U.S. DEPARTMENT OF ENERGY | Office of Science

Roundtable on Research Opportunities in the Physical Sciences Enabled by Cryogenic Electron Microscopy
May 4-6, 2021

Co-Chairs: Amanda Petford-Long (Argonne National Laboratory),

Ben Gilbert (Lawrence Berkely National Laboratory)

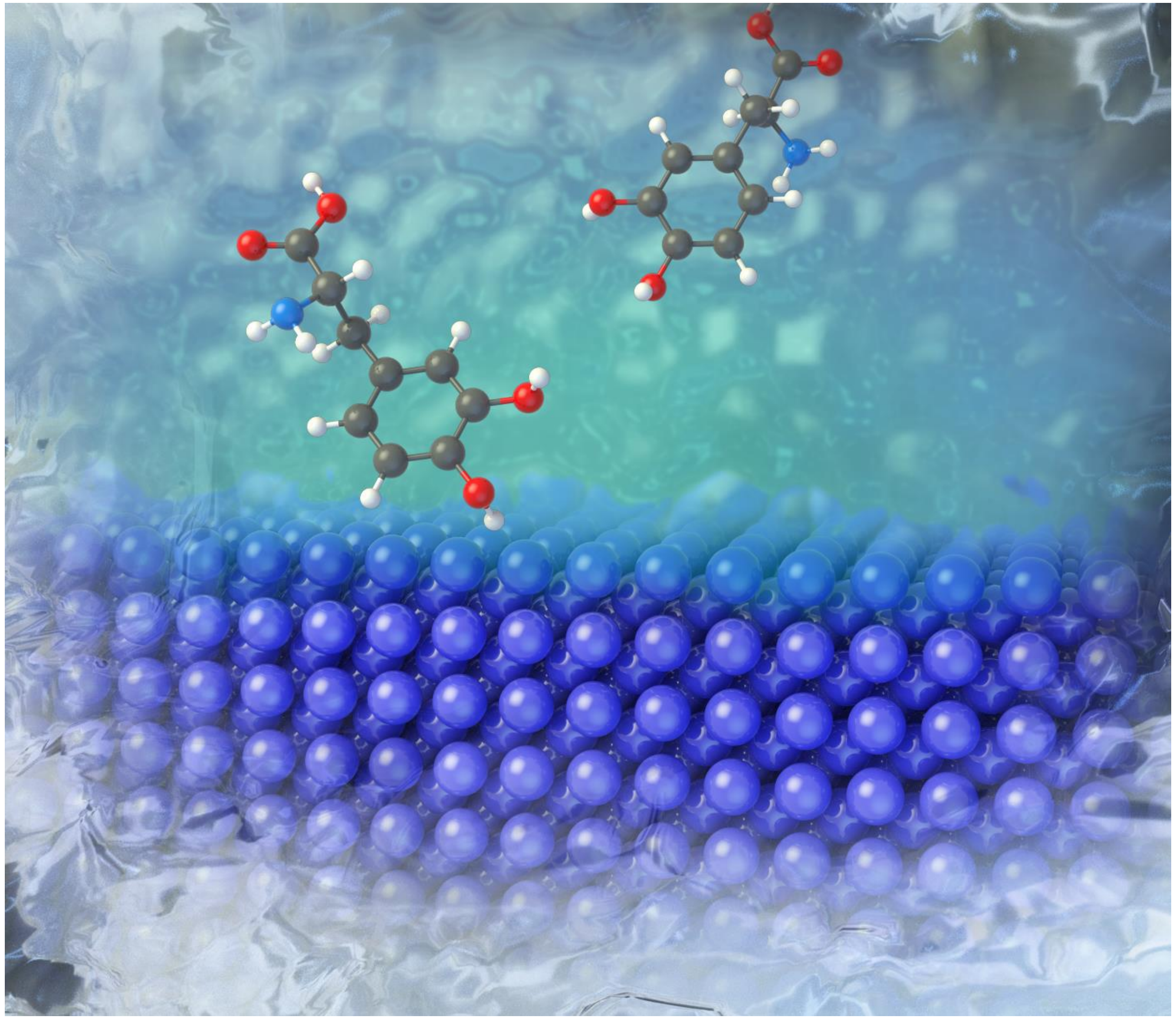
Briefing to the Basic Energy Sciences Advisory Committee

