Campus map — University of California Merced, 5400 N. Lake Road, Merced, CA 95340

Our sponsors

NSF — National Science Foundation, DMR-2328076

IOP Publishing — *Journal of Physics: Condensed Matter* and *Electronic Structure*

U.S. DEPARTMENT OF ENERGY — Tentative

UCMERCED GRADUATE DIVISION

UCMERCED SCHOOL OF NATURAL SCIENCES

UCMERCED DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

UCMERCED DEPARTMENT OF PHYSICS

Organizing committee

- David Strubbe (chair), Dept. of Physics, University of California, Merced
- Aurora Pribram-Jones, Dept. of Chemistry and Biochemistry, University of California, Merced
- Steven G. Louie, Dept. of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory
- Jeffrey B. Neaton, Dept. of Physics, University of California, Berkeley and Lawrence Berkeley National Laboratory

Steering committee

- Susan Atlas (University of New Mexico)
- Jerry Bernholc (North Carolina State University)
- Marco Buongiorno Nardelli (University of North Texas)
- Roberto Car (Princeton University)
- David Ceperley (University of Illinois at Urbana-Champaign)
- James Chelikowsky (University of Texas at Austin)
- Mei-Yin Chou (Academia Sinica, Taiwan)
- Natalie Holzwarth (Wake Forest University)
- Steven Louie (University of California, Berkeley/Lawrence Berkeley National Lab)
- Richard Martin (University of Illinois at Urbana-Champaign/Stanford University)
- Normand A. Modine (Sandia National Laboratories)
- Andrew Rappe (University of Pennsylvania)
- John A. Rehr (University of Washington)
- David A. Strubbe (University of California, Merced)
- Cyrus Umrigar (Cornell University)
- David Vanderbilt (Rutgers University)
- Lucas K. Wagner (University of Illinois at Urbana-Champaign)
- Shiwei Zhang (College of William & Mary/Flatiron Institute)

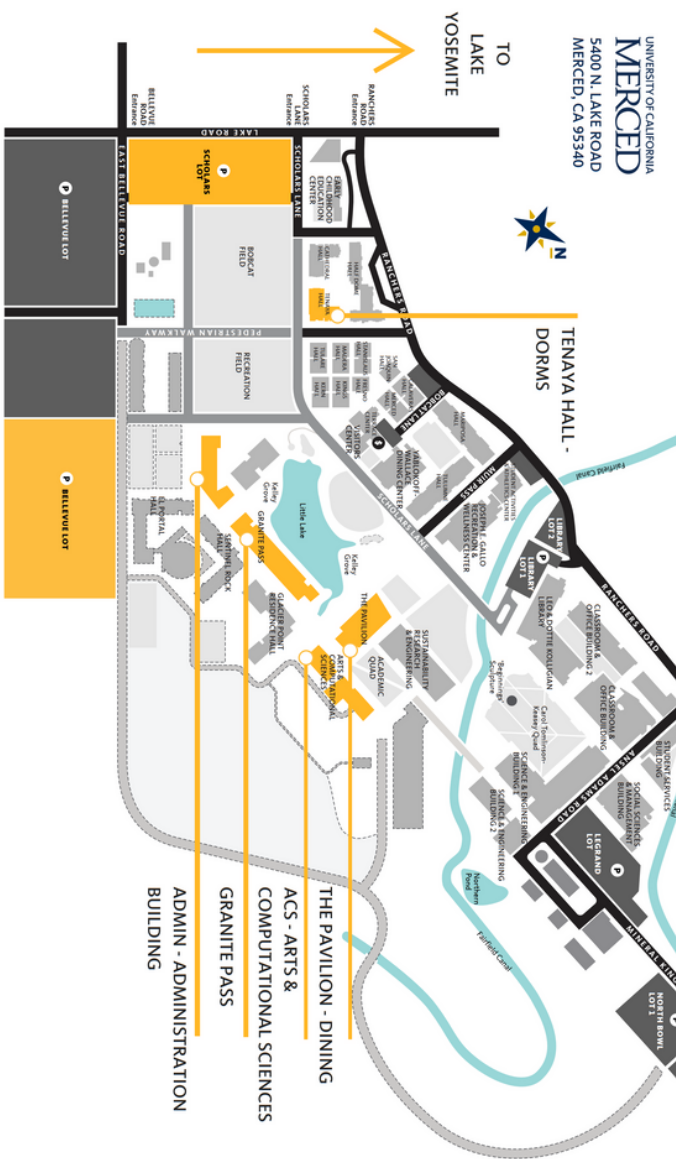# 35th Workshop on Recent Developments in Electronic Structure Methods

