# 29th AACGE Western Section
## Conference on Crystal Growth & Epitaxy

**Stanford Sierra Camp, Fallen Leaf Lake, CA**

**June 7-11, 2026**

# Welcome to
# Stanford Sierra Conference Center

The following information will help you during your stay at our lakeside retreat and enjoy your visit to the fullest!

The best way to keep in touch with the office and home is to bring a laptop with wireless capability. Our wireless network is available throughout the camp, including lodge rooms, meeting rooms, and common areas in the main lodge, as well as in the cabins.

Cell service is spotty and inconsistent at Fallen Leaf Lake so plan to be without cell reception during your stay.

You can receive phone messages at 530-541-1244 and receive faxes at 530-541-2212.

Registration, registration payment, and registration concerns can be emailed to aacg@comcast.net. Visit www.crystalgrowth.org to register and/or pay online.

We post phone messages and faxes on the guest message board across from the office. Check out time on departure day is 10:00.

Our website is www.stanfordsierra.com.

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# 2026 Sponsors

AACGE-West would like to gratefully acknowledge funding from:


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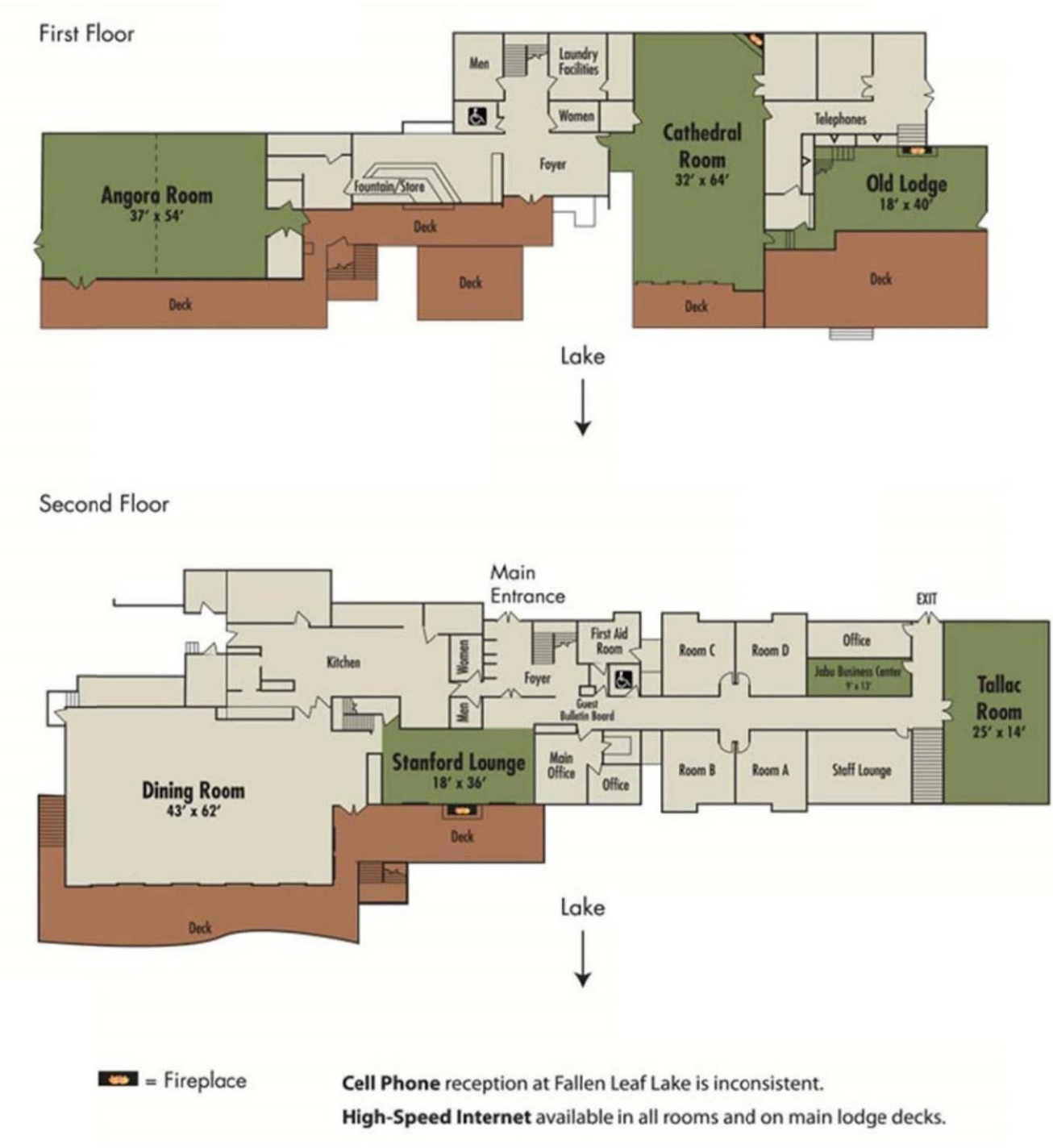
# Main Lodge Facilities



# Program Guide

## Sunday, June 7, 2026

| | | |
|---|---|---|
| Stanford Lounge | 15:00 – 18:00 | Camp Check-in & Conference Registration |
| Old Lodge Deck | 16:30 – 18:00 | Welcome Reception |
| Dining Room | 18:00 – 19:30 | Dinner |
| Cathedral Room | 19:30 – 21:00 | Epitaxial Crystal Growth |

## Monday, June 8, 2026

| | | |
|---|---|---|
| Dining Room | 7:30 – 9:00 | Breakfast |
| Cathedral Room | 9:30 – 10:30 | Fundamentals of Crystallization |
| | 10:30 – 11:00 | Break |
| Cathedral Room | 11:00 – 12:00 | Fundamentals of Crystallization |
| Dining Room | 12:00 – 13:30 | Lunch |
| | 13:30 – 16:00 | Camp Activities Unscheduled Time |
| Angora Room | 16:00 – 18:00 | Posters |
| Dining Room | 18:00 – 19:30 | Dinner |
| Cathedral Room | 19:30 – 20:15 | Plenary Lecture I |
| Cathedral Room | 20:20 – 21:10 | Colloidal Crystallization |

## Tuesday, June 7, 2026

| | | |
|---|---|---|
| Dining Room | 7:30 – 9:00 | Breakfast |
| Cathedral Room | 9:30 – 10:30 | Session |
| | 10:30 – 11:00 | Break |
| Cathedral Room | 11:00 – 12:00 | AI/ML for Crystal Growth |
| Deck | 12:00 – 12:15 | Meeting Photo |
| Dining Room | 12:00 – 13:30 | Lunch |
| | 13:30 – 16:00 | Camp Activities<br>Unscheduled Time |
| Angora Room | 16:00 – 18:00 | Podcast |
| Dining Room | 18:00 – 19:30 | Dinner |
| Cathedral Room | 19:30 – 20:15 | Plenary Lecture II |
| Cathedral Room | 20:20 – 21:10 | Colloidal Crystallization |

## Wednesday, June 8, 2026

| | | |
|---|---|---|
| Dining Room | 7:30 – 9:00 | Breakfast |
| Cathedral Room | 9:30 – 10:30 | Biological & Biomimetic Materials |
| | 10:30 – 11:00 | Break |
| Cathedral Room | 11:00 – 12:30 | Biological & Biomimetic Materials |
| Dining Room | 12:00 – 13:30 | Lunch |
| | 13:30 – 16:00 | Camp Activities<br>Unscheduled Time |
| Angora Room | 16:00 – 17:00 | Student Panel |
| Dining Room | 17:30 – 19:30 | Dinner |
| Cathedral Room | 19:30 – 21:10 | Epitaxial Crystal Growth |

## Thursday, June 9, 2026

| | | |
|---|---|---|
| Dining Room | 7:30 – 9:00 | Breakfast |
| Cathedral Room | 9:30 – 10:30 | Fundamentals of Crystallization |
| | 10:30 – 11:00 | Break |
| Cathedral Room | 11:00 – 12:00 | Fundamentals of Crystallization |
| Dining Room | 12:00 – 13:30 | Lunch &<br>Camp Departure |

# Program

## Sunday, June 7, 2026

19:30 – 21:00 Epitaxial Crystal Growth I
Cathedral Room
Chair: Ganesh Balakrishnan

19:30 – 20:00 Atomic-scale characterization of growth and overgrowth of III-V semiconductor nanostructures. **– Invited –**
Rainer Timm, Lund University

20:00 – 20:20 Strain- and instability-driven lateral compositional modulation of compound semiconductors – can we make use of it?
Sang Han, University of New Mexico

20:20 – 20:40 Engineering epitaxial quantum dots for telecommunication wavelength single photon emitter applications.
Ganesh Balakrishnan, University of New Mexico

20:40 – 21:00 Epitaxial oxidation sequences in titanium and scandium nanoislands.
Pip Knight, Massachusetts Institute of Technology

## Monday, June 8, 2026

| | |
|---|---|
| 9:00 – 10:30 | Fundamentals of Crystallization I |
| Cathedral Room | |
| Chair: | Kristen Fichthorn |
| 9:00 – 9:30 | Two-step crystallization and polymorph selection in 3-chloromandelic acid. **– Invited –**<br>Michael Gruenwald, University of Utah |
| 9:30 – 9:50 | Molecular origins of competing nucleation pathways in complex environments.<br>Nikhil Rampal, LLNL |
| 9:50 – 10:10 | Observations on the oxygen ion behavior in high temperature solutions.<br>Vincent Fratello, Retired |
| 10:10 – 10:30 | Unprecedented packing polymorphism of oxindole: an exploration inspired by crystal structure prediction.<br>Xiaolong Zhu, Merck |
| 10:30 – 11:00 | Break |
| 11:00 – 11:20 | Replacement of the Ostwald rule of stages to predict the sequence of appearance of crystal polymorphs.<br>Peter Vekilov, University of Houston |
| 11:20 – 11:40 | Dynamic studies of material properties at the Lawrence Livermore National Laboratory.<br>Thomas Lockard, LLNL |
| 11:40 – 12:00 | Iron acquisition and mineral transformation by cyanobacteria living in extreme environments.<br>David Kisailus, University of California, Irvine |

## Monday, June 8, 2026

16:00 – 18:00 Poster Session
Angora Room
Chair: Jong Seto

P1 Optimizing TiO2 anatase crystal thin film growth for photocatalysis.
Gabriella Chavez, San Francisco State University

P2 Investigating the effects of fluoride concentration on anatase titanium dioxide thin films and their application to PEC OER.
Brandon Le, San Francisco State University

P3 Automated grain boundary detection and AI-based morphological analysis of TiO2 thin films from AFM imaging.
Jorge Coronado-Sarmiento, San Francisco State University

P4 A novel 8-chambered hydrothermal synthesis reaction vessel: a case study of photocatalysis research with polycrystalline anatase thin films.
Milo Sack, San Francisco State University

P5 Thermal decomposition-driven growth mechanism of hBN in a Li flux.
Jonathan Valenzuela, Lehigh University

P6 A multiscale framework for Heme crystallization inhibition: from single-molecule step-capping to parasite suppression.
Jesus Cleto, University of Houston

P7 Whiplash dynamics-based deposition of nanoparticles for thin film growth.
Dhruvaite Upmanyu, Pingree School

P8

P9

P10

## Monday, June 8, 2026

| | |
|---|---|
| 19:30 – 21:10 | Plenary Lecture & Colloidal Crystallization I |
| Cathedral Room | |
| Chair: | Talid Sinno |

19:30 – 20:15 Dislocation and 2D nucleation mechanisms in large organic and inorganic crystals grown from solution. **– Plenary I –**
Natalia Zaitseva, LLNL

20:20 – 20:50 Cracking colloidal crystallization: classical nucleation and growth with a twist. **– Invited I –**
Benjamin Rogers, Brandeis University

20:50 – 21:10 FFT-based analysis of quantum dot superlattices.
Ken Seungmin Hong, Brown University

## Tuesday, June 9, 2026

| | |
|---|---|
| 9:00 – 10:30 | Artificial Intelligence & Machine Learning for Crystal Growth |
| Cathedral Room | |
| Chair: | Katie Colbaugh & Moneesh Upmanyu |
| 9:00 – 9:30 | High-fidelity atomistic simulations of alloy solidification. **– Invited –**<br>Rodrigo Freitas, Massachusetts Institute of Technology |
| 9:30 – 9:50 | Data-driven coarse-graining: Discovering continuum scale models from atomistic simulations.<br>Amit Samanta, LLNL |
| 9:50 – 10:10 | Predicting antimalarial activity modes in hematin crystallization using a priori machine learning.<br>Hariharan Annadurai, University of Houston |
| 10:10 – 10:30 | Identifying useful nanocrystal morphologies using advanced sampling techniques and machine learning.<br>Kirsten Fichthorm, Penn State University |
| 10:30 – 11:00 | Break |
| 11:00 – 11:20 | A comparative study of PIML and general ML/AI approaches for industrial crystal growth.<br>Katie Colbaugh, Leucite |
| 11:20 – 11:40 | Nucleation and growth of grain boundary phases.<br>Timofey Frolov, LLNL |
| 11:40 – 12:00 | Machine Learning and Artificial Intelligence for Chemistry and Materials.<br>Teresa Head-Gordon, University of California, Berkeley |

## Tuesday, June 9, 2026

12:00 – 12:15 Group Photo
Outside Deck
Chair: Luis Zepeda-Ruiz

11:45 – 12:00 All attendees invited for our group photo.

## Tuesday, June 9, 2026

16:00 – 18:00 Podcast
Angora Room
Chair: Dhruvaite Upmanyu

16:00 – 18:00 Everyone is encouraged to be interviewed.

## Tuesday, June 9, 2026

19:30 – 21:10 Plenary Lecture & Colloidal Crystallization II
Cathedral Room
Chair: Talid Sinno

19:30 – 20:15 Self-assembly and crystallization at protein-inorganic interfaces.
**– Plenary II –**
James DeYoreo, PNNL

20:20 – 20:50 Computational self-assembly of diverse colloidal crystal and cluster structures. **– Invited –**
Julia Dshemuchadse, Cornell University

20:50 – 21:10 Can hydrodynamic interactions explain anomalously fast nucleation in weakly-supersaturated colloidal fluids?
Talid Sinno, University of Pennsylvania

## Wednesday, June 10, 2026

| | |
|---|---|
| 9:00 – 10:30 | Biological & Biomimetic Materials |
| Cathedral Room | |
| Chair: | Jong Seto |

| | |
|---|---|
| 9:00 – 9:30 | Control over crystallization from metastable mineral precursors by manipulation of polyelectrolytes. **– Invited –**<br>Thomas Schroeder, North Carolina State University |
| 9:30 – 9:50 | High-resolution structural studies at the interface of biology and materials science.<br>Brent Nannega, Arizona State University. |
| 9:50 – 10:10 | Clustering of Zn in ectopic biominerals at the biological interfaces in the temporomandibular joint and the kidney.<br>Sunita Ho, University of California, San Francisco |
| 10:10 – 10:30 | Template-directed toxicity sink: molecular mechanisms of lithium-mediated Aβ42 oligomer–fibril interconversion.<br>Radhika Sunil Menon, University of Houston |
| 10:30 – 11:00 | Break |
| 11:00 – 11:30 | Mesoporous frameworks engineered from crystallizable collagen-mimetic peptide amphiphiles. **– Invited –**<br>Andrea Merg, University of California, Merced |
| 11:30 – 11:50 | The structural landscape of amyloid-β oligomerization by high-speed AFM.<br>Nghia Nguyen, University of Houston. |
| 11:50 – 12:10 | Organization and complexation of an extracellular matrix protein with Ca2+ ions.<br>Jong Seto, Arizona State University |
| 12:10 – 12:30 | Programming Crystal Composition through Polymer-Controlled ACC Transformation.<br>Stephan Wolf, Friedrich-Alexander University |

## Wednesday, June 10, 2026

16:00 – 17:30 Poster Award Talks & Career Panel Discussion
Angora Room
Chair: Luis Zepeda-Ruiz

16:00 – 16:15 Poster Awards talks.

16:15 – 17:30 Career Panel Discussion.

## Wednesday, June 10, 2026

19:30 – 21:00 Epitaxial Crystal Growth II
Cathedral Room
Chair: Ganesh Balakrishnan

19:30 – 20:00 Modeling SiGe quantum dot variability induced by interface disorder re-constructed from multi-perspective microscopy. **– Invited –**
Ezra Bussman, Sandia National Laboratory

20:00 – 20:30 Oxide thin films for electronic and optical applications. **– Invited –**
Wilfrid Prellier, Centre National de la Recherche Scientifique (CNRS)

20:30 – 20:50 Analytical x-ray solutions for thin film and wafer analysis.
Destiny Lopez, Malvern Panalytical

20:50 – 21:10 Correlating epitaxial growth and electronic properties of crystalline high-k metal oxides on 2D materials.
Rishabh Kothari, Massachusetts Institute of Technology

## Thursday, June 11, 2026

| | |
|---|---|
| 9:00 – 10:30 | Fundamentals of Crystallization II |
| Cathedral Room | |
| Chair: | Kristen Fichthorn |

| | |
|---|---|
| 9:00 – 9:30 | From colloidal nano building blocks to higher order architectures.<br>**– Invited –**<br>Ou Chen, Brown University |
| 9:30 – 9:50 | The Impact of Wadsley defects and cation disorder on improving $MoNb_{12}O_{33}$ diffusion.<br>Cristopher Sturgill, University of South Carolina |
| 9:50 – 10:10 | Solvent-dependent relative stability of crystal forms.<br>Rohith Pulluri, University of Houston |
| 10:10 – 10:30 | Coupling catalyst activity and degradation: modeling oxygen evolution reaction with surface dissolution on IrO2(110).<br>Rhys Bunting, LLNL |
| 10:30 – 11:00 | Break |
| 11:00 – 11:20 | Atomic-scale insights into calcite dissolution kinetics in nonstoichiometric solutions and the role of $Mg^{2+}$ ions.<br>Shuhong Song, PNNL |
| 11:20 – 11:40 | Crystallization entropy: constituents and contributions to crystal form stability.<br>Alejandro Veliz, University of Houston |
| 11:40 – 12:00 | Morphological Stability of Recrystallization Fronts in Polycrystals: Impurity Effects.<br>Moneesh Upmanyu, Northeastern University |

# Abstracts

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**Sunday, June 7, 2026**
**19:30 – 21:00 Epitaxial Crystal Growth**

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Atomic-scale characterization of growth and overgrowth of III-V semiconductor.
Rainer Timm, Lund University

III-V semiconductor nanostructures, with their superior charge carrier mobility and a direct and tunable band gap, are promising for next generation devices in electronics, photonics, energy harvesting, and quantum information. They offer a large flexibility in forming material, doping, or crystal phase heterostructures. III-V nanowires are especially interesting both from an application and crystal growth perspective, as they combine a complex interplay of lateral and radial growth, can crystallize in structures that are not stable in bulk, and can act as templates for growth of novel nanostructures.
We are using scanning tunnelling microscopy and spectroscopy (STM/S) as well as synchrotron-based X-ray photoelectron spectroscopy (XPS) in various setups for studying growth, atomic structure, and electronic properties of III-V semiconductor nanostructures at the atomic scale. Here, I will show STM/S results highlighting different stages of nanowire growth and overgrowth, where we map nanowires across axial heterostructures between different materials, doping level, or different crystal phase, and correlate the surface structure and local electronic properties, down to quantum size effects. Nanowire crystal phase heterostructures can act as templates for radial overgrowth with atomic-scale control, enabling the growth of novel types of nanostructures monitored by STM: Figure 1 shows the surface of a GaAs nanowire which has been exposed to Bi atoms, resulting in the self-selective growth of well-ordered GaBi 1D and 2D nanostructures on the surface of the wurtzite segment, while only individual Bi atoms or small Bi clusters were incorporated in the zincblende surface.
Bismuth incorporation in III-V semiconductor surfaces also leads to interesting growth phenomena upon 2D film growth. I will show examples of self-limiting Bi growth on InSb(111)B and of a honeycomb surface structure of Bi atoms on GaAs(111)B, which – in contrast to conventional Bismuthene – form strong covalent bonds to the As atoms of the underlying GaAs, but are only weakly bond to each other. These structures are promising for non-trivial topological behavior at room temperature and large Rashba splitting.

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Strain- and instability-driven lateral compositional modulation of compound semiconductors - can we make use of it?
Sang Han, University of New Mexico

Phase instability and interatomic diffusion in epitaxially grown III–V semiconductors are generally associated with materials degradation and eventual device failure. Here, we explore whether these same processes can instead be used to produce lateral compositional modulation and

bandgap engineering. Using GaAsSb/InP as a model system, we examine the evolution of a lattice-matched GaAsSb epilayer during high-temperature annealing. Rather than conventional spinodal decomposition alone, we observe pronounced migration of Sb from the GaAsSb epilayer into the InP substrate and counter-diffusion of P from the substrate into the epilayer. This intermixing produces InSb-rich tips and facets of pyramidal nanostructures together with InGaAsP regions that replace the original GaAsSb layer. High-resolution x-ray diffraction, Raman spectroscopy, scanning transmission electron microscopy, and energy-dispersive x-ray spectroscopy collectively indicate that the transformation is driven by liquid-assisted phase separation associated with transient molten InSb, providing an alternative mechanism to previously proposed solid-state spinodal decomposition. By applying external biaxial strain through stressed SiNx capping layers, the net strain during annealing can be tuned from compressive to tensile. A critical strain appears to exist that strongly alters the resulting morphology, producing a transition from deeply penetrating intermixed domains to laterally confined InSb/InGaAsP layers while substantially slowing the kinetics of degradation. These results demonstrate that phase instability and interdiffusion can be directed by strain and may provide a route to controlled lateral compositional modulation in compound semiconductors.

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Engineering epitaxial quantum dots for telecommunication wavelength single photon emitter applications.

Ganesh Balakrishnan, University of New Mexico

Epitaxial III–V quantum dots (QDs) are promising candidates for single-photon emitters, but conventional InAs/GaAs systems are limited in achieving emission at telecommunication wavelengths. This work explores alternative epitaxial growth pathways using arsenide and antimonide material systems to extend emission beyond 1.3 μm while maintaining control over morphology and optical properties.

InAs growth on InP substrates is investigated as a reduced lattice-mismatch system that enables thicker planar growth prior to three-dimensional island formation. On InP (001), anisotropic surface diffusion leads to elongated quantum dash structures, whereas growth on InP (311)B suppresses this anisotropy and promotes the formation of isolated, symmetric quantum dots exhibiting single-dot emission. Growth parameters such as coverage and growth rate are shown to critically influence the dimensional transition and dot density.

GaSb quantum dot formation on GaAs is also examined under varying stoichiometric conditions. Sb-rich growth results in strain-relaxed islands mediated by misfit dislocation arrays, while group-III-rich conditions favor coherent Stranski–Krastanov growth. Interdiffusion during capping can further modify dot morphology, leading to ring-like structures and altered optical behavior.

These results highlight the role of epitaxial growth conditions, substrate orientation, and strain management in tailoring quantum dot structure and emission properties. The study provides insight into growth mechanisms enabling long-wavelength QDs and supports their integration into quantum photonic devices.

Epitaxial oxidation sequences in titanium and scandium nanoislands.
Pip Knight, Massachusetts Institute of Technology

Understanding epitaxial oxidation processes is crucial to many areas of nanoscience that require control of surface structure or utilize oxidation as a synthetic step to a final nanostructure. For example, in industrial chemical reactions catalyzed by metal nanoparticles, the surface structure of the catalytic nanoparticle depends on the gas environment and is crucial to surface catalytic activity1. Meanwhile in microelectronics, oxidized metal seed layers are proposed to enable the growth of homogeneous gate oxide films on challenging substrates like 2D materials2, so controlling the phase and epitaxy of the oxide seed is essential for controlling these same properties of the film. However, detailed studies of epitaxial oxidation are challenging for more reactive metals because without an ultra-high vacuum (UHV) growth and imaging environment, it is not possible to capture the first stages of oxidation, such as suboxide formation. Furthermore, a detailed study of epitaxial oxidation sequences requires epitaxial, single crystalline metal as a starting material, ideally in a well-defined morphology.

In our work, we aim to understand the oxidation sequences of reactive metals. To do this, we grow flat, epitaxial nanoislands and films of the metals on suspended multilayer graphene (Gr) substrates to use as the starting point for oxidation studies. We focus on the hexagonal close-packed metals titanium (Ti) and scandium (Sc), which are both promising high k dielectric oxides for microelectronics3,4. The metals are grown by electron beam deposition in UHV, then transferred in the same vacuum system to our UHV transmission electron microscope (TEM) where the phase transformations are conducted in situ. By making movies of the phase transformation, we can understand morphology changes and use in situ electron diffraction to track the formation of new crystallographic phases. We find that the sequence of daughter phases that form in each case are epitaxial, and we examine the crystallographic relationships between the sequence of suboxide phases to understand the atomic scale reaction pathway. We also indirectly probe the relative diffusivities of oxygen compared with the metal for each case by observing with in situ TEM whether the nanoscale Kirkendall effect occurs. Finally, we extend our study of in situ metal-gas reactions by discussing prospects for nitride formation reactions.

References:

1. Yokosawa, Tadahiro, Frans D. Tichelaar, and Henny W. Zandbergen. "In-Situ TEM on Epitaxial and Non-Epitaxial Oxidation of Pd and Reduction of PdO at P= 0.2–0.7 bar and T= 20–650° C." European Journal of Inorganic Chemistry 2016.19 (2016): 3094-3102.

2. Kim, Hoijoon, et al. "Ultrathin monolithic HfO2 formed by Hf-seeded atomic layer deposition on MoS2: Film characteristics and its transistor application." Thin Solid Films 673 (2019): 112-118.

3. Kim, Taikyu, et al. "Atomic layer growth of rutile TiO2 films with ultrahigh dielectric constants via crystal orientation engineering." ACS Applied Materials & Interfaces 16.26 (2024): 33877-33884.

4. Lebedev, M. S., et al. "Optical properties and charge transport of textured Sc2O3 thin films obtained by atomic layer deposition." Applied Surface Science 478 (2019): 690-698.

**Monday, June 8, 2026**
**9:00 – 12:00 Fundamentals of Crystallization I**

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Two-step crystallization and polymorph selection in 3-chloromandelic acid.
Michael Gruenwald, Department of Chemistry, University of Utah

Predicting which crystal structures emerge from solution remains a central challenge in crystal engineering and pharmaceutical solid-form design. State-of-the-art computational methods can enumerate thermodynamically plausible crystal structures, but they often predict many metastable polymorphs, few of which are experimentally realized. Here, we revisit the crystallization of 3-chloromandelic acid. We demonstrate that a metastable polymorph, recently observed only in co-crystallization experiments, can be reproducibly obtained from a range of solvents through fast crystallization at large supersaturation. Spectroscopic analyses and molecular simulations reveal that the structural motifs of this polymorph are pre-organized in highly concentrated, amorphous solution environments from which crystallization occurs. These findings establish a direct link between solution-phase structure, crystallization pathway, and polymorph selection, suggesting new strategies for the targeted discovery of metastable crystal forms.

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Molecular origins of competing nucleation pathways in complex environments.
Nikhil Rampal, LLNL

Crystal nucleation from aqueous solutions is often explained using classical nucleation theory (CNT). However, increasing evidence shows that crystals can also form through more complex, non-classical pathways, such as ion clustering and amorphous precursor phases. In this study, we use classical molecular dynamics simulations at constant chemical potential to examine barite ($BaSO_4$) nucleation under two levels of supersaturation.
Our results show that nucleation begins from a shared set of disordered structures that evolve into a cross-linked intermediate. From this point, the system can follow one of two paths: barrier-free formation of an amorphous solid, or crystallization through a small additional activation barrier. Which path is taken depends on the degree of supersaturation.
To test and extend these findings, we train an equivariant graph neural network (EGNN) on structures generated from the simulations and apply it to experimental pair distribution function data. This allows us to interpret early-stage structural features that are difficult to resolve through experiments alone. Overall, this work provides a transferable framework for studying nucleation and phase transformations in chemically complex systems.

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Observations on the oxygen ion behavior in high temperature solutions.
Vincent Fratello, Retired

Crystal growth from molten salt oxides requires a good understanding of the mechanism of solution. Solvents commonly consist of a Lewis base (electron pair donor, in this case O2-) and a Lewis acid solvent additive to reduce the melting temperature, limit evaporation, and affect the solubility of various Lewis base ingredients in the solute. Fischer, Linzen, et al. had previously investigated the oxygen ion concentration of melts with various Lewis acids in various Lewis bases, particularly PbO. Their results have been systematized here and applied to the crystal growth of lead zirconate titanate (PZT) from various solvents including some containing P2O5. Using this formalism explains how P2O5 reduces the solubility of TiO2 and ZrO2 in the melts. It also accounts for the difference in solubilities of TiO2 and ZrO2 in lead oxide-fluxed melts. This results in an understanding that the solvent is not so much lead oxide as the free O2- liberated therefrom by ionization. The O2- available for solution is fixed by the combination of the PbO ionization in the liquid and the complexing by coordination with a strong binding Lewis acid solvent additive. Without available O2- to coordinate with and dissolve weaker binding Lewis acid solutes, they cannot come into the solution. This gives guidance on how to formulate a wide variety of melts using the right combination of a Lewis base solvent, Lewis acid solvent additive, and various Lewis acid solute ingredients.

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Unprecedented packing polymorphism of oxindole: an exploration inspired by crystal structure prediction.
Xiaolong Zhu, Merck

Crystal polymorphism, characterized by different packing arrangements of the same compound, strongly ties to the physical properties of a molecule. Determining the polymorphic landscape is complex and time-consuming, with the number of experimentally observed polymorphs varying widely from molecule to molecule. Furthermore, disappearing polymorphs, the phenomenon whereby experimentally observed forms cannot be reproduced, pose a significant challenge for the pharmaceutical industry. Herein, we focused on oxindole (OX), a small rigid molecule with four known polymorphs, including a reported disappearing form. Using crystal structure prediction (CSP), we assessed OX solid-state landscape and thermodynamic stability by comparing predicted structures with experimentally known forms. We then performed melt and solution crystallization in bulk and nanoconfinement to validate our predictions. These experiments successfully reproduced the known forms and led to the discovery of four novel polymorphs. Our approach provided insights into reconstructing disappearing polymorphs and building more comprehensive polymorph landscapes. These results also establish a new record of packing polymorphism for rigid molecules.

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Replacement of the Ostwald rule of stages to predict the sequence of appearance of crystal polymorphs.
Peter Vekilov, University of Houston

Polymorphism is a fundamental property of crystals whereby a single compound may adopt numerous crystal structures with distinct properties. This structure multiplicity leads to materials with distinct physical properties (e.g., solubility, catalytic activity) that impact their performance in numerous applications. About 75% of the compounds deposited in the Cambridge Structural Database (CSD) crystallize in more than one structure. Crystal structure polymorphism manifests a free energy landscape, which, in contrast to that for protein folding, has not been optimized by evolution and contains not one minimum, but multiple local minima with similar free energies. Crystal structure multiplicity is magnified by the propensity of crystals to incorporate solvent molecules, creating solvates. Crystal polymorphs appear and transform via pathways that are not fully dictated by their stabilities. Observed trends often contradict the Ostwald rule of stages, according to which less stable polymorphs appear first, emphasizing how current state-of-the-art theories of crystallization cannot predict stable crystal structures and the transitions between them.
We rely on the premise that the polymorph to appear first is the one with the fastest rate of nucleation. In turn, the main parameter, which determines the nucleation barrier and the nucleation rate, is the surface free energy of the interface between the nucleus and the crystallization medium. We present an analytical model for the scaling of the nucleation barrier $\Delta G^*$ with the crystallization enthalpy $\Delta H^o_{cryst}$. Results with mefenamic acid support these scaling relations. We experimentally measure the nucleation rates of the individual crystal forms and evaluate $\Delta G^*$. As a measure of their relative stabilities we use their solubilities to evaluate the crystallization free energies $\Delta G^o$. The crystallization enthalpies $\Delta H^o_{cryst}$ of the individual crystal forms are measured from the temperature correlation of their solubilities. Our analysis predicts that solvates would have lower nucleation barriers and form first, elucidating the mechanism behind the persistence of solvates in the crystallization practice.
Our analysis predicts that solvates would have lower nucleation barriers and form first, elucidating the mechanism behind the persistence of solvates in the crystallization practice. This model represents an innovative strategy to predict and control intercrystalline transformations. Filling this gap in current state-of-the-art models will significantly impact the pharmaceutical and chemical industries.

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Dynamic studies of material properties at the Lawrence Livermore National Laboratory.
Thomas Lockard, LLNL

Dynamic and high-pressure material properties are important across a wide range of conditions, from ambient environments to the Earth’s core and stellar interior conditions. National Labora-

tories have been deeply involved in understanding the fundamental physical properties of materials. The work presented here will discuss integrated experimental and theoretical efforts investigating the effects of grain boundaries and crystalline phase changes. Though not exclusive the experimental campaigns highlighted here will be X-ray diffraction, strength by Rayleigh-Taylor instability growth, temperature by Extended X-ray Absorption Fine Structure (EXAFS) and Ramp equation of state (EOS) experiments. Specific cases investigating solid-solid and liquid-solid phase transitions and effects from material strength from grain boundaries will be shown. Improving our understanding and predictive capabilities by coupling experimental and modeling theories is generally related to EOS properties such as pressure, density, or temperature. As a material is compressed, changes phase or exhibits strength these physical properties and associated crystal structures grant a better view into the underlying mechanisms.

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**Monday, June 8, 2026**
**19:30 – 20:15 Plenary I**

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Dislocation and 2D nucleation mechanisms in large organic and inorganic crystals grown from solution.
Natalia Zaitseva, LLNL

Until recently, low-temperature solution growth had been used primarily for the growth of crystals from aqueous solutions. One of the most notable applications of this technique was the development of the technology for producing meter-scale KDP ($KH_2PO_4$) crystals for the world's largest laser facility, the National Ignition Facility (NIF). KDP is a classical inorganic crystal that grows predominantly by the dislocation mechanism and has been extensively studied in both theoretical and experimental works. The unprecedented scale of these crystals created a strong demand for rapid growth at high supersaturation and stimulated the development of specialized techniques that, for the first time, enabled in situ observation of surface structures and growth phenomena occurring simultaneously on multiple faces of large, naturally faceted crystals.
More recently, scientific and industrial interest has shifted toward organic crystals with unique optical and scintillation properties promising for applications in radiation detection, high-energy nuclear physics, and advanced information technologies. For many of these materials, solution growth is preferred because their low symmetry and tendency toward thermal decomposition make melt-growth techniques impractical. In addition, the poor solubility of most organic compounds in water requires a transition from classical aqueous systems to growth from organic solvents.
This transition has revealed substantial differences in crystal-growth behavior. Experimental observations show that the majority of pure organic compounds grow predominantly through two-

dimensional (2D) nucleation mechanisms which, contrary to conventional expectations, can dominate crystal-face growth even at very low supersaturations despite the confirmed presence of screw dislocations. Furthermore, different faces of the same crystal may grow by different mechanisms, independently of supersaturation or dislocation structure. These growth modes create major challenges for controlling defect formation and for implementing rapid-growth technologies required for future large-scale production.
This presentation will discuss the differences between classical dislocation-controlled growth and alternative growth mechanisms in large organic crystals, with emphasis on experimental observations, theoretical models, and computer simulations that can provide insight into defect formation, growth stability, and the future development and practical applications of organic single crystals.

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**Monday, June 8, 2026**
**20:20 – 21:10 Colloidal Crystallization I**

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Cracking colloidal crystallization: classical nucleation and growth with a twist.
W. Benjamin Rogers, Brandeis University

Colloidal crystals are widely believed to self-assemble via classical nucleation and growth, following dynamical pathways analogous to those of atoms and simple molecules. A central challenge in the programmable self-assembly of colloids is to understand whether this framework quantitatively describes the crystallization dynamics of micrometer-sized colloidal particles. In this talk, I will describe how we combine microfluidics-based experiments and theory to develop a complete understanding of the crystallization dynamics of DNA-coated colloids. Specifically, I will show that the nucleation and growth kinetics of DNA-coated colloids are fundamentally different from those of atoms or small molecules, owing to an effective friction that arises from transient DNA hybridization. By incorporating this effective friction into classical theories, such as classical nucleation theory, we can predict the absolute rates of nucleation and crystal growth with quantitative accuracy. I will emphasize how this quantitative picture of the crystallization dynamics can be used in practice to design new non-equilibrium protocols for making macroscopic photonic materials from colloids and then conclude by showing how our techniques can be extended to ask new fundamental questions about nucleation and growth using other material systems, like DNA origami. Taken together, these experiments constitute one of the most well-controlled studies of colloidal nucleation and growth to date, and represent a key step forward in the creation of functional crystalline materials from colloids.

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FFT-based analysis of quantum dot superlattices.
Ken (Seungmin) Hong, Brown University

Complex superlattices (SLs) formed from colloidal quantum dots (QDs) require combination of various analysis techniques, such as electron tomography and X-ray scattering, to reveal accurate structure information. Among those, electron diffraction and fast Fourier transformation (FFT) provide quick access to the structural information through reciprocal space analysis. However, conventional approaches are limited to global characterization due to averaging of signals, making local structural resolution challenging purely from reciprocal space analysis.
In this work, we develop a 4D FFT analysis technique that captures information from four basis vectors – two real space vectors and two reciprocal space vectors – to characterize QD SLs both locally and globally. In this approach, a TEM image is divided into equally sized square regions and an FFT is performed on each region individually. This then enables spatially resolved analysis structural information such as lattice constant, homogeneity through quantitative comparison of neighboring FFTs, and phase boundary identification. By combining local information from multiple TEM images, we can also extract statistical information. This method provides a quick and accessible framework for structural characterization of SLs, not limited to QDs but applicable to any nanocrystal assemblies.

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**Tuesday, June 9, 2026**
**9:00 – 12:00 Artificial Intelligence $ Machine Learning for Crystal Growth**

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High-fidelity atomistic simulations of alloy solidification.
Rodrigo Freitas, Massachusetts Institute of Technology

Atomistic simulations now achieve electronic-structure fidelity at the mesoscale, reshaping how these methods can be used to understand fundamental aspects of solidification. In this talk I will present recent work from my research group that uses high-fidelity atomistic simulations to study solidification in metallic alloys. I will discuss how machine learning potentials enable atomistic studies of increasingly complex chemistries with high fidelity, and I will highlight how these methods provide direct insight into the thermodynamic and kinetic processes governing solid-liquid interfaces, including chemical partitioning, solute trapping, and interfacial transport. Together, these developments establish atomistic simulation as a predictive framework for uncovering the fundamental physics of solidification and point to a broader role for these methods in informing materials processing.

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Data-driven coarse-graining: Discovering continuum scale models from atomistic simulations.
Amit Samanta, LLNL

Understanding solid nucleation in liquids and the dynamics of solid–liquid interfaces under extreme non-equilibrium conditions (e.g., large temperature gradients) remains a major challenge, particularly in regimes where conventional continuum models break down. Advances in high-performance computing have enabled atomistic simulations of systems containing billions of atoms, providing direct access to these phenomena at unprecedented scales. Here, we present a physics-informed, data-driven framework to discover governing partial differential equations (PDEs) for predictive phase-field (PF) and phase-field crystal (PFC) models directly from large-scale molecular dynamics (MD) simulations. Atomistic data are first coarse-grained into scalar fields, from which spatial and temporal derivatives are computed to construct a candidate library of terms. Sparse regression techniques are then employed to identify the underlying PDEs. The resulting models for crystallization and solid–liquid interface dynamics are validated against MD simulations, demonstrating strong agreement. These results highlight the potential of data-driven approaches to bridge atomistic and continuum scales in modeling complex materials phenomena.
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and funded by LDRD Program at LLNL under project tracking code 25-ER-002.

Predicting antimalarial activity modes in hematin crystallization using a priori machine learning.
Hariharan Annadurai, University of Houston

Resistance to frontline antimalarial drugs has created an urgent need for new strategies to disrupt key biological processes in Plasmodium parasites, the causative agents of malaria. One of the most effective drug targets is hematin crystallization, a detoxification pathway essential for parasite survival. Efforts to rationally design hematin crystallization inhibitors and potential antimalarials are stalled by the lack of understanding of how the structure of an organic molecule defines its molecular mode of action in inhibiting hematin crystallization. By predicting how compounds interfere with crystal growth rather than merely whether they inhibit it, our findings enable a more strategic and targeted approach to antimalarial development. We present a general model that correlates the molecular structures of antimalarial drugs to their inhibition mode of action. We categorize growth-active sites on hematin crystal surfaces by subtle differences in their atomic structures and identify the molecular properties that underlie the selective binding of known drugs to these sites. We use the found properties to predict the likely behavior of potential antimalarials. To test the model, we formulate an a priori prediction of the inhibition mechanism mobilized by an FDA-approved antimalarial, tafenoquine, before testing in an experiment. These analyses consistently identify tafenoquine as a kink blocker—a prediction confirmed by experimental measurements of crystal growth dynamics. This work establishes a novel quantitative framework for predictive mechanistic classifications of crystal growth inhibitors, opening new directions for rational drug repurposing, synergistic combination therapy, and the design of next-generation antimalarials.

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Identifying useful nanocrystal morphologies using advanced sampling techniques and machine learning.
Kristen Fichthorn, Penn State

Metal nanocrystals have the capability to revolutionize established technologies and will feature in many upcoming technologies. For most established applications, there is ample evidence that the efficacy of a nanocrystal is sensitive to its shape and fine details of its structure. Thus, there is significant impetus to be able to predict and characterize fine details of nanocrystal structure. We use parallel tempering molecular dynamics (MD) simulations, accelerated MD, and machine learning (ML) to quantify equilibrium shapes of Ag, Cu, Ag-Cu, Pt, Pd and Pt-Pd nanocrystals. In our approach, we describe the nanoparticles with Machine Learning Force Fields (MLFF) with high fidelity to first-principles density functional theory. We find equilibrium nanocrystal shapes can change significantly with temperature, indicating that the nanocrystal shape with the minimum potential energy (at zero K) is not necessarily the shape seen at a higher temperature in an experiment. Moreover, the preferred nanocrystal shapes at low temperatures change drastically with size. These qualitative features have significant ramifications for experiments: It can be vastly more important to understand the free energies of nanocrystals than potential energies. The shapes of fcc metal nanoparticles are typically quantified in terms of perfect morphologies: octahedron, icosahedron, decahedron, etc., but such shapes only arise for certain “magic numbers” of atoms that give the crystal a perfect shape. Here, we analyze and quantify both ideal

and non-ideal nanoparticle morphologies using ML. We classify distinct shape classes with seemingly little order to the eye, and these can have the minimum energy. Our work uncovers catalytically significant morphologies for bimetallics, which include single-atom alloys, core@shell, and patchy particles. Our approach has much promise for understanding and categorizing nanocrystal shapes and designing synthesis and processing routes for achieving these shapes.

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TBD
Katie Colbaugh, Leucite

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Nucleation and growth of grain boundary phases.
Timofey Frolov, LLNL

Grain boundaries (GBs) profoundly influence the properties and performance of materials, emphasizing the importance of understanding their structure and properties. Recent advances in atomistic structure prediction methods and atomic-resolution microscopy have demonstrated that GBs can exist in multiple competing phases and exhibit first-order phase transformations that can lead to dramatic changes in materials properties.
GB phase transformations represent examples of nucleation and growth in two dimensions, where a new interfacial phase nucleates and propagates within the grain boundary plane. Similar to surface phase transitions, the transformation proceeds through the formation and migration of a 1D line defect separating two distinct two-dimensional phases. However, GB phase transformations possess unique characteristics because they are internal interfaces embedded within an elastic crystalline solid. Little is known about the topological nature of these GB line defects, their energy, anisotropy, mobility and how these properties influence nucleation and growth of a new GB phases.
In this talk, I will present a recently developed nucleation theory that quantifies the energetics of grain boundary phase transformations and describes the elastic nature of grain boundary phase junctions. The work will show that the line defects separating competing GB phases are not merely 1D phase boundaries, but also dislocations with a climb component and elastic line forces carrying both Burgers vector content and force monopoles. These elastic contributions strongly influence the nucleation barrier, metastability, and kinetics of GB phase transformations. I will also discuss recent computational and experimental studies of segregation-induced GB phase transformations in multicomponent alloys, including the emergence of unusual interfacial states with icosahedral symmetries. Finally, I will highlight the role of advanced grand-canonical structure prediction methods in enabling systematic exploration of GB phase behavior in multicomponent systems.

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Machine Learning and Artificial Intelligence for Chemistry and Materials.
Teresa Head-Gordon, Departments of Chemistry, Bioengineering, and Chemical and Biomolecular Engineering, University of California, Berkeley

The size of chemical space is vast. This makes application of first principles quantum mechanical and advanced statistical mechanics sampling methods to identify binding motifs, conformational equilibria, and reaction pathways extremely challenging, even when considering better physical models, algorithms, or future exascale computing paradigms. If we could develop new and robust machine learning approaches, ideally grounded in physical principles or heuristic scaling laws, we would be able to better tackle many fascinating but quite difficult chemical, biological, and materials systems. At present, the application of machine learning to (bio)chemistry and materials is still in its infancy, and I will describe end-to-end deep learning applications ranging from potential energy surfaces and property predictions to chemical to biophysical systems, and the emergent properties of chemistry from large language models.

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**Tuesday, June 9, 2026**
**19:30 – 20:15 Plenary II**

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Self-assembly and crystallization at protein-inorganic interfaces.
Jim De Yoreo, PNNL

From harvesting solar energy to capturing CO2 to purifying water, living organisms have solved some of the most vexing challenges now faced by humanity. They have done so by creating a vast library of proteins and other macromolecules that can assemble into complex architectures and direct the mineralization of inorganic components to produce materials characterized by a hierarchy of structure. While the high information content contained within the intricate sequences of the proteins is crucial for accomplishing these tasks, self-assembly and mineralization are nonetheless constrained to proceed according to the physical laws that govern all such processes, even in synthetic systems. An understanding of the mechanisms by which biological systems successfully manipulate those laws to create hierarchical materials would usher in an era of materials design to address our most pressing technological challenges. In this talk, I will present the results of recent research using in situ atomic force microscopy, in situ transmission electron microscopy to directly observe interfacial structure, protein self-assembly, and nanocrystal formation in biomolecular and biomimetic systems, including protein-directed nucleation of calcium carbonate and surface-directed nucleation of two-dimensional protein assemblies. The underlying interactions and structural controls that lead to the observed behavior are understood by applying molecular-to-coarse grain simulations. The results elucidate the mechanisms

by which the interface between biomolecules and materials directs nucleation, self-assembly and crystal growth, leading to unique materials and morphologies. These findings reveal the importance of electrostatics, epitaxial relationships, interfacial solvent structure, and shape complementarity — or, more generally, the balance of protein-substrate-solvent interactions — in determining how organized materials emerge in these systems.

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**Tuesday, June 9, 2026**
**20:20 – 21:10 Colloidal Crystallization II**

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Computational self-assembly of diverse colloidal crystal and cluster structures.
Julia Dshemuchadse, Cornell University

Colloidal metamaterials can adopt a wide range of intricate structures via nanoparticle self-assembly, with promising applications in plasmonics and photonics. The properties of the resulting clusters or extended structures are highly tunable through their geometry. Colloidal nanoparticles are often modeled as hard and spherical; however, particles that are functionalized with ligands, carry surface charges, or that are made from deformable materials violate this assumption. Using coarse-grained molecular dynamics simulations, we model the assembly of small clusters and mesoscopic crystal structures composed of soft spheres. Softness and particle sizes strongly affect the geometries of the assembled cluster and crystal structures. By connecting the effects of particle properties to the assembled structures, our findings will guide targeted synthesis and growth of novel and tunable colloidal materials in the future.

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Can hydrodynamic interactions explain anomalously fast nucleation in weakly-supersaturated colloidal fluids?
Ying-Shuo Peng, University of Pennsylvania

Although molecular simulations have been extremely useful for unraveling some of the mechanistic details of colloidal crystal nucleation, a longstanding issue is that simulations consistently underpredict nucleation rates in weakly supersaturated hard-sphere systems, sometimes by orders-of-magnitude [1]. This is true for both direct simulations of crystal nucleation and enhanced sampling approaches [2,3]. Recently, hydrodynamic correlations between particles due to the solvent have drawn attention as a potential explanation for this mystery. Yet, computational studies that include hydrodynamic interactions (HIs) have mostly shown relatively small effects that arise due to the impact of HIs on single particle attachment kinetics on an already-formed critical

nucleus [4,5].

Here, we consider the impact of HIs on density fluctuations in a metastable colloidal fluid as a potential explanation for the discrepancy between simulation and experiment. Brownian Dynamics (BD) simulations are used to simulate systems without HIs, while Multiparticle Collision Dynamics (MPCD) [6] simulations are used to capture the effect of HIs. We first employ the total intermediate scattering function, F(k,t), to study the impact of HIs on density fluctuations. Our results reveal that in MPCD, density fluctuations decay much more slowly than in BD, suggesting that the enhanced lifetime of pre-critical density fluctuations due to HIs may be crucial for forming large nuclei, especially under weak supersaturation conditions. Moreover, we find that the density-field-stabilizing effect from HIs becomes even more pronounced at larger length scales (lower wavevectors), higher volume fractions, and weaker interparticle interactions—all of which are characteristic of the weakly supersaturated hard-sphere regime where simulation-experiment discrepancies are most severe [1]. We also find that HIs alter the mobility of the colloidal fluid along certain collective directions identified by Principal Component Analysis. Specifically, we find that HIs promote mobility along highly cooperative directions, while inhibiting mobility along non-cooperative directions. We tie these two elements together into a simple model of nucleation to suggest a plausible mechanistic explanation for the long-standing discrepancy.

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[2] K. E. Blow, D. Quigley, and G. C. Sosso, J. Chem. Phys. 155, 040901 (2021).
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[5] M. Tateno, T. Yanagishima, J. Russo, and H. Tanaka, Phys. Rev. Lett. 123, 258002 (2019).
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Control over crystallization from metastable mineral precursors by manipulation of polyelectrolytes.
Thomas Schroeder, North Carolina State University

Minerals often crystallize from solution via pathways that involve metastable amorphous intermediate phases. The lifetime of these phases can be greatly extended by multiply-charged additives such as antiscalants and biomacromolecules. In some cases, such additives direct the formation of viscoelastic mineral-dense droplets that can wet substrates before nucleation, imparting morphological control down to the nanoscale; such “polymer-induced liquid precursors” have been implicated in biomineralization processes such as the intrafibrillar mineralization of collagen during bone growth.
This talk will present our recent progress on manipulating precursors to crystalline minerals in solution. Inspired by observations in the collagen system, we have developed a strategy for triggering the crystallization of carbonate salts on-demand and in controlled patterns from metastable solutions by exploiting the polyelectrolyte character of the stabilizing additives. We have found it productive to consider polyelectrolyte-stabilized liquid precursors as complex coacervates. By creating conditions in which the polyelectrolytes experience a strong driving force to leave behind their ionic cargo, we demonstrate that we can controllably destabilize precursor phases, yielding prompt crystal formation in solutions that would otherwise remain fully amorphous for several days. We find that confining the destabilizing conditions to specific locations enables crystallization in patterns; further, varying the solution composition in a manner that modulates coacervate driving forces impacts the effectiveness of the trigger. This study provides an unconventional conceptual framework for understanding and manipulating additive-mediated precursors that suggests both relevance to physiological processes and new possibilities for manipulating crystallization processes in engineered contexts.

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High-resolution structural studies at the interface of biology and materials science.
Brent Nannenga, Arizona State University

From biological molecules to inorganic materials, high-resolution structural approaches are key to understanding how these systems function. This presentation will focus on the use of advanced electron microscopy methods and the intersection of these approaches in the fields of structural biology and materials science. We will present the use of single particle cryo-EM to study the protein-inorganic interface of the model biomineralization protein ferritin. This approach produced a 2.85 Å structure of the ferritin-iron oxide nanoparticle complex where key protein-nanoparticle interactions could be visualized. Additionally, the cryo-electron microscopy method of microcrystal electron diffraction will be presented along with applications for crystallographic

analysis of biomolecules and materials.

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Clustering of Zn in Ectopic Biominerals at the Biological Interfaces in the Temporomandibular Joint and the Kidney.

Sunita Ho, University of California San Francisco

Ectopic biominerals occur in multiple organs and their cause remains unknown. The pathobiology and physicochemical characteristics of ectopic minerals have been investigated over several decades (1, 2). Osteoarthritis and nephrolithiasis, two distinctly different and globally prevalent common diseases are clinically diagnosed by exploiting mineral density variations in the temporomandibular joint (TMJ) and the kidney using X-rays. Mechanical overloading can tip the TMJ into chronic oxidative stress and disrupt the homeostatic balance within tissues and across interfaces (3). Chronic oxidative stress resulting from metabolic disorders, hypoxia, hyperosmolality, and drug and toxic exposure can occur in patients with nephrolithiasis (renal stone) in a kidney (4). Despite the obvious organ-specific disparities in these tissues and their function, the common denominator in osteoarthritis and nephrolithiasis is elevated chronic oxidative stress. Ensuing pathobiology is identified as elevated levels of reactive oxygen, nitrogen, and sulfur species with irreversible cell damage (autophagy and apoptosis). Resulting byproducts include “cell debris” and increased extracellular Zn levels due to apoptosis and/or autophagic degradation of metallothioneins (MTs), proteins that are involved in the control of available zinc in cells (5). In this study, we will analyze the interfaces across dissimilar cartilage and bone of the TMJ, and the mineralized papillary tissue/zone (MPZ) and calcium oxalate (CaOx) stone in a kidney by using high resolution microspectroscopy. Spatial maps of elements, and coordination chemistry of sulfur (S) and zinc (Zn) at cartilage-bone and the MPZ and stone interfaces were acquired to illustrate oxidative stress. Surgically removed osteoarthritic condyles with minimal cartilage revealed Zn-rich nodules. Quantifiable levels of S, Zn, calcium (Ca), and phosphorus (P) were identified with laser ablation-ICPMS from cartilage to bone. Multiple sulfur species within the OA cartilage and bone, and MPZ and stone were observed using X-ray absorption near edge spectroscopy and X-ray fluorescence imaging. The commonly identified CaOx stones also contained appreciable levels of sulfur and zinc. Higher levels of organic and inorganic sulfates were observed in OA cartilage and bone compared to control, and in CaOx stones. Zn-rich nodules in OA cartilage and mineralized papilla contained Zn bound phosphates, and to a lesser extent carbonates and sulfates with the remainder being the commonly reported hydroxylapatite in tissues with no discernable cells. Elevated Zn (compared to controls) with increased organic and inorganic S-species suggest that the chemistry across the interfaces from distinctly different diseased organs is similar. These nuances in S-species from regions containing lower and higher Zn levels in osteoarthritic yet sulfated cartilage of the TMJ and MPZ with CaOx stone in the kidney will be discussed within the context of pathobiomineralogy.

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Template-directed toxicity sink: molecular mechanisms of lithium-mediated Aβ42 oligomer–fibril interconversion.

Radhika Sunil Menon, University of Houston

The self-assembly of Amyloid-beta 42 (Aβ42) into supramolecular aggregates is a hallmark of neurodegenerative disorders such as Alzheimer's disease, facilitating molecular-level insights into aggregation kinetics and pathways. