



2024 West Coast Theoretical Chemistry Meeting

May 5, 2024

University of California, Merced

Arts and Computational Sciences Building, Room 120 (ACS 120)

Breakfast (8:00 – 8:35 AM), ACS 120

Poster presenters should use this time to get set up.

Morning Session 1 (8:35 – 10:20 AM), ACS 120

Session Chair: Thomas Markland, Stanford University

8:35 - 8:40 : Opening remarks

8:40 – 9:20 : Nicole Adelstein, San Francisco State University
Techniques for Multiscale Simulations of Solid-Solid Interfaces

9:20 – 9:40 : Diptarka Hait, Stanford University
Can excited states of radical ions act as photoredox catalysts?

9:40 – 10:20 : Dean Tantillo, University of California, Davis
Organic reactions with bifurcating reaction coordinates - What, why, why care?

Coffee Break (10:20 – 10:50 AM), ACS 120

Poster presenters should use this time to get set up.

Morning Session 2 (10:50 – 11:50 AM), ACS 120

Session Chair: Tim Kowalczyk, Western Washington University

10:50 – 11:30 : Grant Rotskoff, Stanford University
From coarse-grained models to conformational ensembles

11:30 – 11:50 : Chenchen Song, University of California, Davis
Simulating photoreactions in biological environments with state averaged CASSCF in AMOEBA polarizable models



Lunch & Poster Session (11:50 AM – 2:00 PM)

Lunch served in Pavilion

Poster session outside the ACS building

Afternoon Session 1 (2:00 – 3:20 PM), ACS 120

Session Chair: Kristi Closser, California State University, Fresno

2:00 – 2:40 : David Limmer, University of California, Berkeley

Taking chemistry far from equilibrium

2:40 – 3:00 : Siddharth Sonti, University of California, Davis

Elucidating the fluxionality and dynamics of zeolite-confined Au nanoclusters using machine learning potentials

3:00 – 3:20 : Imam Wahyutama, University of California, Merced

Conjugation and symmetry effects in ultrafast charge migration

Coffee Break (3:20 – 3:50 PM), ACS 120

Poster presenters should use this time to put posters away.

Afternoon Session 2 (3:50 – 5:15 PM), ACS 120

Session Chair: Lee-Ping Wang, University of California, Davis

3:50 – 4:30 : Ashley Ringer McDonald, Cal Poly San Luis Obispo and Molecular Science Software Institute

What can the MolSSI do for you? Resources, programs, and software from the Molecular Sciences Software Institute.

4:30 – 5:10 : Xiao Wang, University of California, Santa Cruz

Periodic wavefunction methods for materials science

5:10 – 5:15 : Closing remarks

(Optional) Tutorial on nanoHUB.org tools for hands-on pedagogical simulations (5:30 – 6:15 PM), ACS 120

Instructor: David Strubbe, University of California, Merced