Amanda Petford-Long

August 24, 2021

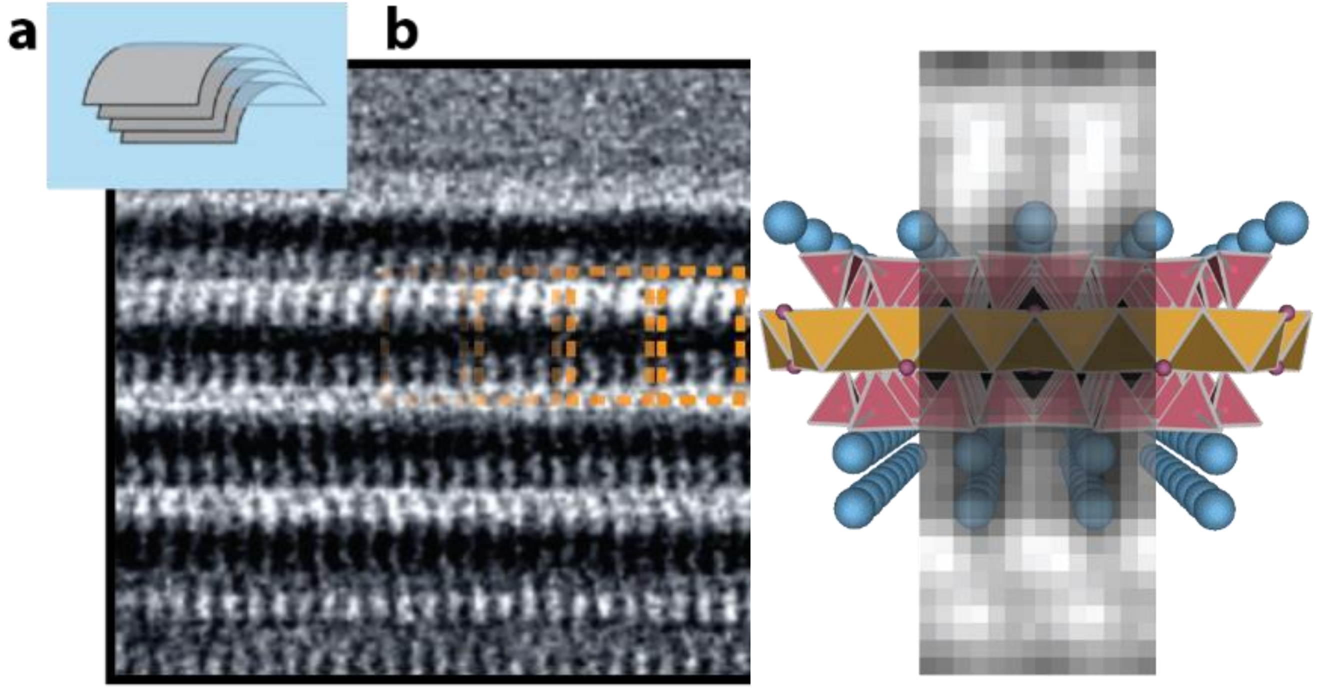
CryoEM Roundtable Workshop Charge

- To identify the key science drivers, research priorities, and research strategies for the BES research portfolio in the area of cryogenic electron microscopy (cryoEM) for the physical sciences.



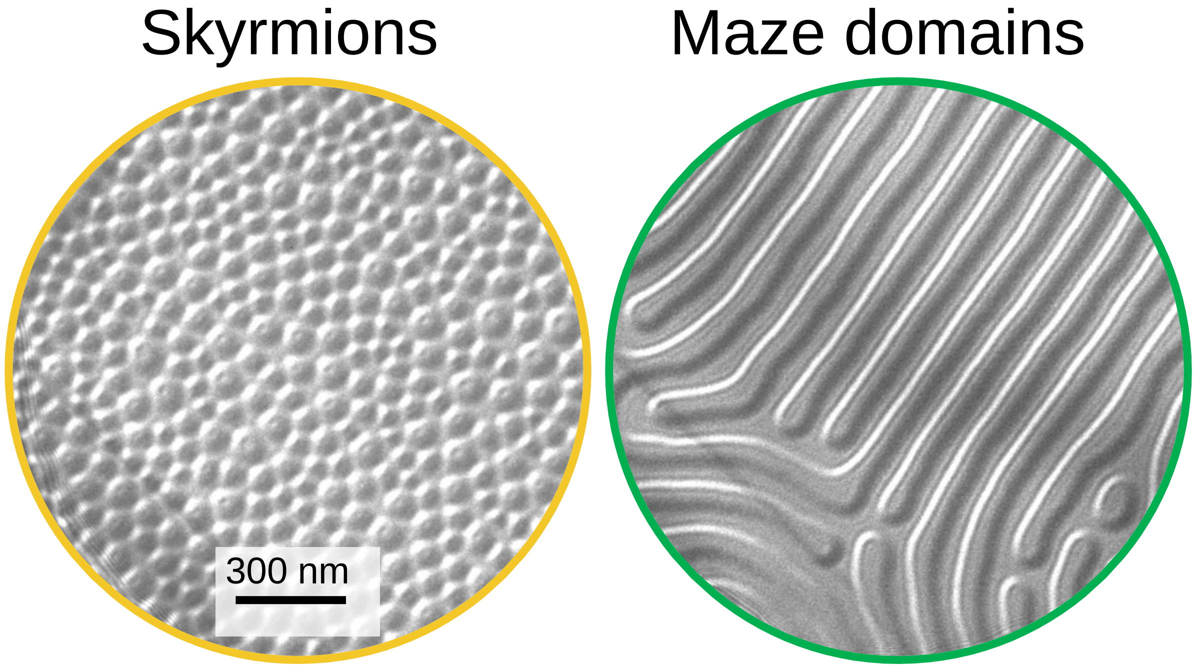
Opportunities enabled by CryoEM

- Understanding materials properties and chemical or biological processes at the atomic- to nano-scale when room temperature analysis is not appropriate



CryoEM imaging of clay layers in aqueous solution shows Na ion adsorption sites above and below one clay layer.

Whittaker, Ren, Ophus, Zhang, Gilbert, Waller, Banfield. 2020.arXiv:2012.09295.



Magnetic domain structure at 100K in Fe_3GeTe_2: cooled in a magnetic field (left) or in zero field (right).

Courtesy of C. Phatak, ANL

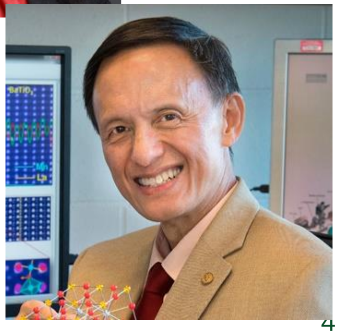
Roundtable Topical Panels

- **Condensed Phase Chemical Dynamics and Reaction**
  - **Lead: Lee Penn, University of Minnesota**

- **Controls of Structure and Function in Soft Matter**
  - **Lead: David Beratan, Duke University**

- **Processes and Chemical Pathways in Energy Materials**
  - **Lead: Shirley Meng, University of California San Diego**

- **Low-temperature Phenomena in Quantum Matter**
  - **Lead: Yimei Zhu, Brookhaven National Laboratory**



Plenary Talks

- *In aqua* High-resolution Imaging of Inorganic and Hybrid Earth Materials

  Jill Banfield, University of California Berkeley

- How Can Cryo-STEM Revolutionize Materials Science?

  Miaofang Chi, Oak Ridge National Laboratory

Priority Research Opportunities

- The initial panels focused on the topical areas outlined previously

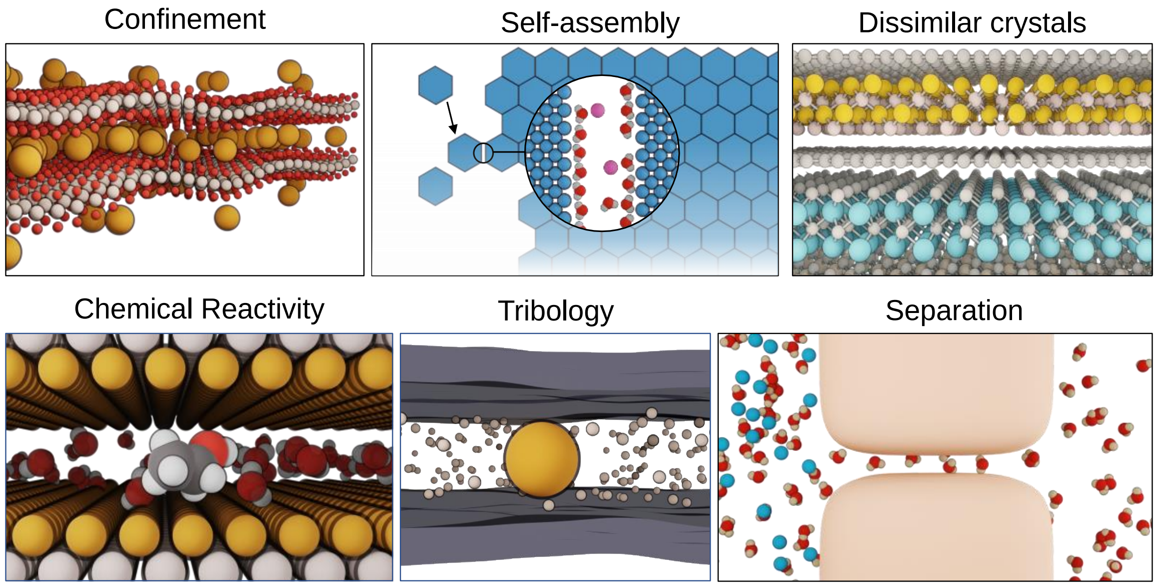
- We then reconfigured the panels to encourage cross-cutting conversations and development of the Priority Research Opportunities(PROs) by the panelists

- The PROs represent areas in which the panelists believe cryoEM will make major contributions to fundamental studies of materials behavior and chemical processes

Priority Research Opportunity 1: **Discover emergent behavior and coupled processes at interfaces**

- Interfaces between different phases of matter play critical roles in many technologies, including energy conversion and storage, as well as microelectronics
- **Key question**: How can we relate the complex and dynamic nature of interfaces to the chemical processes and physical behavior that they support?

- CryoEM will play an essential role by elucidating structure and chemistry at the atomic to the nanoscale and in 3D
- Also by linking this to the interface **function** through *in situ* experiments that probe frozen chemical states and physical behavior that only occurs at low temperatures.



Priority Research Opportunity 2: **Elucidate the role of heterogeneity in hierarchical systems**

- Hierarchical systems are ones in which structure and composition at different length and time scales interact to influence their mesoscale and macroscopic behavior
- **Key question**: How can we discover the dominant interactions across length and time-scales that control behavior in hierarchical systems?
- The use of cryoEM to understand how the different components in hierarchical systems interact will be key to elucidating their behavior
- CryoEM will also lead to an understanding of the way in which hierarchical systems form and heterogeneity emerges

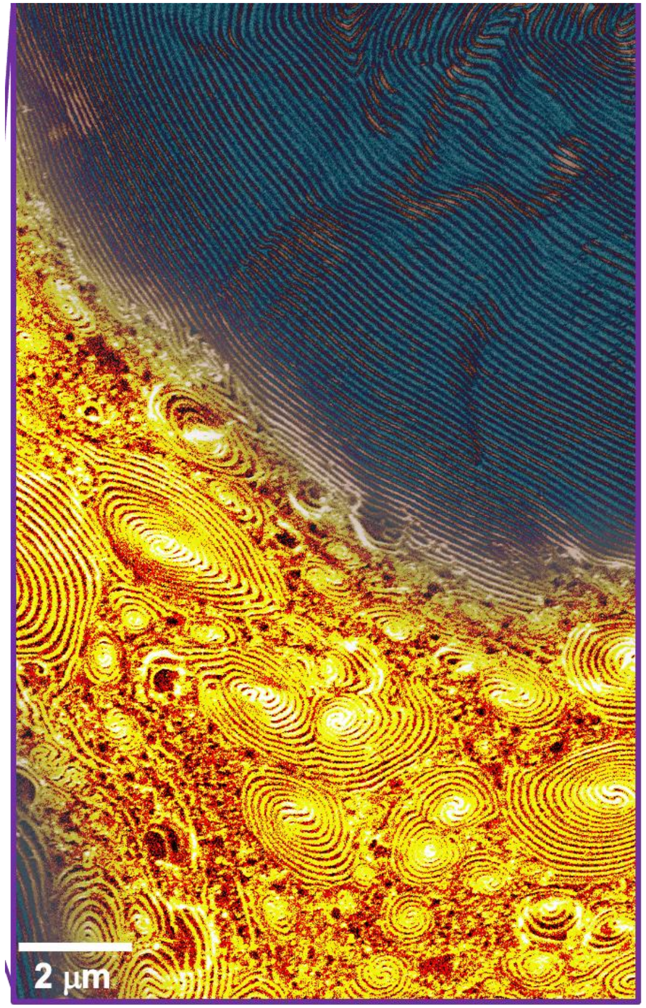
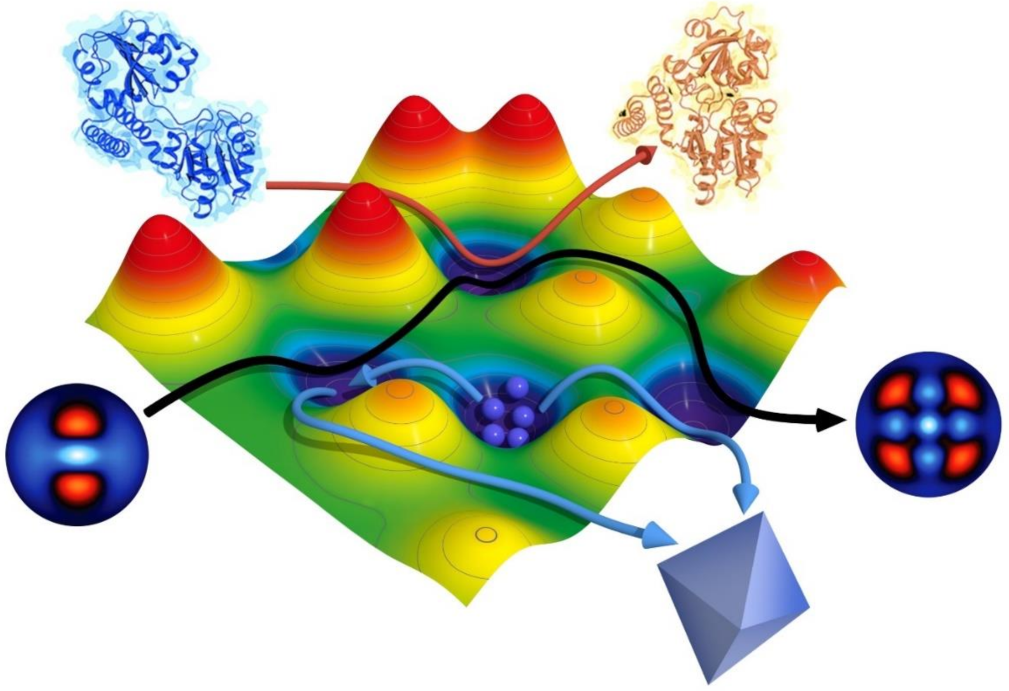


Figure adapted from: Maslyn et al., *Macromolecules* 54, 4010 (2021).

PRO 3: **Understand the evolution of matter in variable environments across length and time scales**

- The dynamic behavior of matter in response to changes to its environment influences many of the properties that we harness for energy-related applications
- **Key questions**: How is matter assembled from its constituent units? How can we map the energy landscape that controls dynamic behavior and processes?

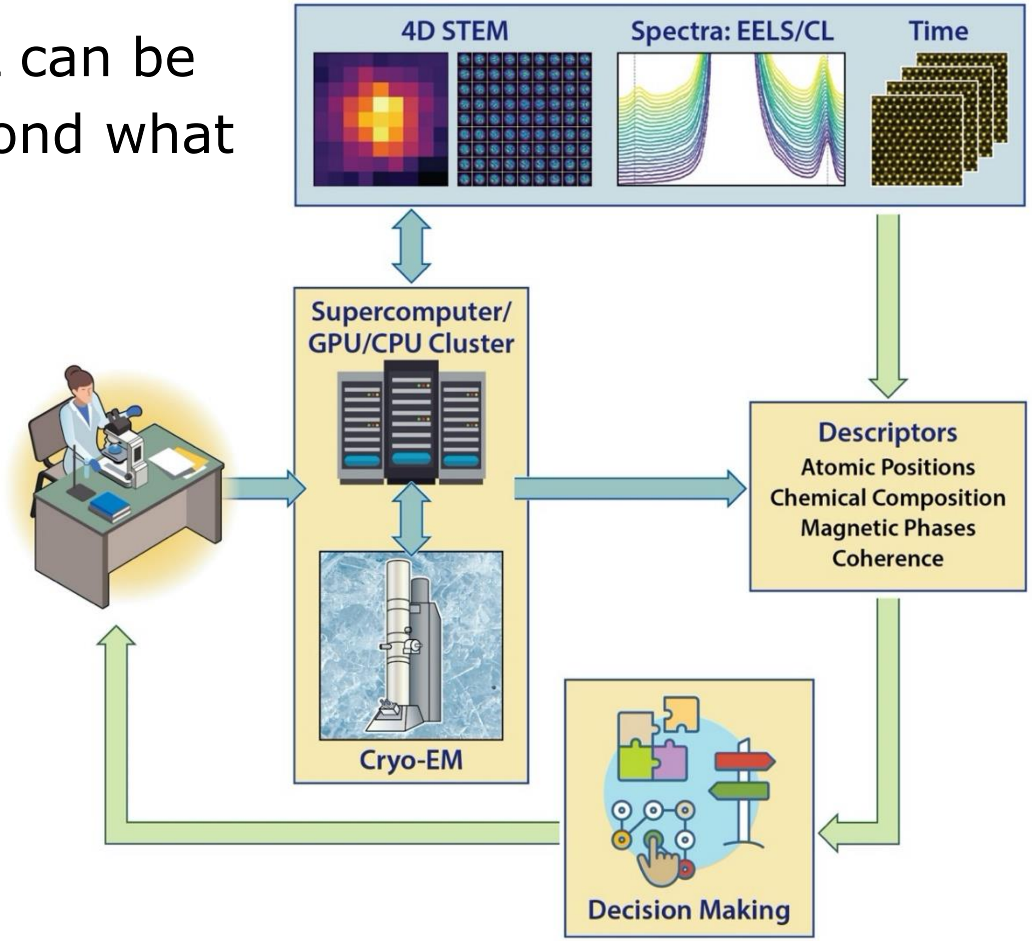
- CryoEM will help understand the energy landscape that controls assembly of matter, the subtleties of chemical transformations, and the dynamics of materials systems excited by an external stimulus.
- Integrating theory, cryoEM experiments, and data science will open exciting approaches to understanding dynamic behavior and harnessing it for applications.



Images of protein conformation adapted from Chu 2018 https://pubs.acs.org/doi/10.1021/acscentsci.8b00274.

PRO 4: **Harness data analytics and automation to expand the role of cryoEM in enabling scientific discoveries**

- CryoEM experiments are very challenging, and approaches are needed that will ensure that best use is made of every electron
- **Key question**: What advances in AI and ML can be harnessed to enable cryoEM to advance beyond what is currently possible?
- Data science and data analytics offer exciting opportunities to revolutionize our use of cryoEM in the physical sciences
- These approaches will dramatically expand the capabilities and impact of cryoEM by capturing phenomena that were previously inaccessible

