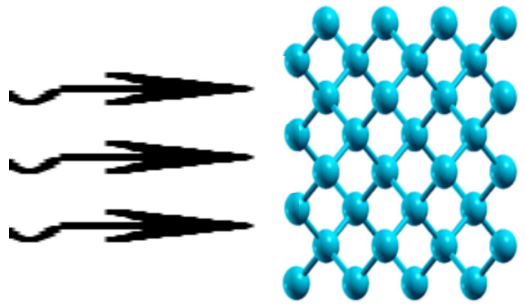
Simulating electronic structure under ultrafast compression with DFT and TDDFT

David A. Strubbe, Department of Physics
University of California, Merced



HEDS
High Energy Density Science Center

High Energy Density Science Seminar
Lawrence Livermore National Laboratory
9 Jan 2020

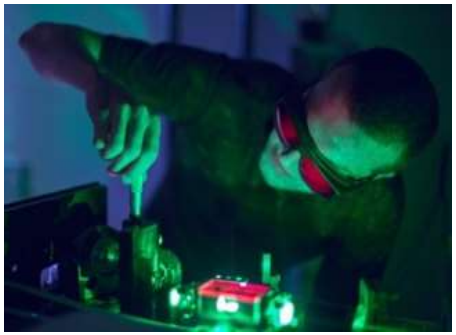
UCMERCED

Founded 2005, 10th campus of the University of California
First US research university of the 21st century
Merced population is about 80,000
60-90 minutes drive from here.

Who We Are

- 17 faculty members (5 women)
- 10 affiliated faculty in other departments
- 64 graduate students (17 women)
  from the Central Valley, San Francisco Bay Area, Southern California, Ohio, Maryland, Iran, India, Nepal, Cyprus, Bangladesh, …
- 60 undergraduate physics majors
- 9000 total undergraduates (55% Hispanic, 75% first-generation college students)
- Hispanic-Serving Institution
- Overall: 700 graduate students, 407 faculty

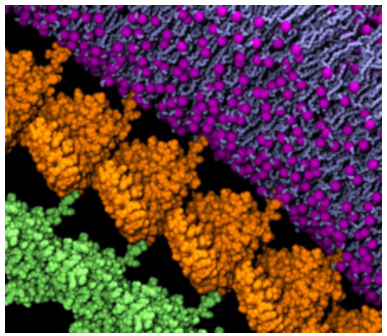
Physics Research Areas and Centers



Atomic, Molecular, and Optical Physics

Experiment
Sayantani Ghosh
Michael Scheibner
Jay Sharping
Roland Winston
Jing Xu

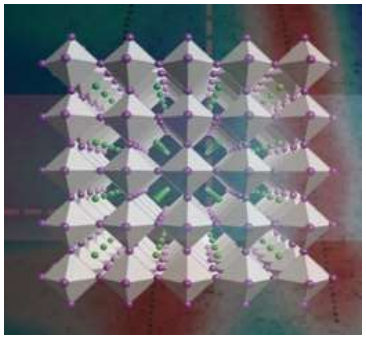
Theory
Chih-Chun Chien
Kevin Mitchell
Lin Tian



