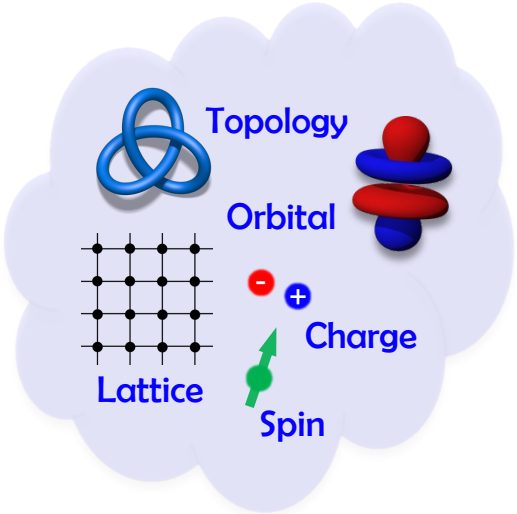
Los Alamos Computational Condensed Matter Summer School 2026

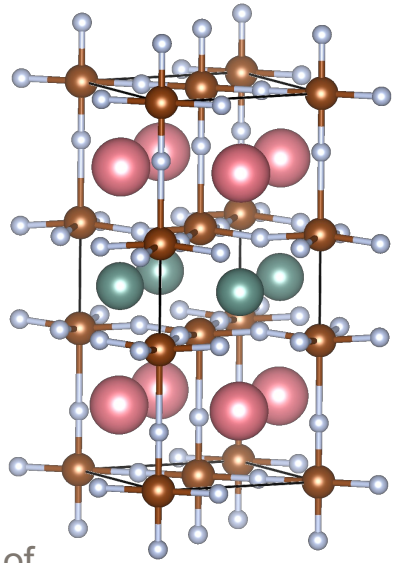
June 15, 2026

Quantum Materials: A Powerful Solution to Current Technological Challenges

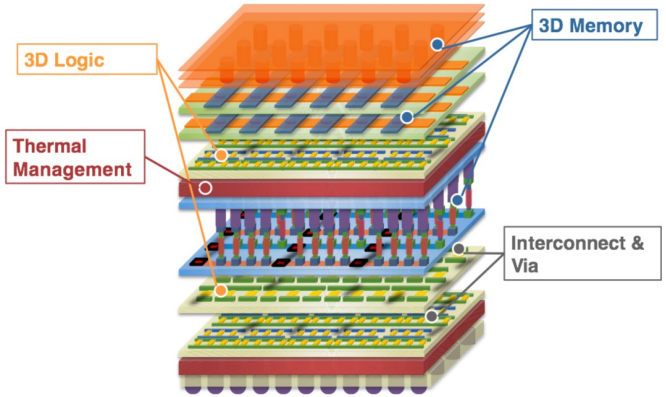
Fundamental Interactions



Materials



Devices



Discovery and Design of Novel Phases of Matter

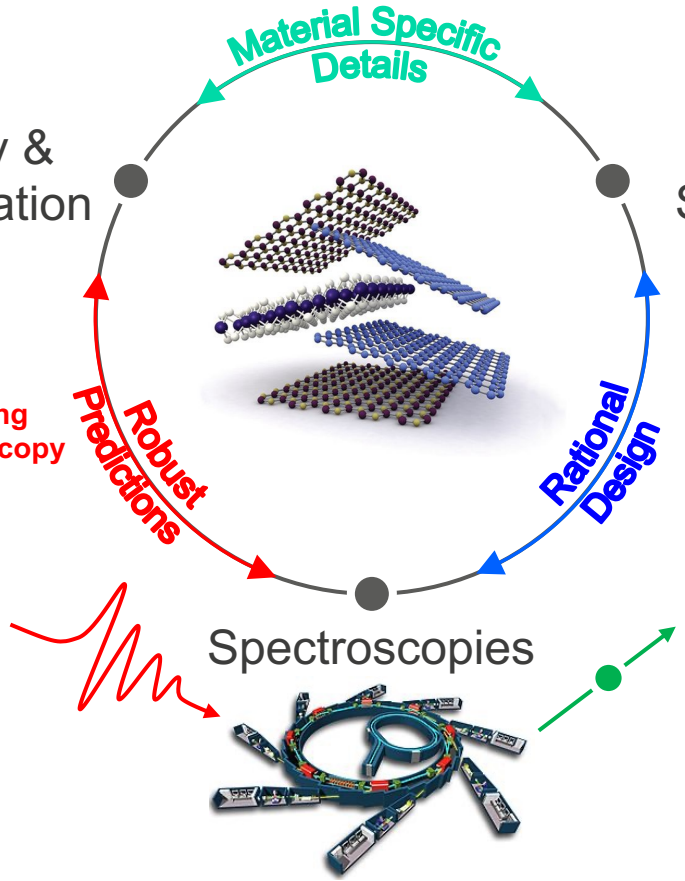
Design of Next generation Devices

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)

Co-Design Approach to Quantum Materials

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



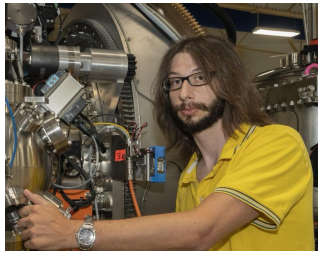
- ARPES
- Neutron Scattering
- Optical Spectroscopy
- RIXS
- STM/S

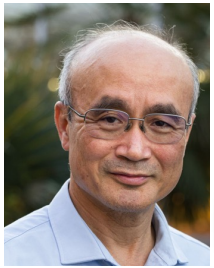
- Data Mining / Analytics
- Machine Learning
- Artificial Intelligence
- Property Optimization and Inverse Design

Students from Around the Nation and Abroad

Summer School Overview







Theory

- *Density Functional Theory*
- *Many-Body Green's Functions*
- *GW+BSE*
- *Dynamical Cluster Approximation*

Computation

- *Electronic and Magnetic Properties*
- *Molecular Dynamics*
- *X-ray Spectroscopy Simulations*
- *Optical Excited States*
- *ML Models, and AI Approaches*

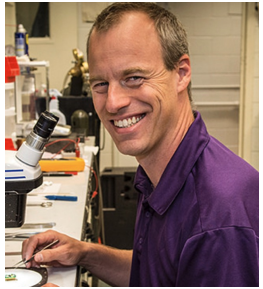
Spectroscopies

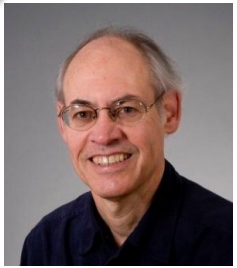
- *ARPES*
- *Optical Spectroscopy*
- *RIXS*
- *Pump-Probe THz*
- *Scanning probe + optical Microscopy*









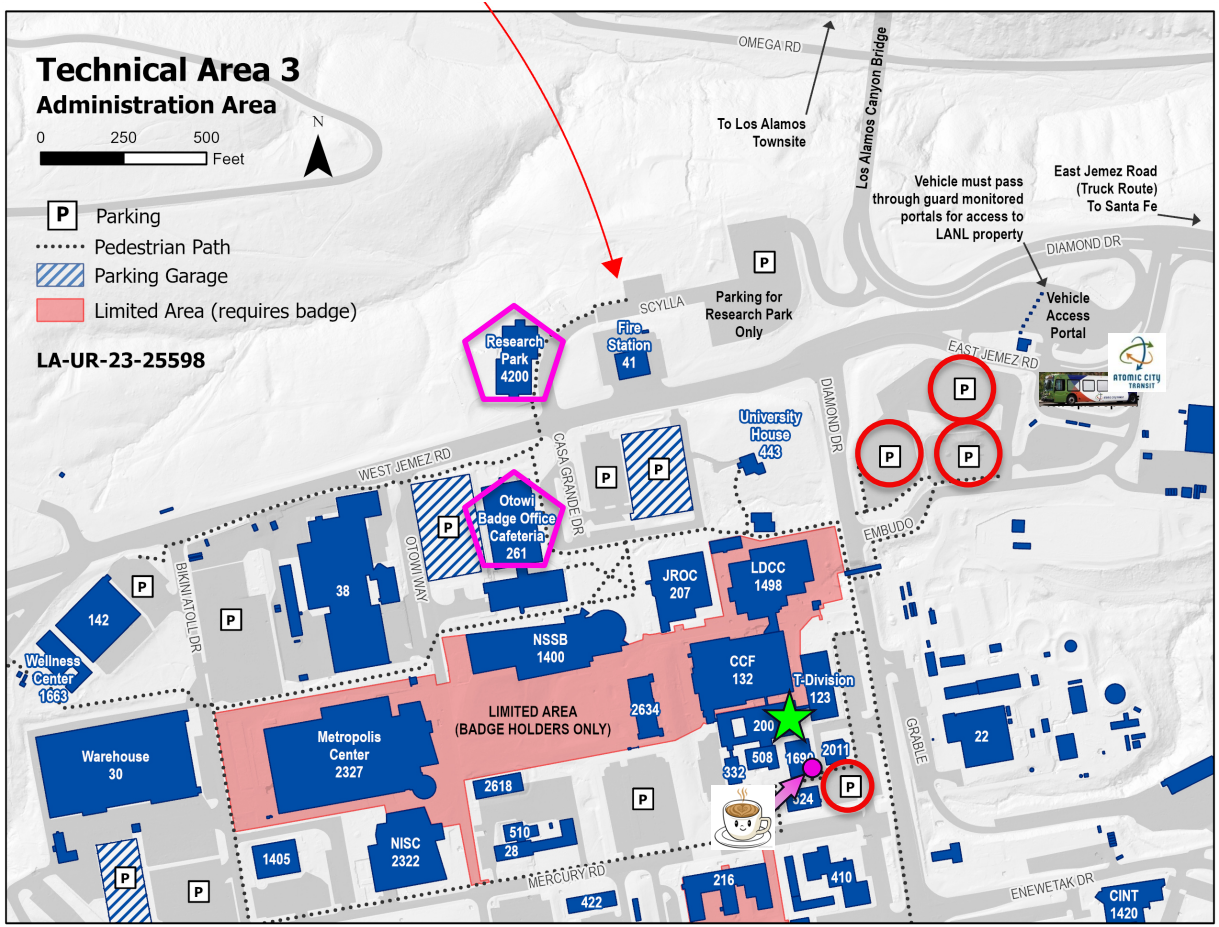


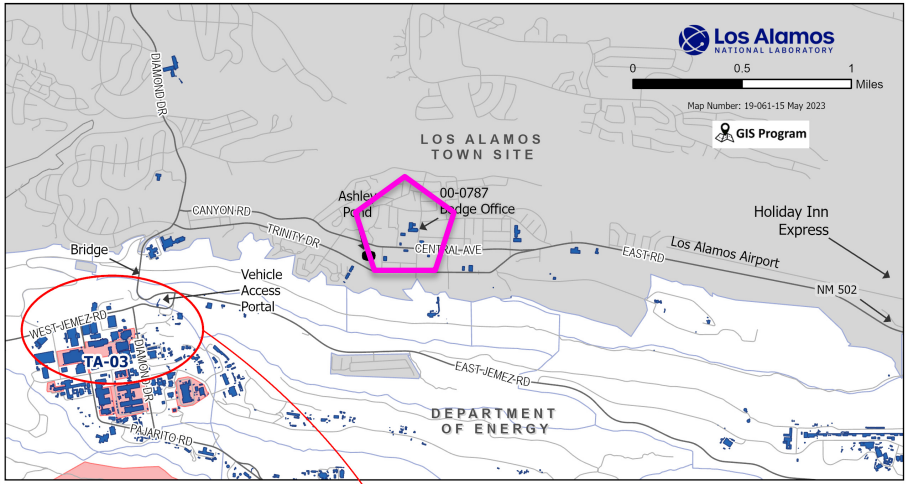
Summer School Schedule

Time	Sunday June 14, 2026	Monday June 15, 2026	Tuesday June 16, 2026	Wednesday June 17, 2026	Thursday June 18, 2026	Friday June 19, 2026	Saturday June 20, 2026
8:30		Badge Office and Account Setup	Predicting Properties from First Principles I: Electronic and Magnetic Properties	When Independent Particle Methods Fail: The Effect of Correlations	Many-Body Primer III: Green's Functions, Spectral Weight, Self-Energy	Overview of Theoretical Spectroscopy	Free Time
9:00							
9:30				Many-Body Primer I: Second Quantization			
10:00			Break	Break	Break	Break	
10:30			Determination of Electronic Structure: Solving the Kohn-Sham Equations	Many-Body Primer II: Second Quantization Cont., Time Evolution Operator, Time-Ordered Product	Many-Body Primer IV: Quasiparticles, Hedin's Equations and Approximations	Ab initio Theoretical Optical Spectroscopy and the Bethe-Salpeter Equation (BSE)	
11:00							
11:30		Lunch					
12:00			Lunch & Poster Session	Lunch	Lunch	Lunch	
12:30							
13:00		Welcome					
13:30		Introduction to the Computational Condensed Matter School	Predicting Properties from First Principles II: Total Energy and Force Applications	Facility Tour: Los Alamos Neutron Science Center	Many-Body Primer V: Models, DMFT, and Embedding Schemes	Experimental Tutorial: Optical Spectroscopy	
14:00		Overview on Condensed Matter					
14:30		Break					
15:00		Density Functional Theory: Fundamentals and Modern Developments	Break		Break	Break	
15:30	Arrival & Check-In		Hands-on: Material Properties from DFT I	Hands-on: Material Properties from DFT II	Hands-on: Green's Functions and Self-Energy Corrections	Hands-on: Computing the Optical Absorption Spectrum of Si	
16:00							
16:30							
17:00	Dinner	Dinner	Dinner	BBQ at North Park	Dinner	Los Alamos Summer Concert Series	

Time	Sunday June 21, 2026	Monday June 22, 2026	Tuesday June 23, 2026	Wednesday June 24, 2026	Thursday June 25, 2026	Friday June 26, 2026	Saturday June 27, 2026
8:30	Free Time	Experimental Tutorial: Angle-Resolved Photoemission Spectroscopy	Theoretical X-ray Spectroscopy: Fundamentals and Applications	LANL Institutes: CINT, IMS, & CNLS	Overview of ML/AI for Materials	ML/AI for Material Discovery	Departure
9:00							
9:30							
10:00		Break	Break	Break	Break	Break	
10:30		The Dynamical Cluster Approximation	Advances in Theoretical X-ray Spectroscopy	Experimental Tutorial: Combining Scanning Probe and Optical Microscopy	AI/ML Architectures	ML/AI for Material Inverse Design	
11:00							
11:30							
12:00		Quantum and Condensed Matter Physics Group Picnic	Lunch	Lunch	Lunch	Lunch	
12:30							
13:00							
13:30		Facility Tour: Center for Integrated Nanotechnology	Experimental Tutorial: Resonant Inelastic X-ray Scattering (RIXS)	Experimental Tutorial: Pump-Probe THz Spectroscopy	Facility Tour: National High-Magnetic Field Laboratory: Pulsed Field Facility	Hands-on: Inverse Design	
14:00							
14:30							
15:00			Break	Travel to Hike		Break	
15:30		Hands-on: The Dynamical Cluster Approximation	Hands-on X-ray Spectroscopy with FEFF10	Hike and Picnic	Hands-on: AI/ML Architectures	Feedback Survey	
16:00						Overview of Reimbursement Process	
16:30							
17:00		Dinner	Dinner		Dinner	Closing Remarks	
17:30						Travel to Banquet	
18:00						Banquet	

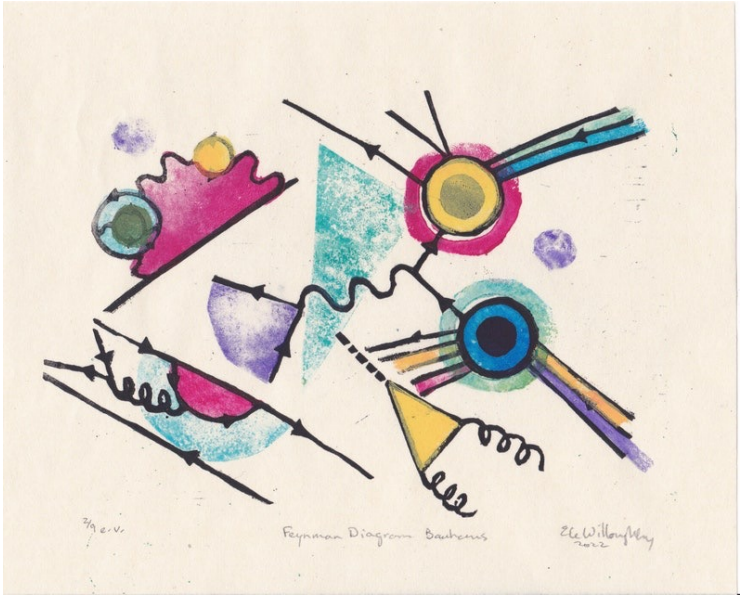
LANL Campus & Key Locations





Posters

- Set up posters for the duration of the school
- Poster ‘Flash Talks’ (Poster Advertisement)
  - Just proceeding Lunch Tuesday June 16.
- Poster Session
  - 12 pm – 1:30 pm (During Lunch) Tuesday, June 16



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

Special Events

BBQ in North Mesa Park

Wednesday
June 17th

Los Alamos Summer Concert

Friday
June 19th

Hike and Picnic

Wednesday
June 24th

Banquet Dinner

Friday
June 26th

Sponsors

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

Organizing Committee

Christopher Lane

Elizabeth Peterson

Roxanne Tutchton

Ying Wai Li

Andrew Jones

Alessandro Mazza

Do not hesitate to reach out with any questions!