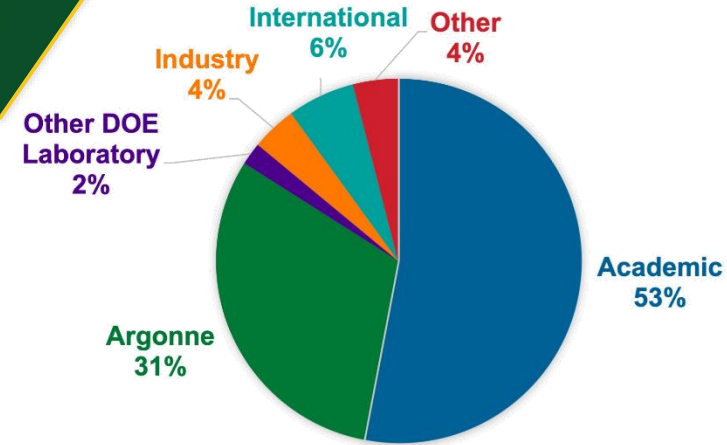
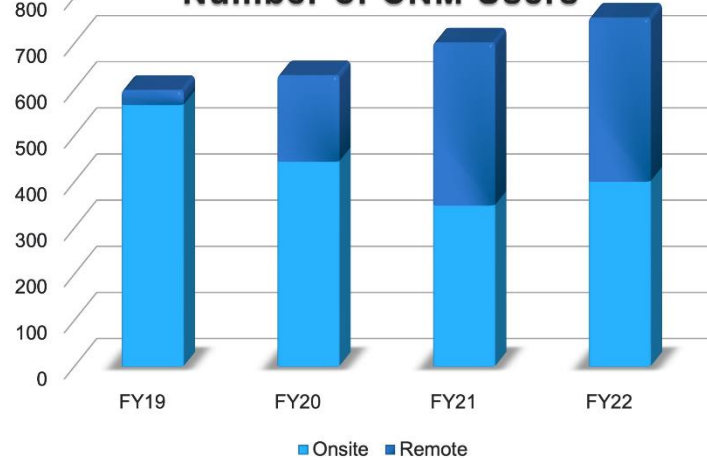


# Center for Nanoscale Materials (CNM) at Argonne

CNM USER AFFILIATION



Number of CNM Users



~300 peer-reviewed publications per year, 55% IF>7 (FY22)

Yearly recap and renewal of instrumentation: ~\$2.5M

MIE Recap: ~\$12M

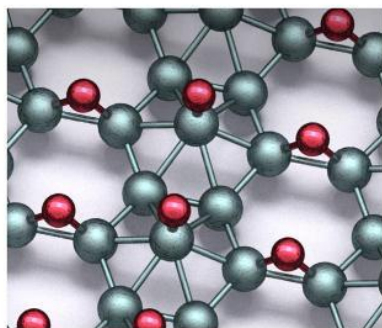
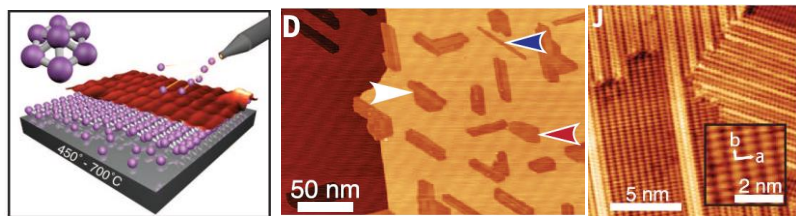
**Ilke Arslan, CNM Director**

Leverage Argonne's DOE User Facilities:

- APS-U (\$800M project, ~100X brilliance in one year – first light in April 2024, entirely new experiments will be possible at CNM Beamline
- Aurora: \$500M exascale computer, a greater diversity of workloads, including machine learning and data-intensive tasks, in addition to traditional simulation and modeling campaigns.

# CNM Scientific Impact

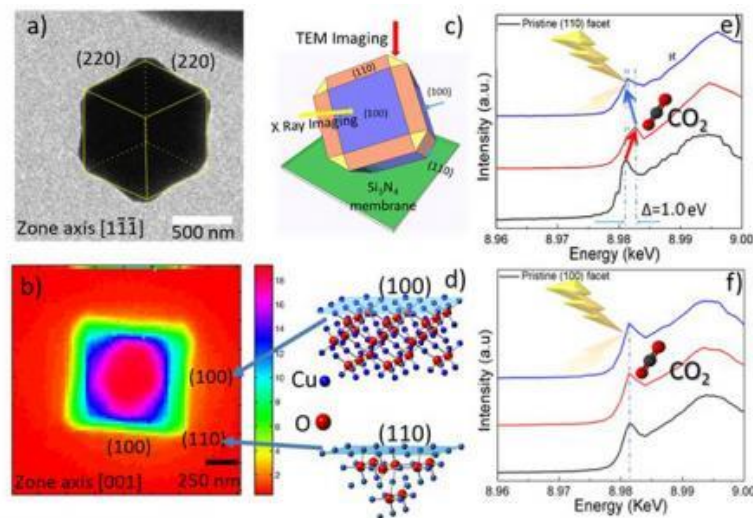
## Discovery of Borophene and Borophane



- First experimental growth and measurement of previously theoretically predicted properties of borophene, with an international team led by the CNM.
- Theoretical modeling on borophane done at CNM, in collaboration with our users at Northwestern.

*Science* **350**, 1513 (2015); *Science* **371**, 1143 (2021)

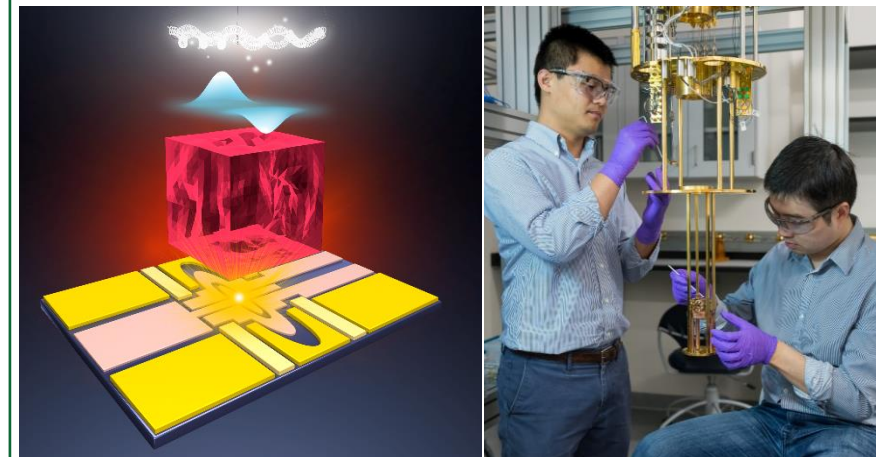
## Selective photocatalytic reduction of CO<sub>2</sub> into methanol fuel



- Single-nanoparticle multimodal *operando* and photoactivated measurements of same exact particle with same holder across TEM and Hard X-ray Nanoprobe used to identify the facet-specific sites in Cu<sub>2</sub>O catalyst capable of selectively reducing CO<sub>2</sub>.
- An internal quantum yield of 70% was determined for the photocatalytic conversion of CO<sub>2</sub> to liquid fuel methanol.

*Nature Energy* **4**, 957 (2019)

