MATERIALS PRIORITIES AT ARGONNE NATIONAL LABORATORY

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Materials and Chemistry Lead

UChicago ▸ Argonne LLC
U.S. DEPARTMENT OF ENERGY
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.
Argonne NATIONAL LABORATORY

Argonne accelerates science and technology for U.S. prosperity and security

- Pivotal discoveries
- Innovative collaborations
- Unparalleled facilities

DIVERSIFIED RESEARCH PORTFOLIO

$1.02 Billion in FY2020

End-to-end, from discovery to application

User facilities integrated with our research

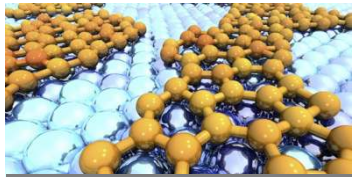
Collaborations within and outside Argonne

ARGONNE IS FOCUSED ON SOLVING BIG PROBLEMS IN SCIENCE AND ENGINEERING

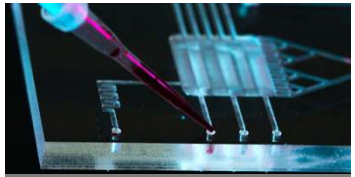
MAJOR INITIATIVES

Hard X-ray Science

Advanced Computing



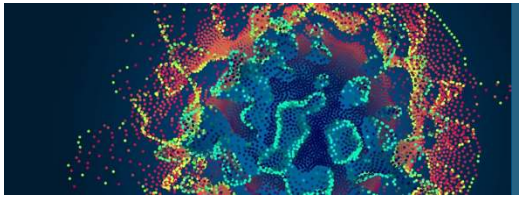
Materials and Chemistry



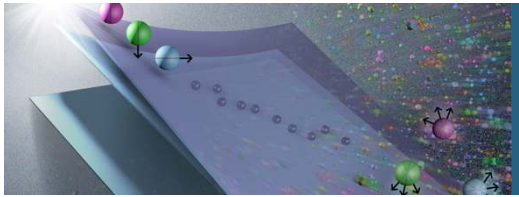
Manufacturing Science & Engineering

Universe as Our Lab

EMERGING INITIATIVES



Artificial Intelligence for Science



Quantum Information Science

ARTIFICIAL INTELLIGENCE FOR SCIENCE

In ten years …

Learned models begin to replace data

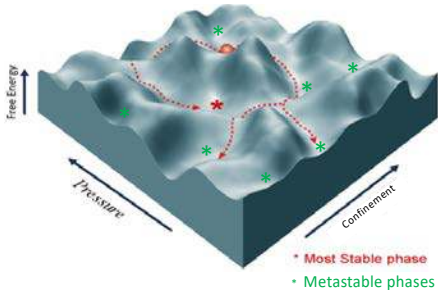
Experimental discovery processes change dramatically