Biophysics and Soft Matter

Experiment
Linda Hirst
Dustin Kleckner
Bin Liu
Jay Sharping
Jing Xu

Theory
Daniel Beller
Kinjal Dasbiswas
Ajay Gopinathan



Condensed Matter (Solid-State) Physics

Experiment
Ray Chiao
Sayantani Ghosh
Michael Scheibner
Jing Xu

Theory
Chih-Chun Chien
David Strubbe
Lin Tian

Solar and Energy Sciences

Sayantani Ghosh
Linda Hirst
David Strubbe
Roland Winston

Sarah Loebman, theoretical astrophysicist, joining fall 2020

Center for Chemical Computation and Theory

CCBM
NSF-CREST
CENTER FOR CELLULAR AND BIOMOLECULAR MACHINES

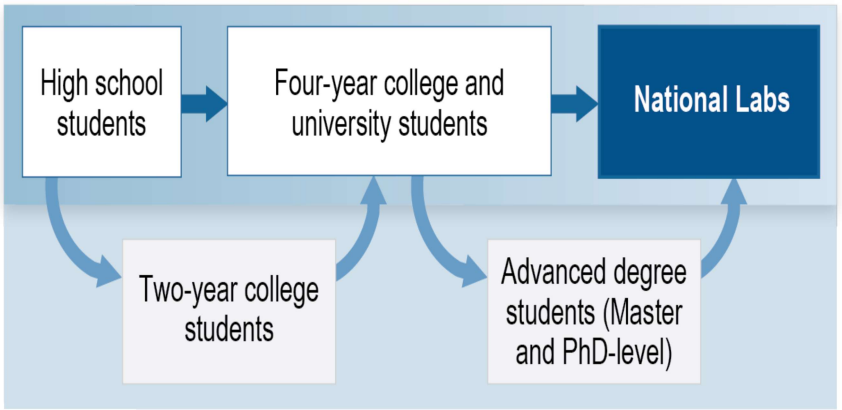
MACES
MERCED NANOMATERIALS CENTER FOR ENERGY AND SENSING

UC Solar
University of California Advanced Solar Technologies Institute

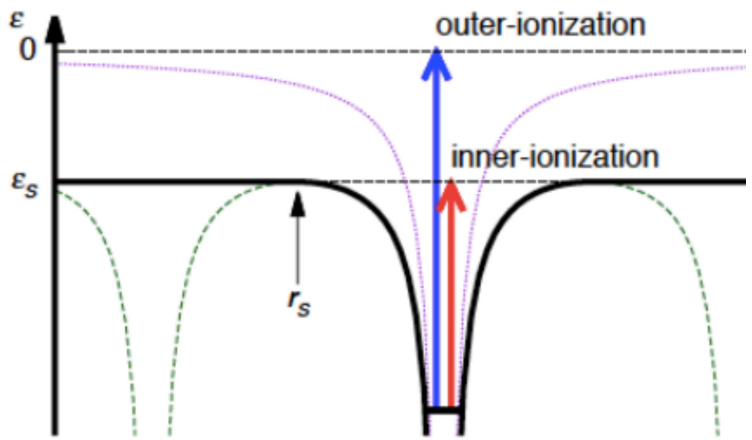
Consortium for High-Energy Density Science (CfHEDS)

- Computational study of matter under extreme temperature and pressure
- Expand education and research opportunities, connect students to careers in national labs, develop curriculum

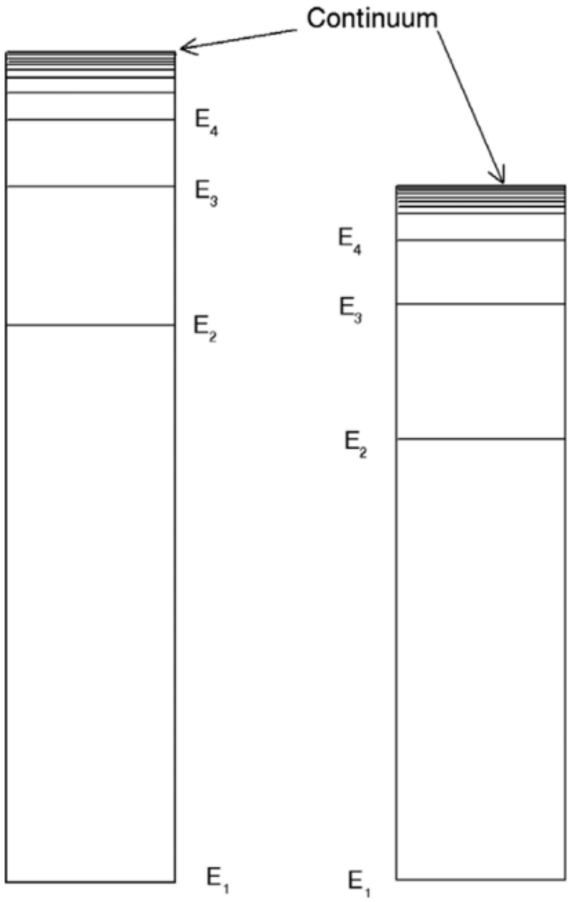
Florida A&M University, Tallahassee, FL (HBCU).
Charles Weatherford (PI) and Ronald Williams.
University of California, Merced (HSI).
David Strubbe and Aurora Pribram-Jones.
Morehouse College, Atlanta, GA (HBCU).
Eddie Red and Wesley Sims.
Lawrence Livermore National Laboratory.
Frank Graziani, Ronnie Shepherd, Tony Baylis.