## A New Qubit Platform

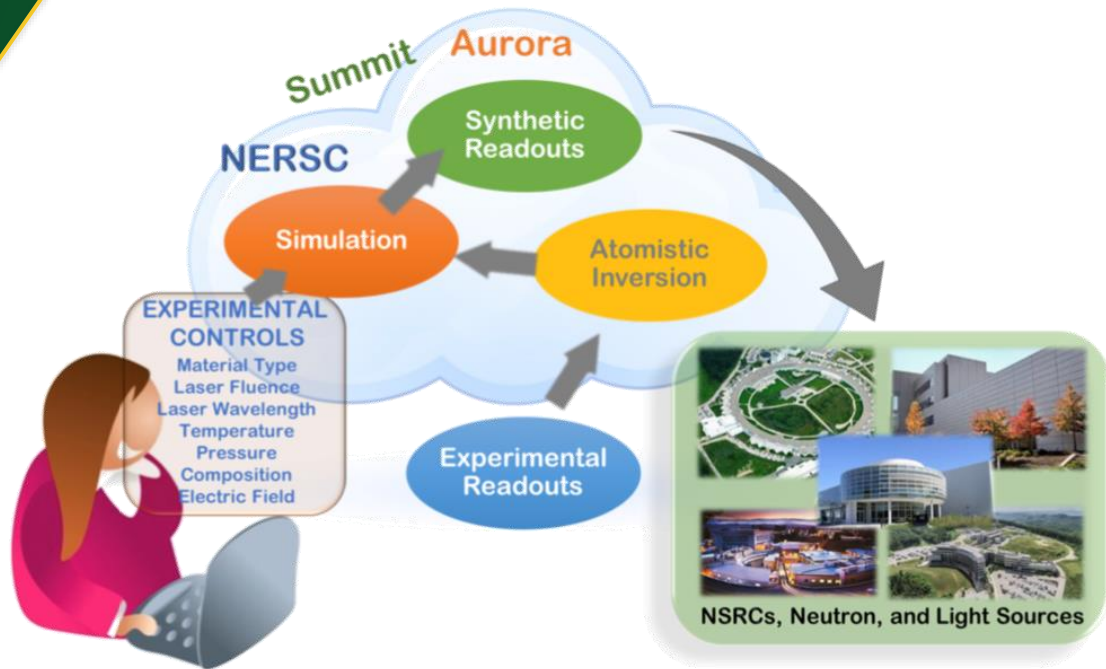


- New qubit platform: Electrons from a heated light filament (top) land on solid neon (red block), where a single electron (represented as a wave function in blue) is trapped and manipulated by a superconducting quantum circuit (bottom patterned chip).
- Relaxation times of 15 μs and phase coherence time over 200 ns were measured in this paper, with subsequent measurements of considerably longer relaxation and coherence times.
- This new qubit platform could transform QIS&T by simultaneously embodying long coherence, fast operation, and large scalability.

*Nature* **605**, 46 (2022)



# Synergy with User Facilities: Digital Twin for Spatiotemporal Experiments



- AI solutions to the inverse problem, i.e., information extraction from time-resolved experiments
- AI/ML Guided multi-fidelity bridging for physically accurate & efficient dynamical simulations
- Shared workflows for seamless information exchange between models and experiments

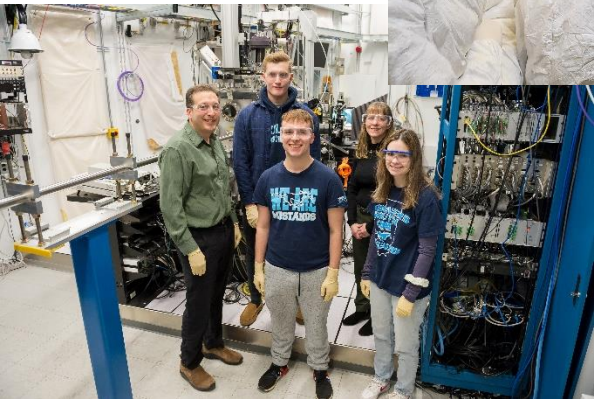
Digital Twin for *In-silico* Spatiotemporal Experiments

Experimental Controls	Experimental Input at time $t_0$	AI Inversion	Digital Simulation	Job Submission	Synthetic Read-out
Material Type: <input type="text" value="Hybrid"/> Composition: <input type="text" value="Al2O3, Au, thiol"/> Temperature: <input type="text" value="1000"/> K Pressure: <input type="text" value="10"/> GPa Laser Fluence: <input type="text" value="2"/> J cm <sup>-2</sup> Laser Wavelength: <input type="text" value="650"/> nm Electric Field: <input type="text" value="1"/> V cm <sup>-1</sup> <input type="button" value="Add Control"/>	CDI  TEM  XPCS  SANS  <input type="button" value="Load Input"/>	   <input type="button" value="Setup"/>	<b>Scale Bridging:</b> <input type="button" value="Model Selection"/> <input type="button" value="Training Data"/> <input type="button" value="AI Optimization"/> <b>Simulations:</b> <input type="radio"/> AIMD <input checked="" type="radio"/> Atomistic MD <input type="radio"/> CG MD <input type="radio"/> Reinforcement Learning <input type="button" value="Setup Simulation"/> <input type="button" value="Uncertainty Quantification"/> <input type="button" value="Add module"/>	<input type="button" value="Leadership Computing"/> <input checked="" type="radio"/> NERSC <input type="radio"/> Aurora <input type="radio"/> Summit <input type="button" value="Mid-Level Computing"/> <input type="radio"/> Carbon <input type="radio"/> CADES <input type="button" value="Submit"/>	    <input type="button" value="Export"/>