13–16 June 2023

UNIVERSITY OF CALIFORNIA MERCED

ES23

Agenda All talks will be in ACS 120

TUESDAY, JUNE 13

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

WEDNESDAY, JUNE 14

9:00 AM	**Welcome remarks: Dean Hrant Hratchian** (ACS 120)
9:10 AM	**Peter Oppeneer:** A first-principles approach to orbital accumulation and orbital transport
9:50 AM	**Sayantani Ghosh:** TBD -- experiments and spectroscopy
10:40 AM	**Break** (Outside ACS 120)
11:05 AM	**Sanghamitra Neogi:** Machine Learning Models to Assist Designing Atomic Environments in Semiconductor Heterostructures and Complex Alloys
11:45 AM	**Trevor David Rhone:** Artificial intelligence guided materials discovery of two-dimensional magnets
12:25 PM	**Lunch** (Pavilion)
12:25 PM	**Steering committee lunch** (Pavilion 104)
1:40 PM	**Emmanuel Fromager:** Ensemble density functional theory of electrons and nuclei
2:20 PM	**Henrik Larsson:** Tensor network states for computing vibrational and electronic states
3:00 PM	**Break** (Outside ACS 120)
3:25 PM	**Yuan Ping:** Spin relaxation, dephasing and diffusion in solids from ab-initio density-matrix dynamics
4:05 PM	**Carsten Ullrich:** (TD)DFT for noncollinear spins: orbital functionals, semilocal approximations, and xc torques

All talks will be in ACS 120

WEDNESDAY, JUNE 14 CONT.

4:45 PM	**Jennifer Cano:** Engineering topological phases with a superlattice potential
6:00 PM	**Dinner for speakers & 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 Öğüt** (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	**Marco Govoni:** TBD -- embedding theory and defects
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	**John Bonini:** Lattice dynamics with broken time reversal symmetry
1:40 PM	**Marco Bernardi:** Frontiers of First-Principles Electron-Phonon Interactions: Spinful, Data-Driven, and Parsimonious
2:20 PM	**Siyuan Chen:** Forces, stress, and geometry optimization with auxiliary-field quantum Monte Carlo
3:00 PM	**Break** (Outside ACS 120)
3:25 PM	**Lenz Fiedler:** Demonstrating temperature transferability of neural network models replacing modern density functional theory
4:05 PM	**Isaac Tamblyn:** A powerful yet inadequate tool - ML for electronic structure
4:45 PM	**Boris Kozinsky:** Machine learning models of many-body atomic and electronic interactions
5:25 PM	**Poster takedown** (ACS Terraces)
6:00 PM	**Banquet, poster awards, announcements** (ADMIN 306)

All talks will be in ACS 120

FRIDAY, JUNE 16

	Housing check-out by noon (Summit Tenaya Housing Office 190)
9:00 AM	**Mit Naik:** Bethe Salpeter equation calculations in moiré superlattices with thousands of atoms in the unit-cell
9:40 AM	**Emanuel Gull:** Electronic Structure – a view from finite-temperature field theory
10:20 AM	**Break** (Outside ACS 120)
10:45 AM	**Marcus Eisenbach:** Scalable First Principles Calculations for Alloys
11:25 AM	**Xavier Andrade:** TBD -- Inq and TDDFT
12:05 AM	**Closing remarks** (ACS 120)
12:15 AM	**Lunch** (Pavilion)

Electronic Structure at UCM

Center for Chemical Computation and Theory (ccCAT)

Consortium for High Energy Density Science (CfHEDS)

Department of Physics

Department of Chemistry & Biochemistry

Materials and Biomaterials Science and Engineering

The meeting will be conducted according to the American Physical Society's Code of Conduct for APS Meetings (see webpage). Please report any concerns to Prof. Strubbe at dstrubbe@ucmerced.edu