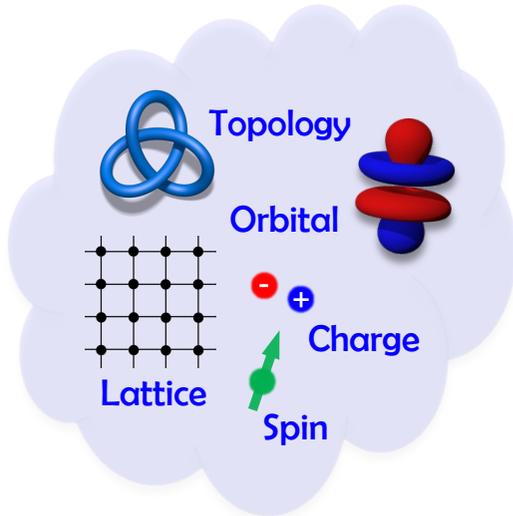# Los Alamos Computational Condensed Matter Summer School
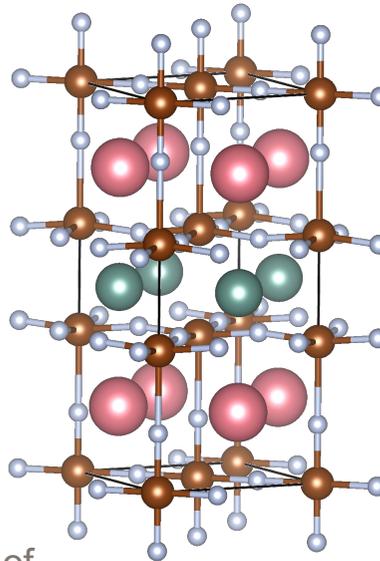