Many questions are pursued semi-autonomously at scale

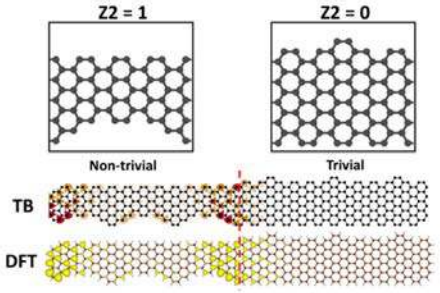
Simulation and AI approaches merge

Theory becomes data for next-generation AI

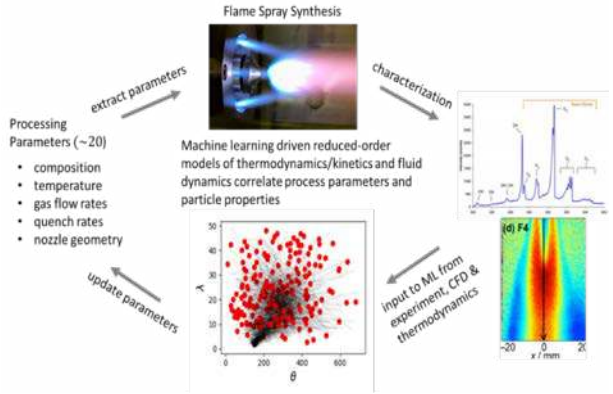
AI + MATERIALS PORTFOLIO



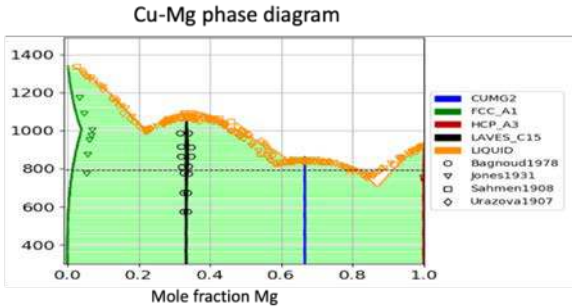
Energy Landscapes



Design of Topological Matter



Process Control

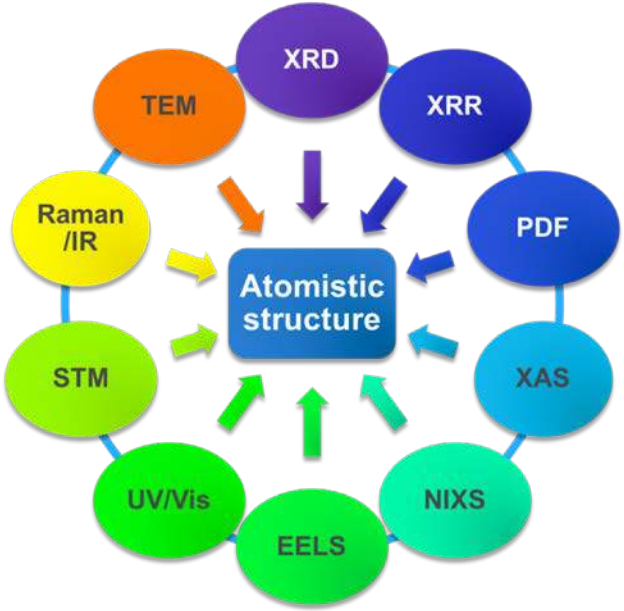


Phase Diagrams

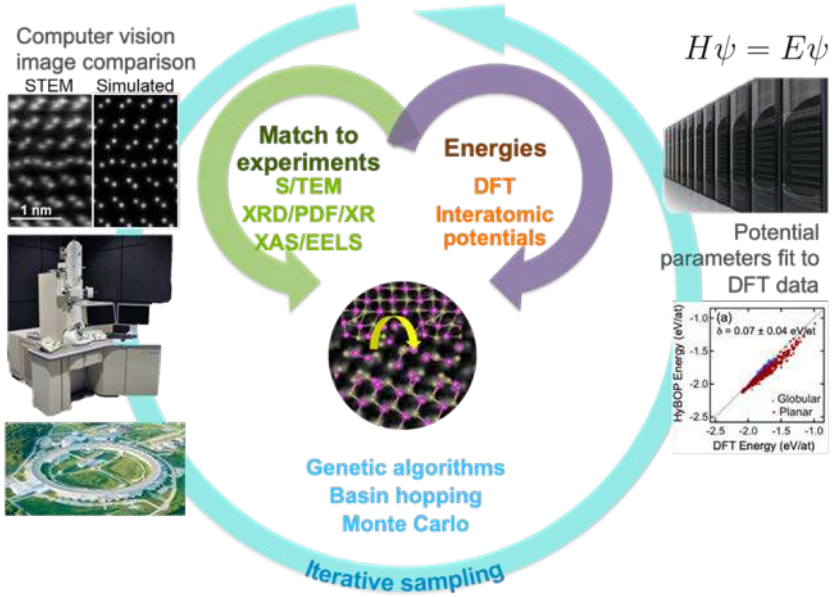
- Image analysis
- X-ray spectroscopy
- Battery lifetime prediction

$4.4 M lab internal investment over 2 years

FANTASTX



Multimodal Data Streams



- Use AI to automate search, learning, and pattern matching
- Use physics to restrict atomic structures to viable solutions

Maria Chan, NST

EXASCALE + AI

Coming in 2021

Early Science

Exascale Computational Catalysis PI: David Bross, Argonne	**Accelerated Deep Learning Discovery in Fusion Energy Science** PI: William Tang, PPPL	**Virtual Drug Response Prediction** PI: Rick Stevens, Argonne

QUANTUM INFORMATION SCIENCE

Chicago Quantum Exchange

Materials discovery for next-generation QIS devices

Quantum sensing

Quantum networking

Computational techniques

CHICAGO QUANTUM EXCHANGE

IBM

HRL LABORATORIES

ColdQuanta

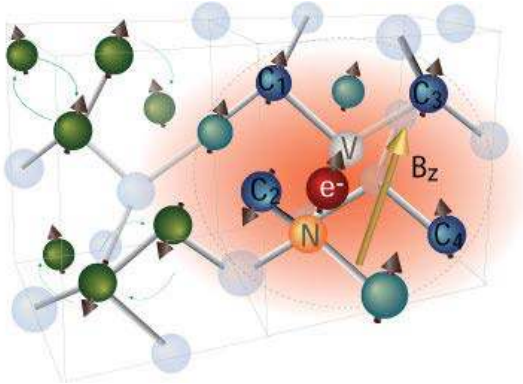
rigetti

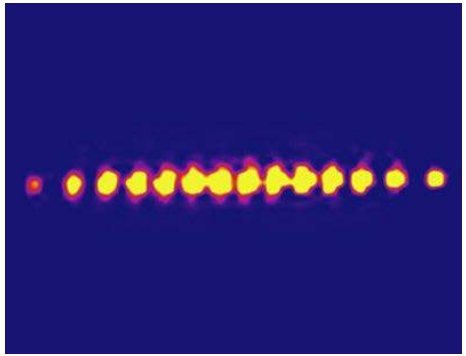
APPLIED MATERIALS make possible

Quantum Opus

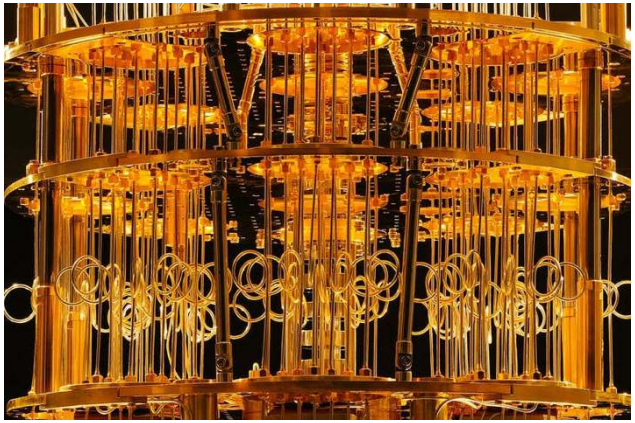
- Lab - University - Industry quantum consortium
- Materials — Devices — Systems
- National Quantum Initiative Hub

QUANTUM NETWORKING





QUANTUM NETWORKING



IBM 53-qubit
quantum computer

QUANTUM NETWORKING

Quantum Network

QUANTUM NETWORKING

- 30 mile Chicago area quantum fiber network, node at Argonne
- Study quantum entanglement in a long-distance fiber network under “real-world” operating conditions
- Generate long distance entanglement in **solid-state matter qubits** with high fidelity and throughput
- **Materials agnostic testbed for fundamental quantum information science:** decoherence, channel capacity, entanglement fidelity, non-locality, quantum noise and errors