pressure ionization

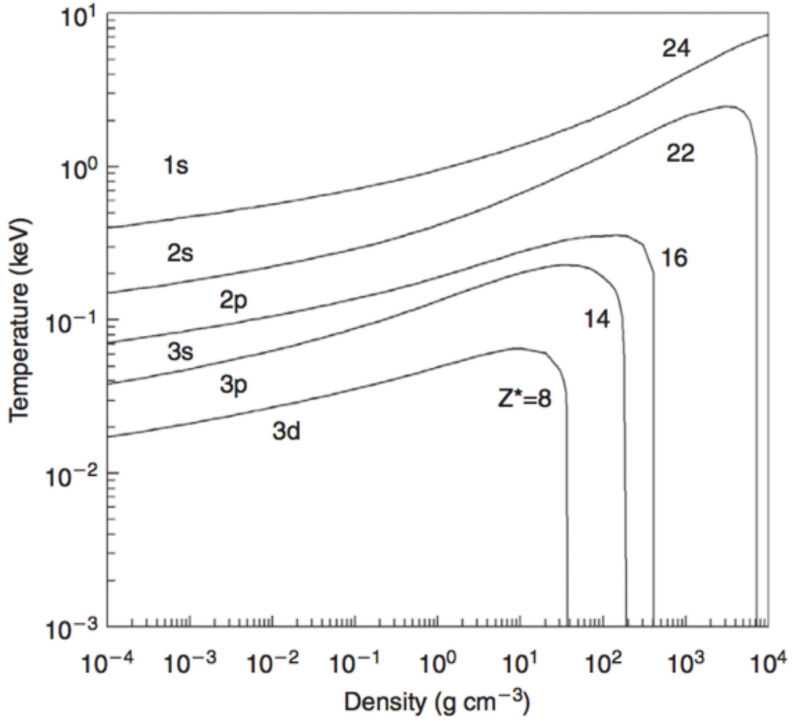


continuum lowering



ionization potential depression

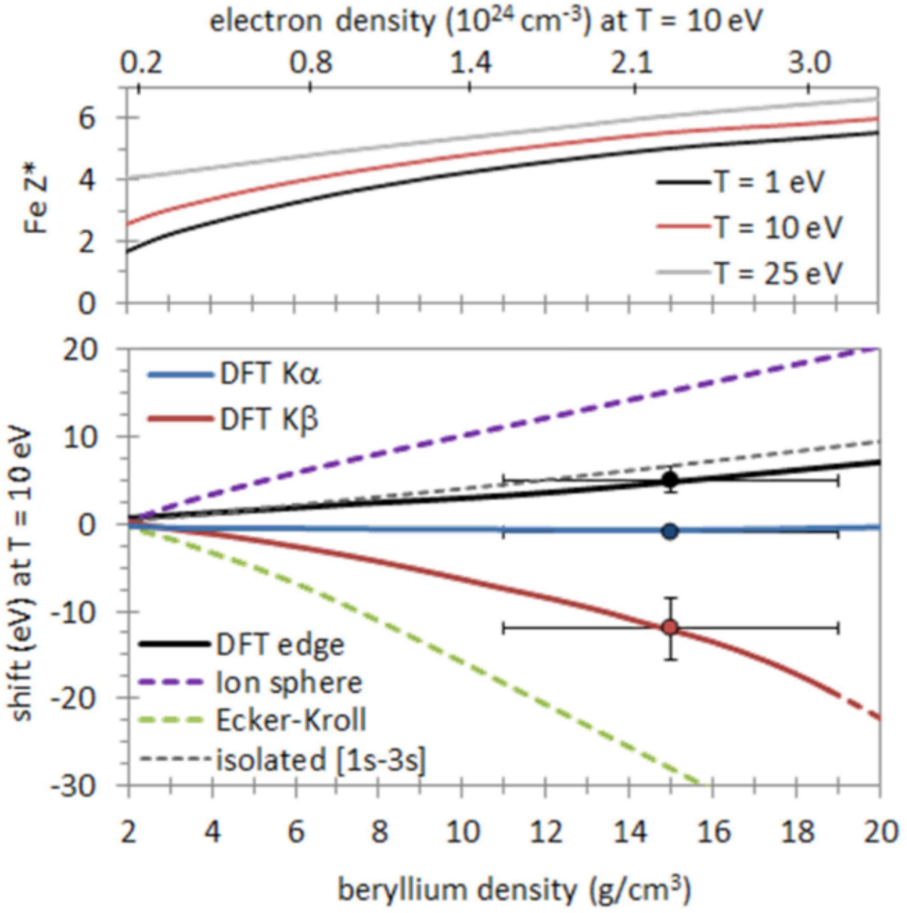
due to pressure and temperature



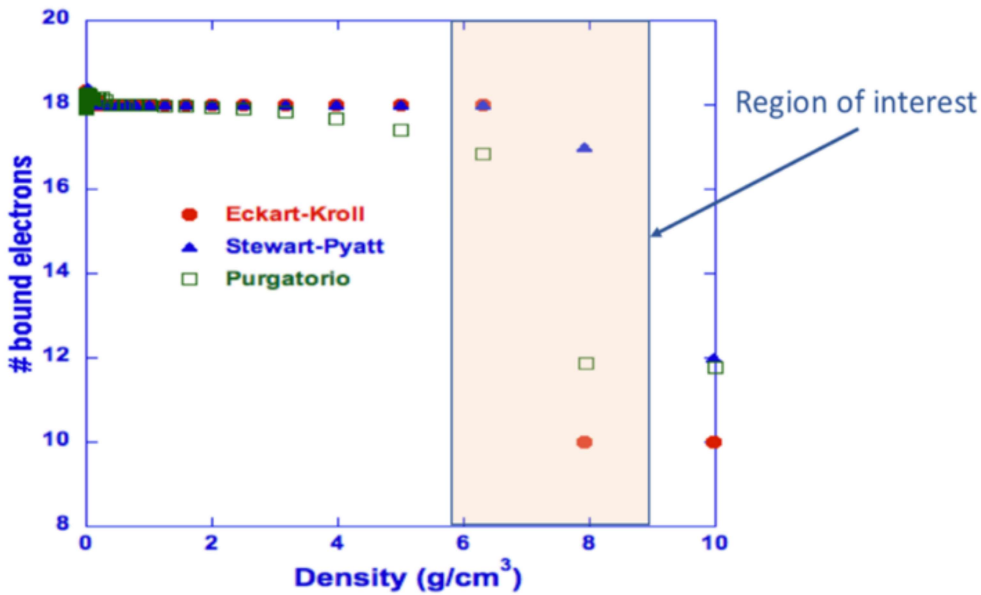
Extreme Physics

Modeling continuum lowering

Empirical models
Density functional theory (DFT)-molecular dynamics (MD) calculations
Neutral pseudo-atom (NPA) MD calculations



Fe in Be (S. Hansen)



Potassium (R. Shepherd)

Basic theoretical technique: density-functional theory (DFT)

Quantum mechanics for *N* electrons ("electronic structure"):
time-independent Schrödinger equation

$$H\Psi = E\Psi, \Psi\left(r_1, r_2, ..., r_N\right)$$

Many-electron Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + V_{\text{nuclei}} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i - r_j|}$$

One-electron Kohn-Sham Hamiltonian:

$$H_{\text{KS}} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{nuclei}} + \frac{1}{2}\int\frac{e^2 n\left(r'\right)}{r - r'}dr' + V_{\text{xc}}\left[n\right]$$

reformulated in terms of density *n*

$$\Psi\left(r_1, r_2, \cdots\right) = \left|\psi_1\left(r_1\right)\psi_2\left(r_2\right)\cdots\right|$$

Reducing to effective one-electron problem. Only for ground state.

Density-Functional Theory (DFT)

One-electron Kohn-Sham Hamiltonian:

$$H_{\mathrm{KS}} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{nuclei}} + \frac{1}{2}\int \frac{e^2 n\left(r'\right)}{r - r'} dr' + V_{\mathrm{xc}}\left[n\right]$$

reformulated in terms of density *n*

Ground state properties: energy, electron density, forces, stresses, equilibrium structure

Time-dependent DFT can calculate optical properties (time-dependent Schrödinger equation).

Approximations to Vxc are limiting. May be able to transcend by machine learning, finding density directly from external potential.

K. Ryczko, D. A. Strubbe, and I. Tamblyn, *Phys. Rev. A* 100, 022512 (2019)

Still a computationally intensive task. Need parallel supercomputers.