LA-UR-26-21604

June 16, 2025

Quantum Materials: A Powerful Solution to Current Technological Challenges

Fundamental Interactions

Topology
Orbital
Charge
Lattice
Spin

Materials

Devices

3D Logic
3D Memory
Thermal Management
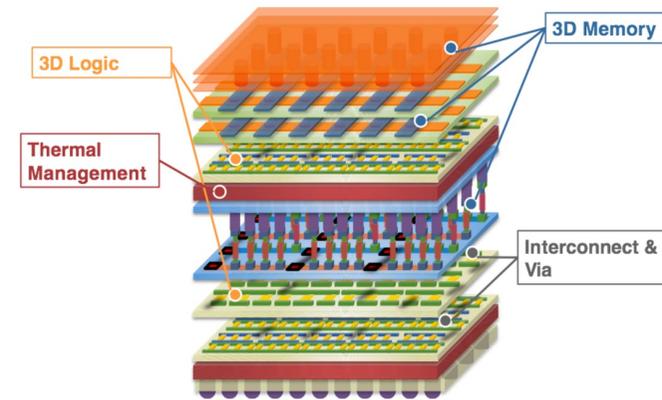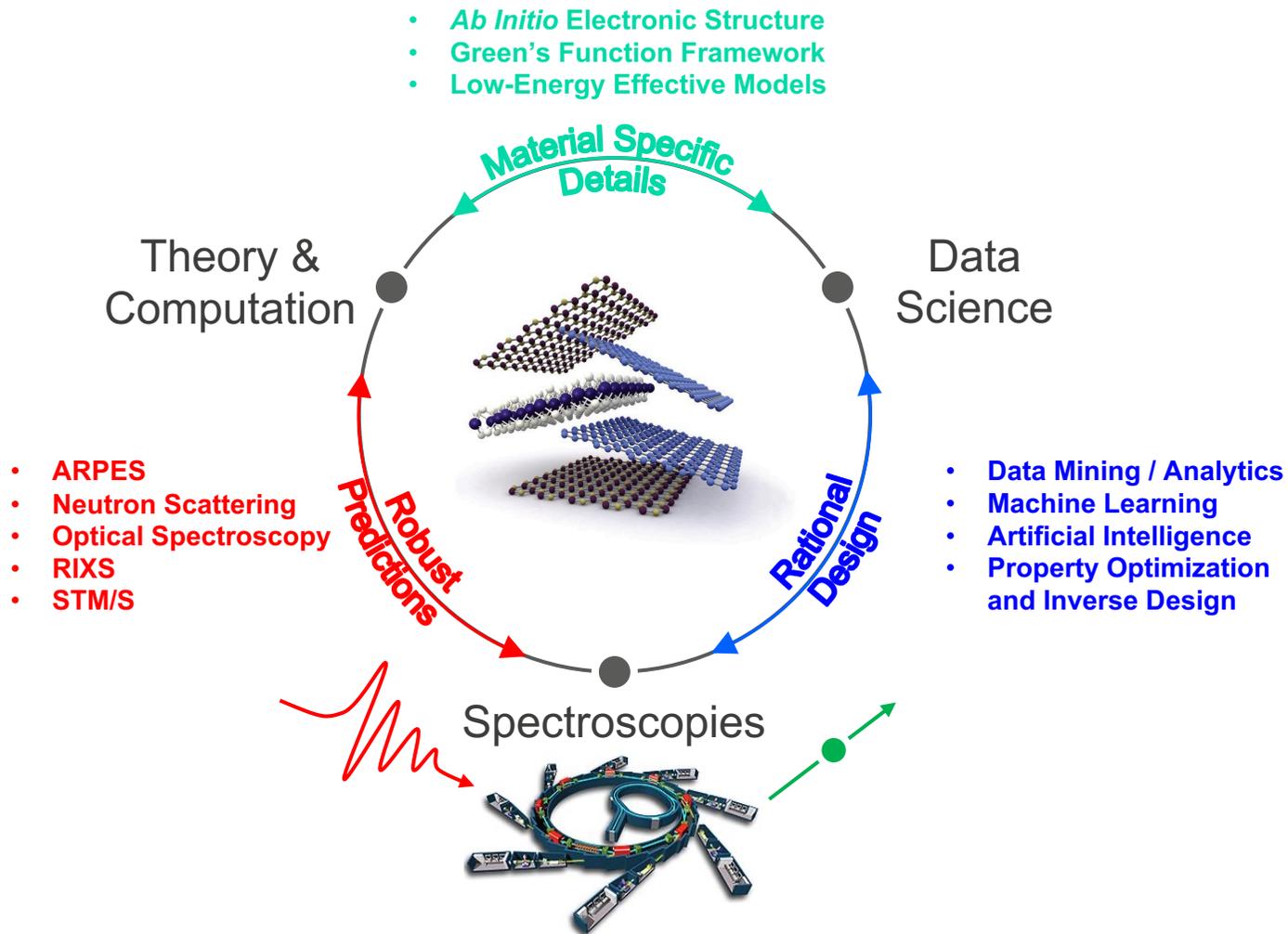Interconnect & Via

Discovery and Design of Novel Phases of Matter

Design of Next generation Devices

Challenge: The properties of naturally occurring materials are not necessarily commensurate with those needed for next-generation devices.

The Rise of Quantum Materials. Nature Physics 12, 105 (2016)
B. Keimer and J. E. Moore Nature Physics 13, 1045–1055 (2017)
R. Cava, N. de Leon, and W. Xie Chem. Rev. 121(5), 2777–2779 (2021)
C. Murray, et al. Basic Research Needs for Microelectronics. USDOE SC (2018)

Los Alamos
NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

Co-Design Approach to Quantum Materials

- *Ab Initio* Electronic Structure
- Green's Function Framework
- Low-Energy Effective Models

Material Specific Details

Theory & Computation

Data Science

- ARPES
- Neutron Scattering
- Optical Spectroscopy
- RIXS
- STM/S

Robust Predictions

Rational Design

- Data Mining / Analytics
- Machine Learning
- Artificial Intelligence
- Property Optimization and Inverse Design

Spectroscopies

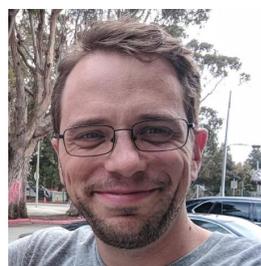June 16, 2025

Summer School Overview
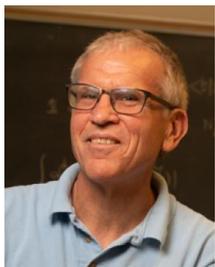
Theory
- *Density Functional Theory*
- *Many-Body Green's Functions*
- *Monte Carlo*
- *Superconductivity*

Computation
- *Electronic and Magnetic Properties*
- *Molecular Dynamics*
- *Spin Dynamics Simulations*
- *Optical Excited States*
- *Data Analytics, Classification Models, and ML Approaches*

Spectroscopies
- *ARPES*
- *Neutron Scattering*
- *Optical Spectroscopy*
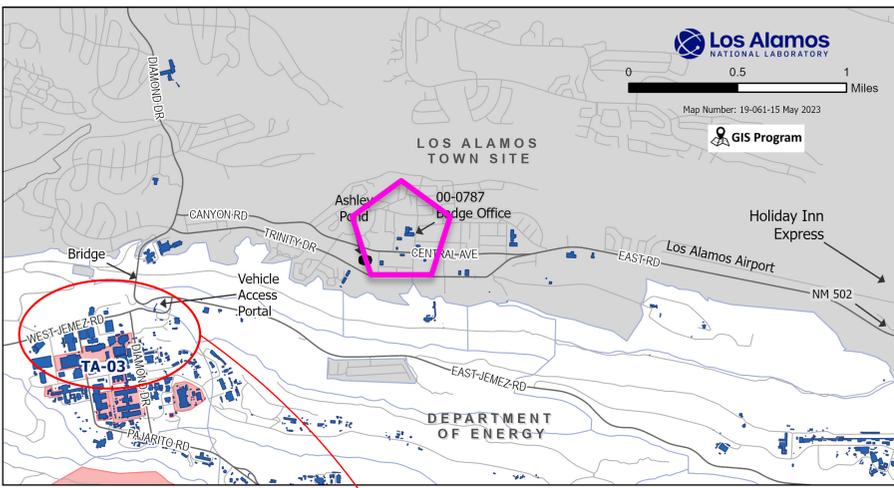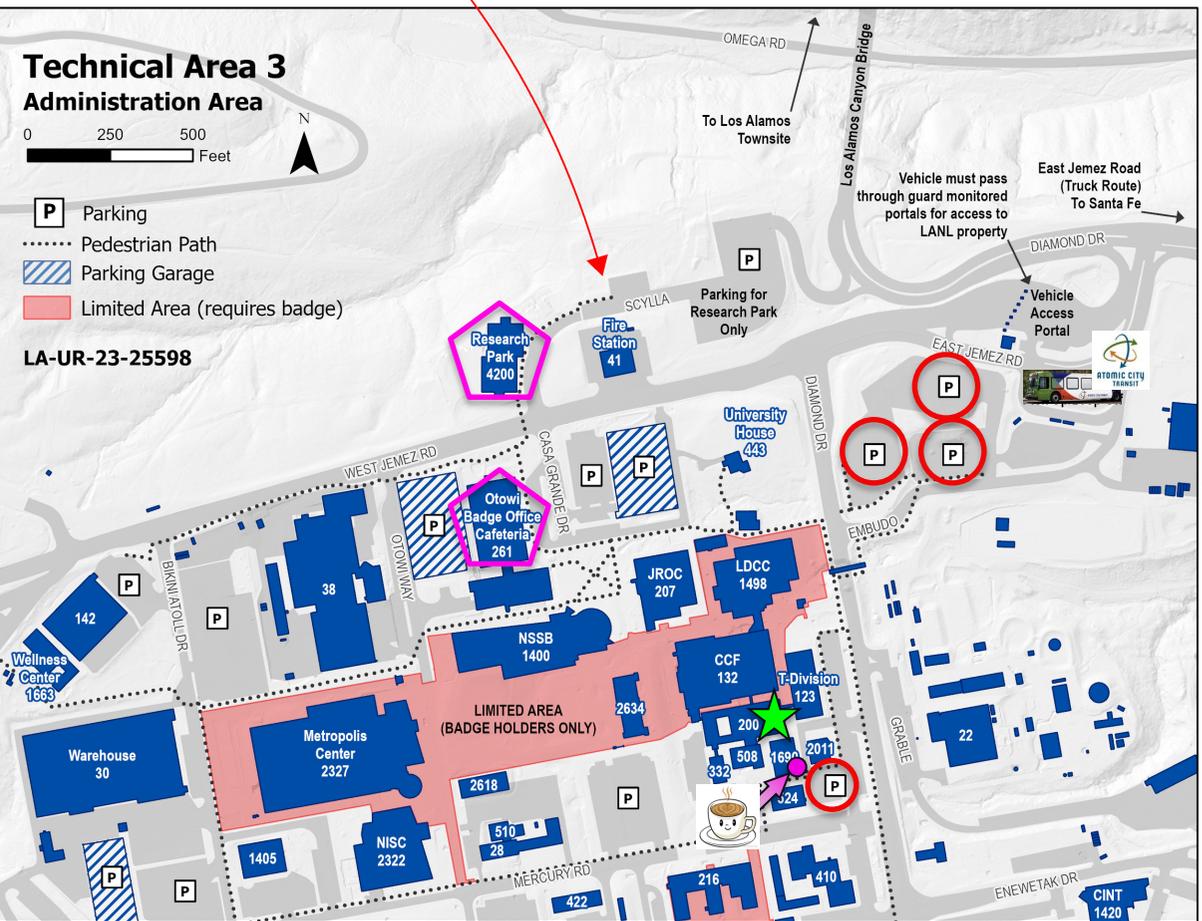- *Quantum Oscillations*
- *High Magnetic Fields*
- *STEM*

June 16, 2025

Summer School Schedule

Time	Sunday June 15, 2025	Monday June 16, 2025	Tuesday June 17, 2025	Wednesday June 18, 2025	Thursday June 19, 2025	Friday June 20, 2025	Saturday June 21, 2025
8:30		Badge Office	Determination of Electronic Structure: Solving the Kohn-Sham Equations	When Independent Particle Methods Fail: The Effect of Correlations	Many-Body Primer II: Spectral weight, Self-Energy, Quasiparticles, Hedin's Equations and Approximations	Theoretical Spectroscopy: Introduction and Overview	
9:00							
9:30							
10:00		Welcome	Break	Break	Break	Break	
10:30		Introduction to the Computational Condensed Matter School	Predicting Properties from First Principles I: Electronic and Magnetic Properties	Many-Body Primer I: Second quantization, Time evolution operator, Time-ordered product, Green's Function	Introduction to Classical and Quantum Monte Carlo	Theoretical Spectroscopy: Optical Spectroscopy	
11:00		Overview on Condensed Matter Physics & Quantum Materials					
11:30							
12:00		Lunch	Lunch & Poster Session	Lunch	Lunch	Lunch	Free Time
12:30							
13:00							
13:30							
14:00		Density Functional Theory: Fundamentals and Applications	Predicting Properties from First Principles II: Total Energy and Force Applications	Angle-resolved photoemission spectroscopy: introduction and applications	Facility Tour I: Los Alamos Neutron Science Center	Experimental Optical Spectroscopy	
14:30							
15:00							
15:30	Arrival & Check-In	Break	Break	Break		Break	
16:00		Hands-on: Introduction to High Performance Computing	Hands-on: Material Properties from DFT	Hands-on: DFT Electronic Bands, Success and Failure	Introduction to Classical and Quantum Monte Carlo Cont.	Hands-on: Optical Spectroscopy	
16:30							
17:00	Dinner	Hands-on: Bonding and the Hydrogen Molecule					
17:30							
18:00		Dinner	Dinner	BBQ	Dinner	Los Alamos Summer	

Time	Sunday June 22, 2025	Monday June 23, 2025	Tuesday June 24, 2025	Wednesday June 25, 2025	Thursday June 26, 2025	Friday June 27, 2025	Saturday June 28, 2025
8:30		Many-Body Primer III: Anderson impurity, DMFT, Embedding schemes	The Hunt for High-Tc Superconductivity: from Discovery to Breakthrough	LANL Institutes: CINT, IMS, & CNLS	ML/AI for Materials: Introduction and Overview	Distinguishing Different Types of Plastic Flow Using Position-and-Velocity Based Principal Component Analysis	
9:00							
9:30							
10:00		Break	Break	Break	Break	Break	
10:30		Electrons Behaving Badly: Experimental Techniques Applied to Electrical Insulators and Neutral Fermions	Low Hanging Fruit in Experimental Plutonium Science Made Sweeter by Computation	Dynamical Spin Response	ML/AI for Materials: Introduction and Overview Cont.	ML Architectures	
11:00							
11:30							
12:00	Free Time	Lunch	Lunch	Lunch	Lunch	Lunch	Departure
12:30							
13:00							
13:30							
14:00		Facility Tour II: Center for Integrated Nanotechnology & MPA-Quantum	Scanning Transmission Electron Microscopy	Neutron Scattering	Facility Tour III: National High-Magnetic Field Laboratory: Pulsed Field Facility	Hands-on XI: ML Architectures	
14:30							
15:00							
15:30			Break	Break		Break	
16:00		Hands-on: Dynamical Mean Field Theory	Hands-on: Superconductivity	Hands-on: Introduction to magnetism simulations using Sunny.jl	Hands-on X: Classification and Learning Models	Overview of Reimbursment Process	
16:30							
17:00						Closing Remarks	
17:30						Travel to Banquet	
18:00		Dinner	Dinner	Dinner	Dinner	Banquet	

U.S. DEPARTMENT OF ENERGY

LANL Campus & Key Locations

June 16, 2025

- Set up posters for the duration of the school

- Poster 'Flash Talks' (Poster Advertisement)
  - ➢ Just proceeding Lunch Tuesday June 17.

- Poster Session
  - ➢ 12 pm - 2 pm (During Lunch) Tuesday, June 17

https://www.etsy.com/people/minouette
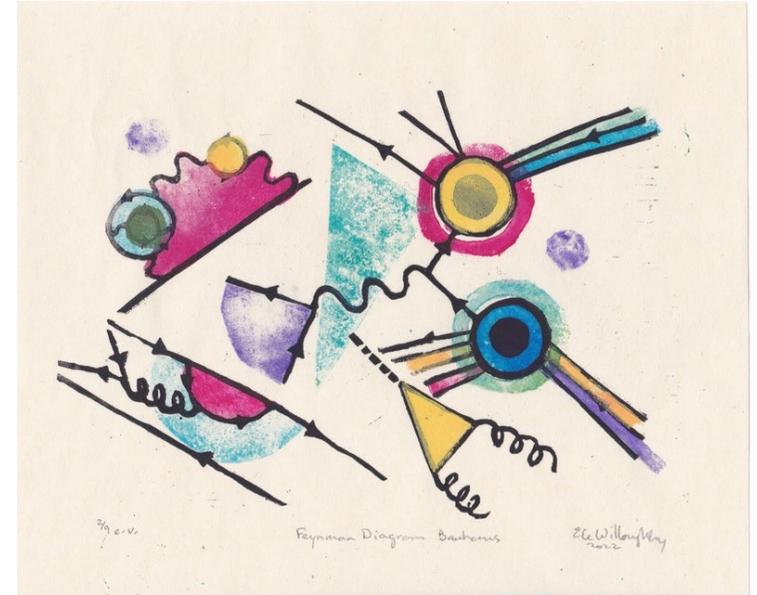
BBQ in North Mesa Park	Los Alamos Summer Concert	Banquet Dinner
Wednesday June 18th	Friday June 20th	Friday June 27th

Institute for
Materials Science

Center for Integrated
Nanotechnologies

Center for
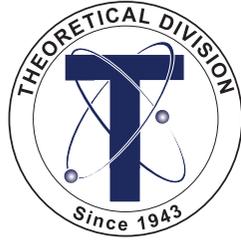Nonlinear Studies

Institute for Complex
Adaptive Matter

Thank You!

https://www.etsy.com/people/minouette

Christopher Lane

Elizabeth Peterson

Roxanne Tutchton

Ying Wai Li

Yue Huang

Johanna Palmstrom

Do not hesitate to reach out with any questions!

June 16, 2025