Argonne node fiber network box

BlueFORS 7 mK dilution refrigerator

Sutter Instruments P-2000 laser-based fiber puller

POLYMER INNOVATION

AI-driven experimental laboratory

Processes to upcycle homogeneous plastic waste

Processes to efficiently transform mixed plastic waste

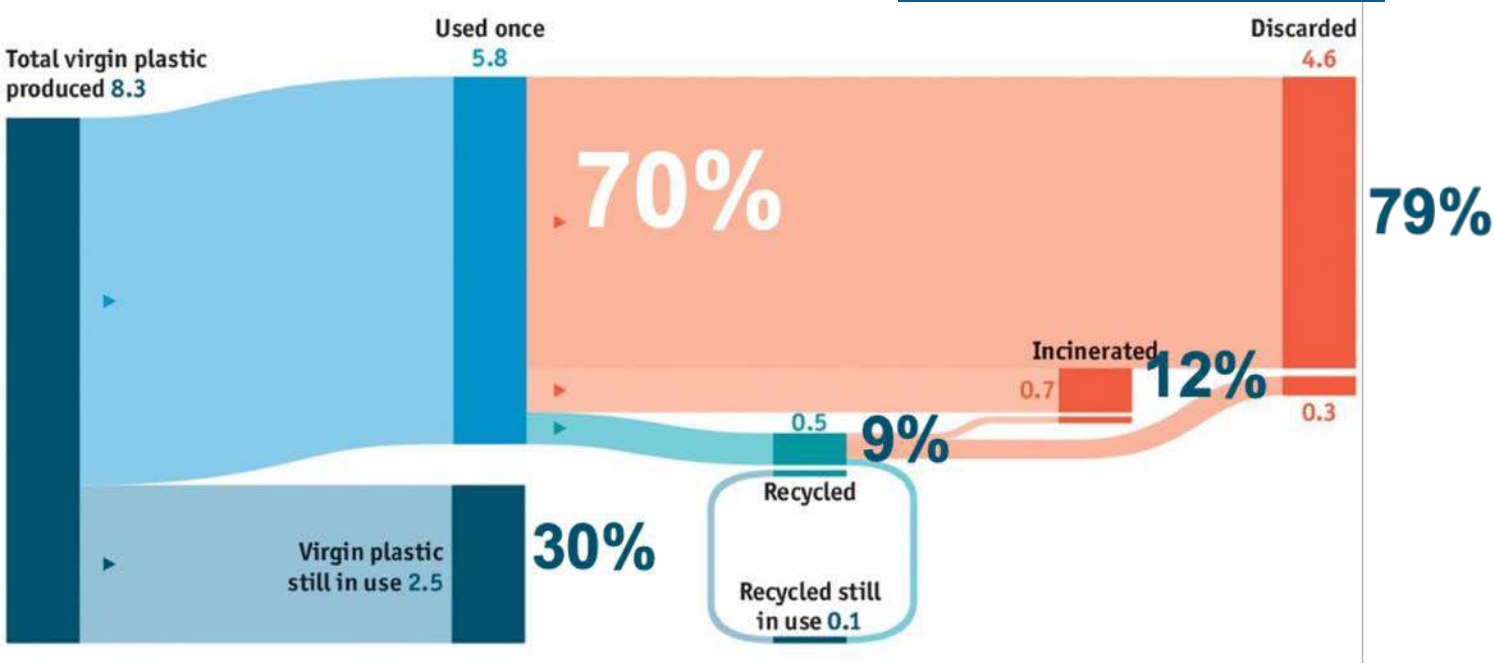
New polymers that minimize waste via chemical circularity

Deeper insights into polymer chemistry and properties

THE PROBLEM

THE PROBLEM

<10% recycled



Source: "Production, use, and fate of all plastics ever made" by R. Geyer et al., Science Advances, 2017

ARGONNE'S APPROACH TO DEALING WITH THE PLASTIC PROBLEM

Design plastics for recycling

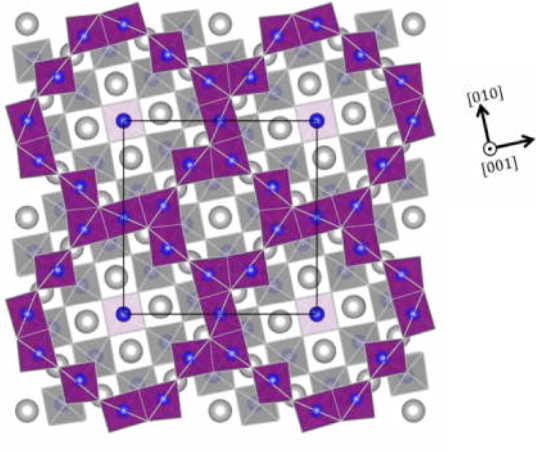
Find inexpensive ways
to **separate mixtures** of plastics

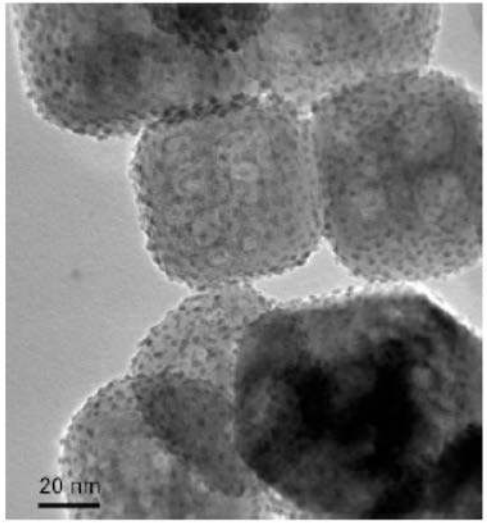
Innovate new ways
to **deconstruct plastics**

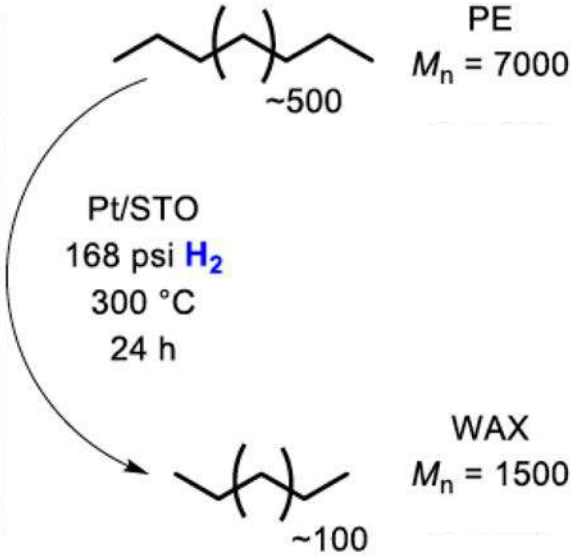
Study environmental impact
of plastic waste

Chopping Polyethylene

Polyethylene Chopping Performance over Supported Platinum Nanoparticle Arrays on Strontium Titanate





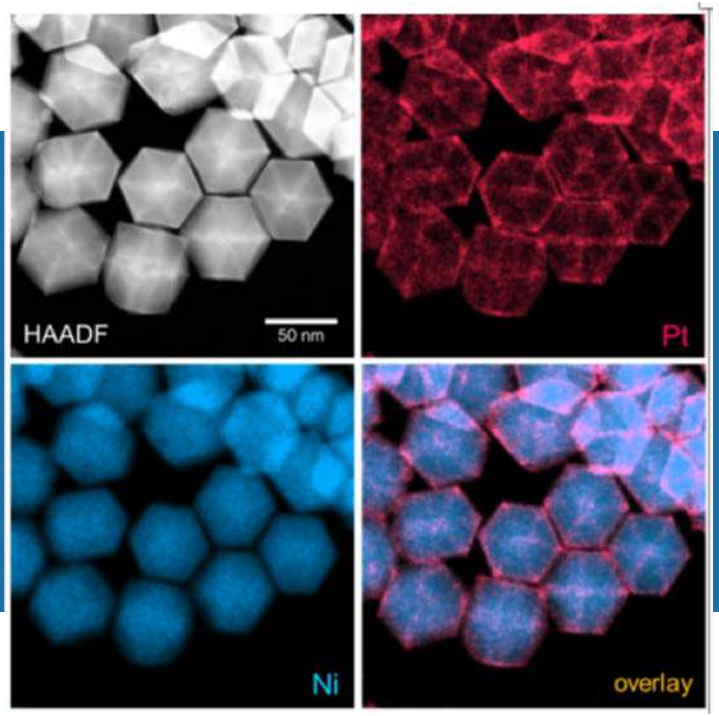


STO nanocrystals treated by ALD

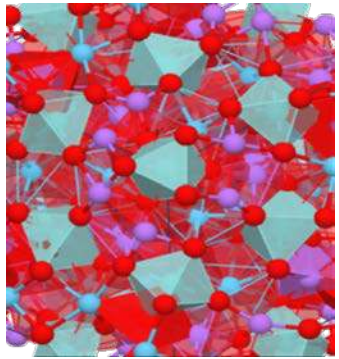
MANUFACTURING SCIENCE AND ENGINEERING

Innovative, high-performance materials offer the potential to transform energy technology

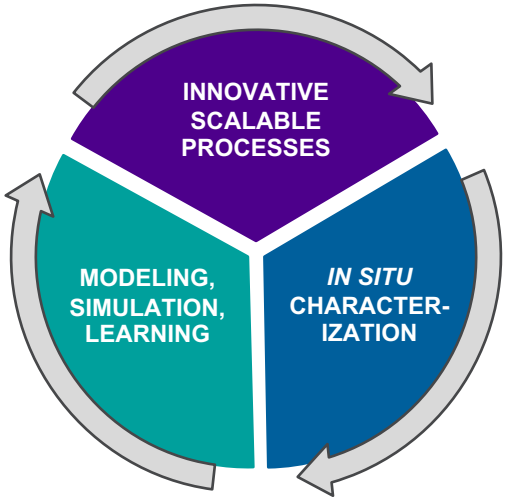
To realize this potential, radically new process technologies are essential



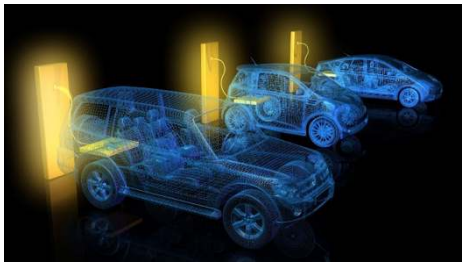
A SCIENCE-BASED APPROACH TO MANUFACTURING



Discovery Science



Scale-up and Manufacturing Process Development



Devices, Systems, and Commercial Technologies

These are highly specialized capabilities requiring unique, co-located facilities and expertise