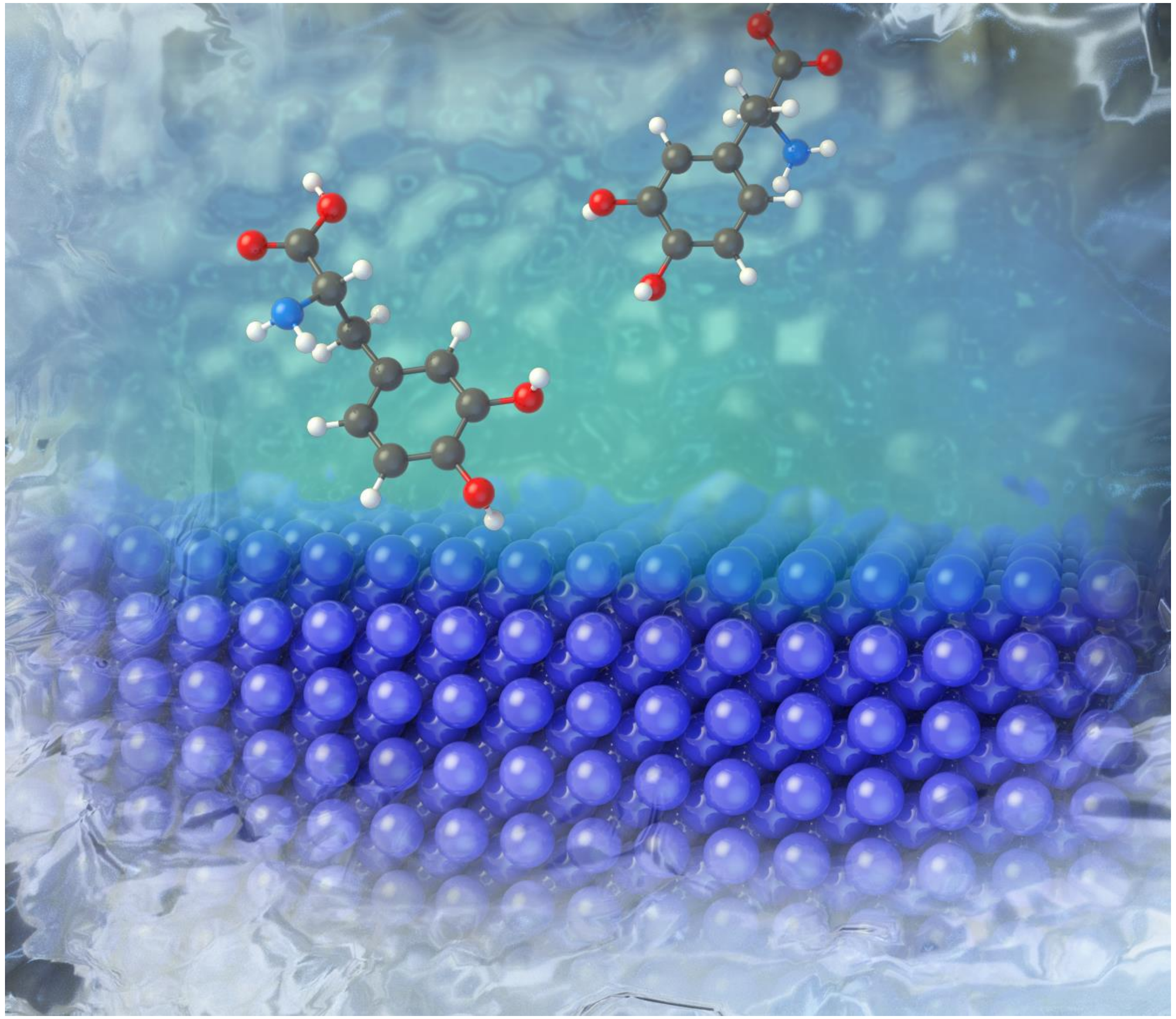


Capability needs

- New approaches to sample preparation, storage and transfer
  - Approaches that preserve critical features such as interfaces and heterogeneity are important if cryoEM is to achieve its full potential
- High stability imaging and spectroscopy at cryogenic temperatures
  - Exploring phenomena such as topological insulator behavior will require atomic-resolution cryoEM of lattice, electronic, and spin structures at variable temperatures down to tens, a few, or even sub-1 K
- In situ and operando experiments to track dynamic behavior
  - Integrating *in situ* excitations, such as electric fields, across a range of temperatures is critical to the exploration of pumped dynamic processes and phase transformations in quantum materials
  - Methods are needed to initiate and study chemical reactions *in situ*—for example, using variable-temperature cryoEM to manipulate reaction rates.
- Integrating data science, theory and correlative methods with cryoEM
  - Developing workflows that integrate experiment, theory, and AI/ML at all stages will be essential
    - Choice of experimental parameters, data acquisition and processing approaches, and data interpretation

Current status

- The Roundtable report is undergoing final edits
- We hope to share it with you soon



Acknowledgements

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- ANL production team

Thank you for your attention

Questions are welcome

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