

**35th Workshop on Recent Developments in Electronic Structure Methods  
University of California, Merced**

**TUESDAY, JUNE 13**

8:00 AM-8:00 PM	Housing check-in	Summits Tenaya Housing Office 190
3:00 PM-6:00 PM	Registration	ACS 238, Physics Lounge
5:00 PM-6:00 PM	Welcome reception	ACS 238, Physics Lounge
6:00 PM-7:00 PM	Dinner	Pavilion
7:00 PM-9:00 PM	Activity: Wiki-editing	GRAN 110
7:00 PM-9:00 PM	Tutorial: nanoHUB	GRAN 120
7:00 PM-9:00 PM	Tutorial: RMG	GRAN 125

**WEDNESDAY, JUNE 14**

9:00 AM	Welcome remarks: Dean Hrant Hrachian, steering committee chair Andrew Rappe	ACS 120
9:10 AM	Talk: Peter Oppeneer, A first-principles approach to orbital accumulation and orbital transport	ACS 120
9:50 AM	Talk: Sayantani Ghosh, The role of nanostructured metal halide perovskite materials in solar energy harvesting	ACS 120
10:40 AM	Break	Outside ACS 120
11:05 AM	Talk: Sanghamitra Neogi, Machine Learning Models to Assist Designing Atomic Environments in Semiconductor Heterostructures and Complex Alloys	ACS 120
11:45 AM	Talk: Trevor David Rhone, Artificial intelligence guided materials discovery of two-dimensional magnets	ACS 120
12:25 PM	Lunch	Pavilion
12:25 PM	Steering committee lunch	Pavilion 104
1:40 PM	Talk: Emmanuel Fromager, Ensemble density functional theory of electrons and nuclei	ACS 120
2:20 PM	Talk: Henrik Larsson, Tensor network states for computing vibrational and electronic states	ACS 120
3:00 PM	Break	Outside ACS 120
3:25 PM	Talk: Yuan Ping, Spin relaxation, dephasing and diffusion in solids from ab-initio density-matrix dynamics	ACS 120
4:05 PM	Talk: Carsten Ullrich, (TD)DFT for noncollinear spins: orbital functionals, semilocal approximations, and xc torques	ACS 120
4:45 PM	Talk: Jennifer Cano, Engineering topological phases with a superlattice potential	ACS 120
5:25 PM	End	
6:00 PM	Dinner for speakers and committee	El Capitan, downtown
6:00 PM	Dinner	Pavilion
7:00-9:00 PM	Preliminary results discussion	GRAN 110
7:00-9:00 PM	Meet the NSF Program Manager, with Serdar Ögüt	GRAN 115
7:00-9:00 PM	Informal gathering at park next to campus	Lake Yosemite

**THURSDAY, JUNE 15**

8:30 AM	Poster setup	ACS Terraces
9:00 AM	Talk: Marco Govoni, TBD -- embedding theory and defects (virtual)	ACS 120
9:40 AM	Group photo	Outside ACS 120
9:50 AM	Break	Outside ACS 120
9:50 AM	Poster session	ACS Terraces
12:00 PM	Lunch	Pavilion
12:00 PM	IOP publishing webinar, over lunch	GRAN 135
1:00 PM	Talk: John Bonini, Lattice dynamics with broken time reversal symmetry	ACS 120
1:40 PM	Talk: Marco Bernardi, Frontiers of First-Principles Electron-Phonon Interactions: Spinful, Data-Driven, and Parsimonious	ACS 120
2:20 PM	Talk: Siyuan Chen, Forces, stress, and geometry optimization with auxiliary-field quantum Monte Carlo	ACS 120
3:00 PM	Break	Outside ACS 120
3:25 PM	Talk: Lenz Fiedler, Demonstrating temperature transferability of neural network models replacing modern density functional theory	ACS 120
4:05 PM	Talk: Isaac Tamblin, A powerful yet inadequate tool - ML for electronic structure	ACS 120
4:45 PM	Talk: Boris Kozinsky, Machine learning models of many-body atomic and electronic interactions	ACS 120
5:25 PM	End, poster takedown	ACS Terraces
6:00 PM	Banquet, poster awards, announcements	ADMIN 306

**FRIDAY, JUNE 16**

	Housing check-out by noon	Summits Tenaya Housing Office 190
9:00 PM	Talk: Mit Naik, Bethe Salpeter equation calculations in moiré superlattices with thousands of atoms in the unit-cell	ACS 120
9:40 PM	Talk: Emanuel Gull, Electronic Structure – a view from finite-temperature field theory	ACS 120
10:20 PM	Break	Outside ACS 120
10:45 PM	Talk: Marcus Eisenbach, Scalable First Principles Calculations for Alloys	ACS 120
11:25 PM	Talk: Xavier Andrade, The INQ code: reinventing the electronic-structure code	ACS 120
12:05 PM	Closing remarks	ACS 120
12:15 PM	Lunch	Pavilion