MANUFACTURING ENGINEERING RESEARCH FACILITY (MERF)

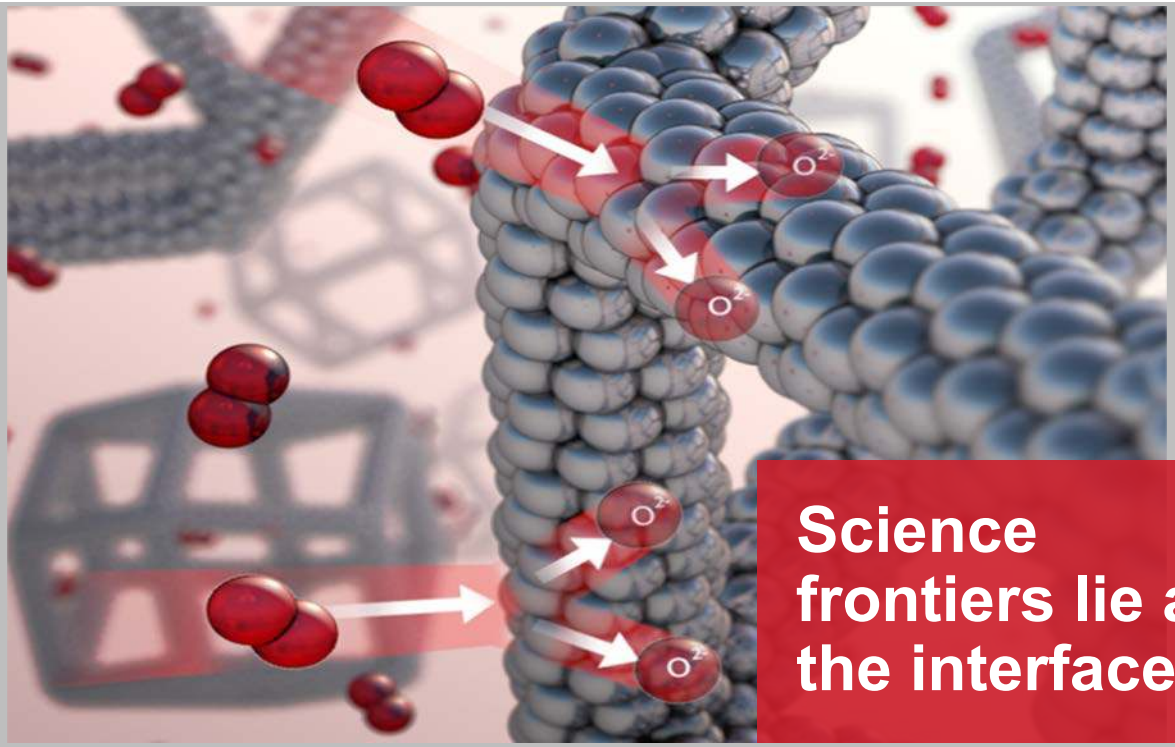
MERF capabilities include:

- Evaluation of emerging manufacturing technologies
- Scale-up of newly discovered materials
- Analysis and refinement of processes for materials synthesis
- Providing kilogram quantities of novel materials to industry for testing
- Development of analytical methods and quality control procedures for new material specifications

