acid Biosensors with Varied Surface Properties
54	Tirthendu Sen	Reversible Photoswitching in Dreiklang: A Theoretical Insight of the Mechanism
55	Victor Fung	Complex-mediated methane conversion over metal oxides from first principles
56	Yalu Chen	Design of High Performance Electrocatalysts for Clean Energy Conversion Guided by Machine-Learning and Quantum Chemistry
57	Yi-Siang Wang	Propagation of Quantum Particle Distributions by Combining Lindblad Master Equation and Surface Hopping
58	Zhenzhuo Lan	Theoretical Studies for CH Bond Activation Mediated by Bio-inspired Dicopper Catalysts
59	Zhi-Hao Cui	Density Matrix Embedding to Realistic Solids