

The Northern California Theoretical Chemistry Meeting
Sunday, May 19, 2019

8:00 am	Breakfast	Tan Hall Lobby
8:45 am	Opening Remarks by Organizers Martin Head-Gordon, Eran Rabani, David Limmer	120 Latimer Hall
Session I – Chair: Ilan Benjamin, UC Santa Cruz		120 Latimer Hall
9:00 am	Teresa Head-Gordon, UC Berkeley <i>“Chemical Reactivity in Complex Environments”</i>	
9:40 am	Tim Zuehlsdorff, UC Merced <i>“Static and dynamic approaches to computing spectral lineshapes”</i>	
10:00 am	Tom Markland, Stanford <i>“Paddling in the deep end: unraveling proton defect dynamics with machine learning and path integrals”</i>	
10:40 am	Coffee Break	Tan Hall Lobby
Session II – Chair: Todd Martinez, Stanford		120 Latimer Hall
11:10 am	Lee-Ping Wang, UC Davis <i>“Recovering from self-consistent field convergence failure in Born-Oppenheimer molecular dynamics with a Car-Parinello monitor”</i>	
11:50 am	Shunda Chen, UC Davis <i>“Controlling Heat Transfer at Nanoscale”</i>	
12:10 pm	Lunch and Poster Session	775 Tan Hall
Session III – Chair: Eric Neuscamman, UC Berkeley		120 Latimer Hall
3:10 pm	Yuan Ping, UC Santa Cruz <i>“Excited State Dynamics for Defects in Two-dimensional Materials for Quantum Information”</i>	
3:50 pm	Alice Walker, Stanford <i>“Mechanistic insights into photodecarboxylation of fatty acids from classical and QM/MM simulations”</i>	
4:10 pm	Coffee Break	Tan Hall Lobby