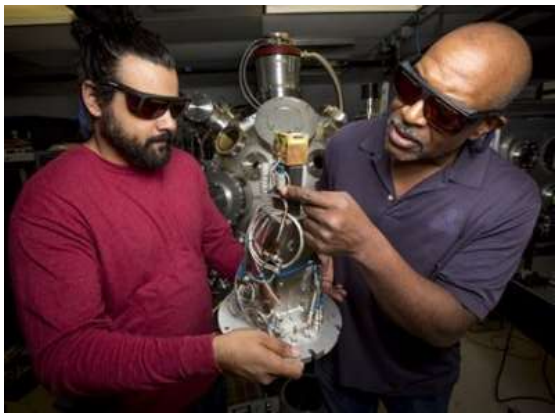
CfHEDS student collaborative research at LLNL

Undergrads from FAMU (laser experiments), Morehouse (materials physics and engineering)

UC Merced physics major: Zach Mauri – computational theory of interaction of light with molecules

FAMU grad students and postdocs:

- Jerry Clark
- Yaye Badjo, Dr. Daniel Gebremedhin, Dr. Edwin Quashie (PhD from FAMU, now at LLNL) -- electronic structure theory
- Jessica Tucker – quantum computing



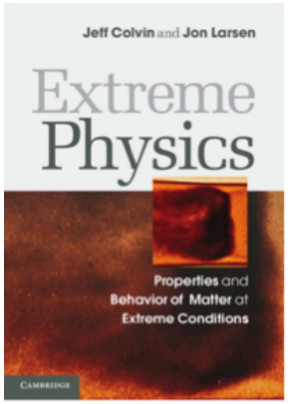
Special education and training opportunities

- Outreach to community colleges (specifically Merced College)
- Webinar on applying for Dept of Energy graduate and postdoctoral fellowships

May: Tour of the National Ignition Facility and discussion of career opportunities at LLNL, for UC Merced students.

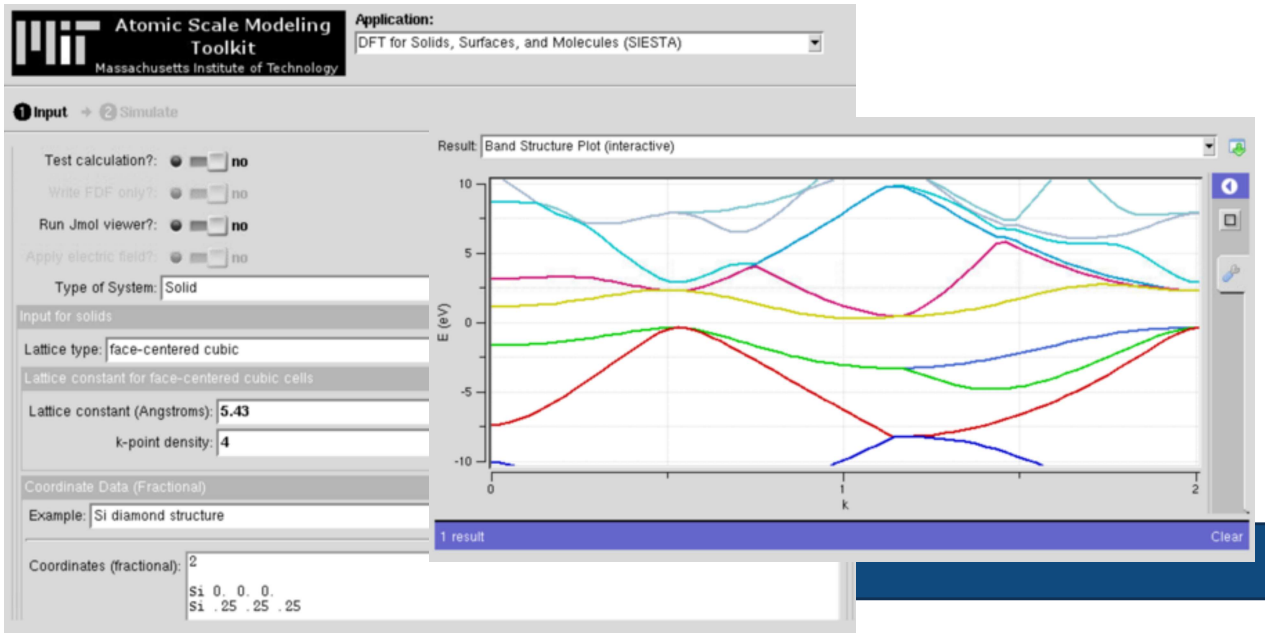
HEDS Education

- 3rd Workshop on Education in HEDS, UC San Diego, Dec 2019: discussing curriculum development, course sharing, distance learning among universities
- Honors General Chemistry lectures on states of matter, intermolecular forces, phase diagrams, and scientific ethics.
- Graduate Condensed Matter Physics: upcoming guest lectures by Jeff Colvin on equation of state
- Formal DFT class: discussion of thermal DFT/TDDFT
- Seminars at UCM: Tammy Ma, Frank Graziani, Attila Cangi (Sandia New Mexico)