MATERIALS AND CHEMISTRY

Rules-Based Approach

- **Science begins with synthesis.**
- Watch and learn
- Growing smarter



Rules-Based Approach

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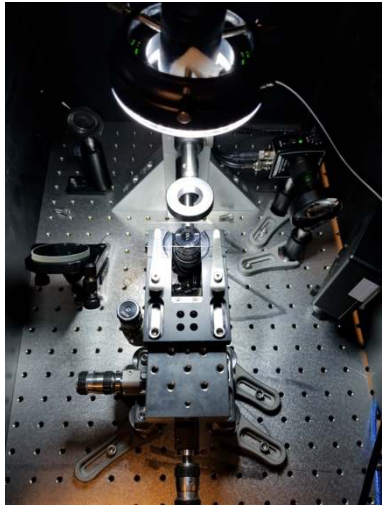
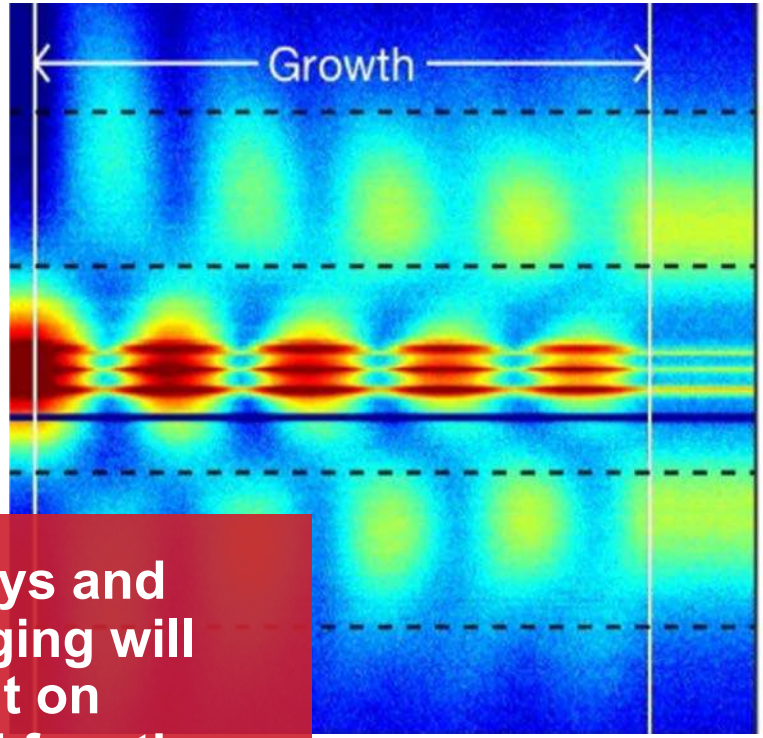


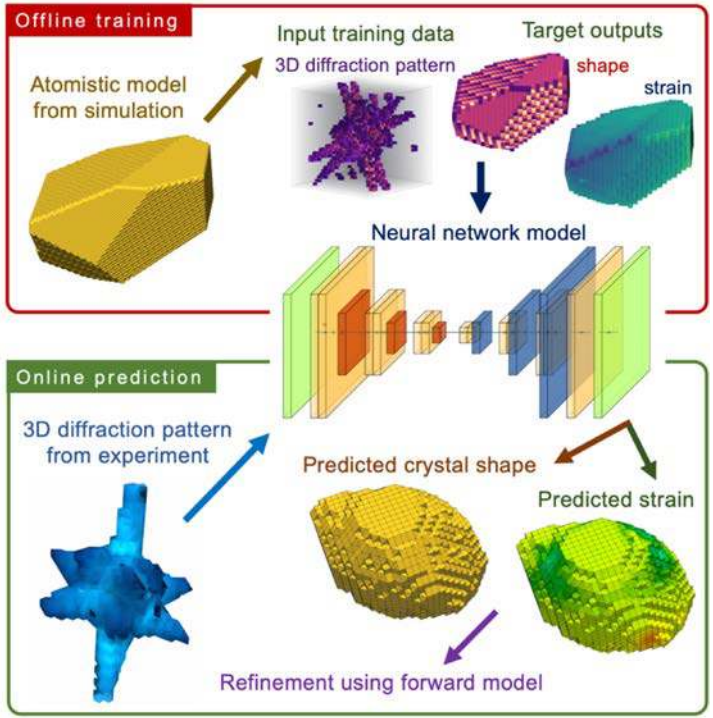


Coherent x-rays and quantum imaging will shed new light on synthesis and function.

Rules-Based Approach

- Science begins with synthesis
- Watch and learn
- **Growing smarter**

AI and data science are poised to revolutionize how we discover and understand matter.



SCIENCE INVESTMENTS

Interfacial Processes:

Ion Transport in Heterogeneous Materials: Using coherent x-rays to probe structure and dynamics of ion motion in liquids and solids

Defect Assemblies and Interactions:

Advanced Characterization of Polytipic SiC for Quantum Technologies: Designing in situ x-ray reactor for SiC growth studies

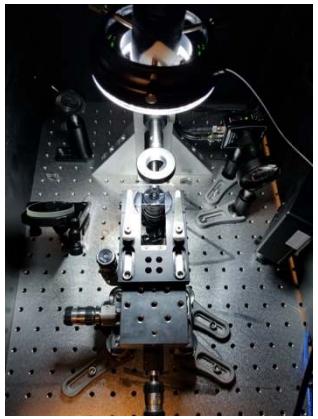
Multiscale Correlations and Hierarchies in Solutions:

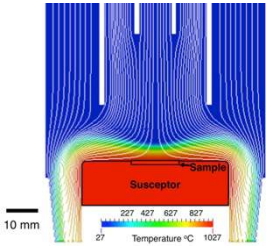
Coupling Data Science and in situ multimodal probes for Materials Synthesis: Predicting and following synthesis and crystallization pathways from melts

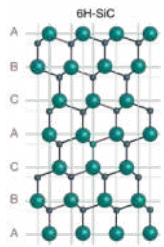
Quantum Materials:

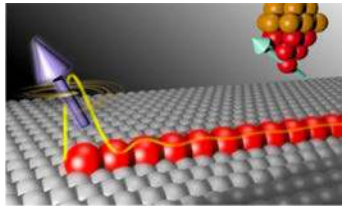
Ultrafast Time-resolved Quantum Ghost Imaging: Using entangled photons to explore dynamic processes via pump-probe

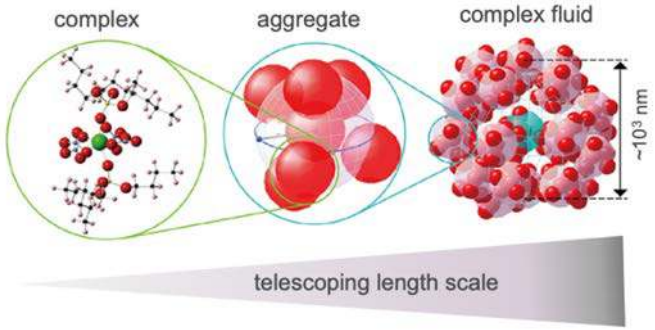
Atomic Synthesis of Artificial Lattices for Quantum Simulation: Creating quantum simulators from precision-placed atoms



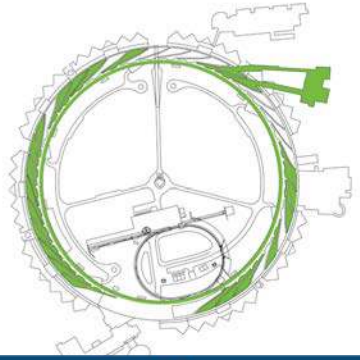


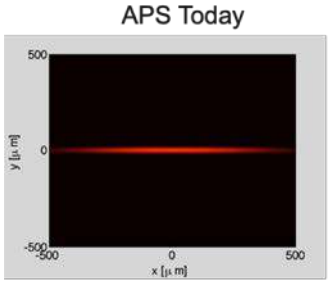




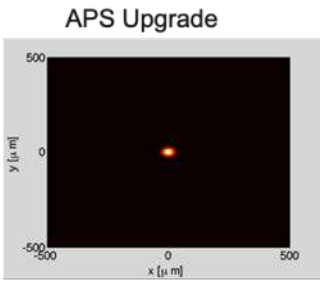


APS-UPGRADE: COHERENT X-RAYS





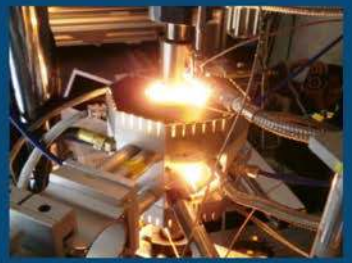
ε_o = 3100 pm



ε_o = 42 pm

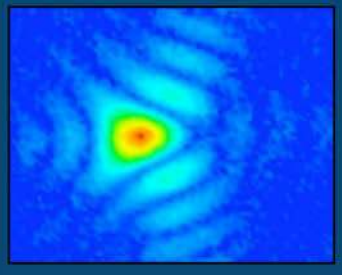
High Energy

Penetrating bulk materials and operating systems



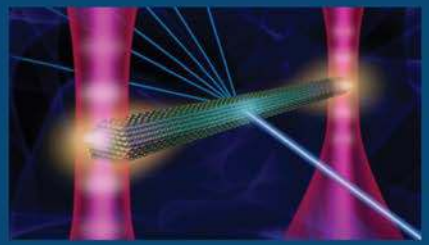
Brightness/Coherence

Highest possible spatial resolution/dynamics



Time-Resolved Studies

Measurements from ~100 ps to seconds



PARTNERSHIPS ADVANCE SCIENCE

WATER

Advanced Materials for Energy-Water Systems Center

- UChicago
- Northwestern

ENERGY STORAGE

Joint Center for Energy Storage Research

- 9 Labs
- 38 Universities

QUANTUM

Chicago Quantum Exchange

- 2 Labs
- 3 Universities

University of Delaware 1743

- Quantum
- Advanced Manufacturing
- Polymer Life Cycle
- AI/Data
- Interface Science