Processing ... 80%

**Collaboration Across Scientific User Facilities:  
CNM, CNMS, MF, CFN, CINT, APS, ALS, SLAC**

# Strengths and Initiatives for CNM User Community



## Strengths of our User Community:

- Training the next generation of STEM Scientists and Engineers
  - Exemplary Student Research Program (high school students)
  - DOE SCGSR Students (graduate students)
  - DOE SULI Students (undergraduate students)
  - GEM Fellowship students, promoting graduate education for minorities.
- Good balance of remote users with 60 different tools and 75 associated computers remotely accessible for tool operation and data analysis in FY22
- Strong engagement with other DOE initiatives: JCESR, Q-NEXT, EFRCs, CMB-S4

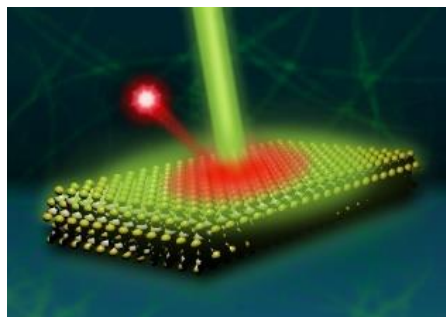
## Current and Future Initiatives:

- Grow users from underrepresented groups, MSIs by giving talks at specific universities, joining MSI specific professional groups, information on how to submit a successful proposal
- Target outreach to MSIs Outreach engagement to promote future scientists and nanoscience with local community (Conferences for Undergraduate Women in Physics (CUWiP) and Science Careers in Search of Women, Nanoscience 101)
- Forming partnerships for RENEW, FAIR, Energy Earthshots, BRaVE, etc.
- Industry Collaboration Committee (ICC) formed to increase industry users
  - Reach out to targeted regional, national and international industry community with capabilities and expertise that are suitable for industry
  - Inviting speakers to CNM colloquium from start-ups and reputed industries
  - Based on feedback from Industry/UEC, propose tools to acquire at CNM that are requested by industry



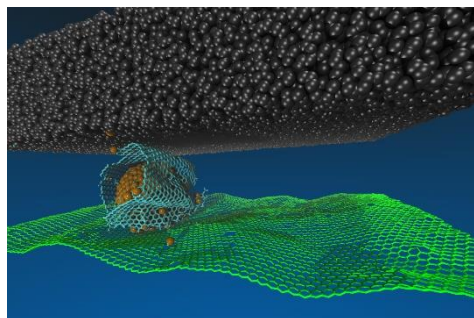
# Future Scientific Opportunities

Quantum coherence by design



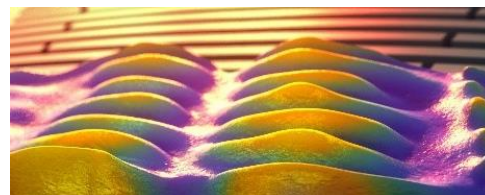
*Quantum Emitters*

Interfaces, assembly and fabrication for emergent properties



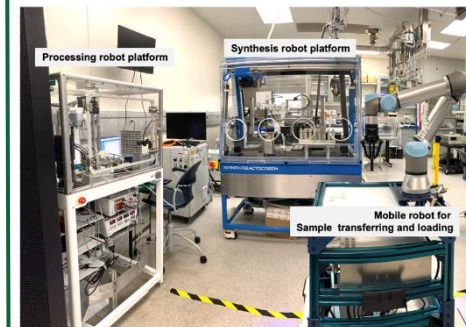
*Macro-scale superlubricity*

Ultrafast dynamics and non-equilibrium processes



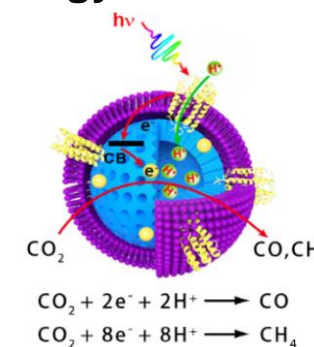
*Visualizing lattice dynamics of acoustics in excited materials*

AI/ML-accelerated analytics and automation



*Autonomous Discovery enabled by AI/ML*

Nanoscale discovery for a sustainable energy future



*Cell-mimic assembly for CO<sub>2</sub> reduction*

*All themes utilize expertise in synthesis, fabrication, characterization and theory*