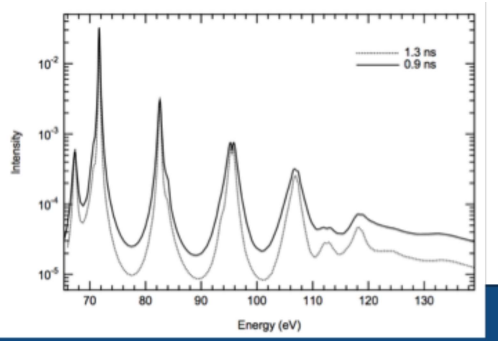


nanoHUB.org for simulation tools

- NSF-supported platform headquartered at Purdue
- Free web-based simulation tools (undergraduate or graduate level)
- Graphical user interface for input and output, to focus on physics
- Using in condensed-matter physics class
- Exploring use for FLYCHK (ionization code) or others in HEDS
- Immediately usable by any students or classes worldwide



https://nlte.nist.gov/FLY/



Outreach

Interview on U Texas El Paso NPR program about HED research for the general public

FAMU STEM Day—800+ K-12 students and parents learn about and participate in STEM experiments.

Morehouse: 20 high-school students in 5-week enrichment program Nuclear, Materials, and Space Science (NuMaSS)

Symposium at Society for the Advancement of Chicano/Hispanic and Native Americans in Science (SACNAS):

"Research in University-National Laboratory Collaborations: The Minority Serving Institution Partnership Program"

David A. Strubbe, University of California, Merced: "Stars, fusion, and shocks: simulation of materials under extreme temperature and pressure"

Yirong Lin, mechanical engineering, University of Texas at El Paso: "Additive manufacturing of functional materials: from nano to micro to meter scale"

Chris Wetteland, materials science and engineering, University of Tennessee, "Using Additive Manufacturing Research to Build the Minority Pipeline"

Aurelia Williams, computer science, Norfolk State University, "Using Cybersecurity Research to Increase the Workforce"

Honolulu, Hawaii. Sat, 2 Nov 2019

Also participated in LLNL panel.

2020 Electronic Structure Workshop at University of California, Merced: June 2-5, 2020

Organizing committee

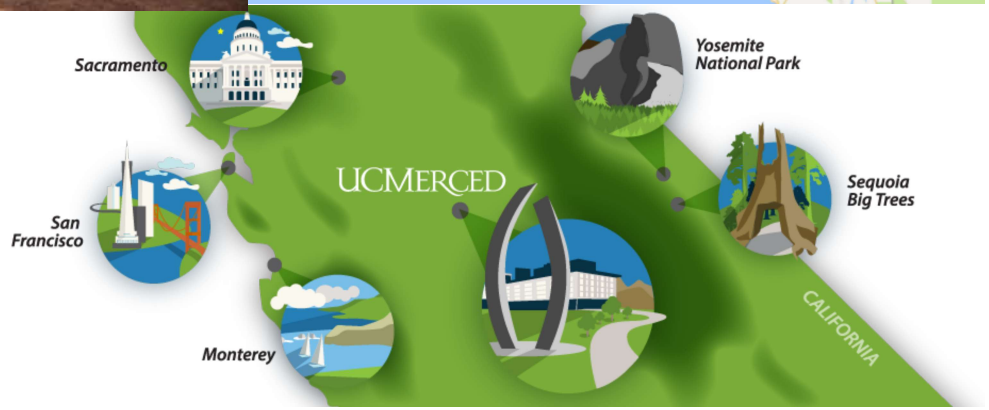
David Strubbe and Aurora Pribram-Jones, UC Merced

Steven Louie and Jeffrey Neaton, UC Berkeley and LBNL

Topics include simulations of warm dense matter.

Hosted in brand-new buildings, banquet at nearby vineyard

https://physics.ucmerced.edu/electronic-structure-workshop



Conclusions

More info on Consortium for High-Energy Density Science: *http://cfheds.ucmerced.edu*

Acknowledgments:

NNSA and UC Merced start-up funds

Computation at NERSC and local MERCED cluster funded by NSF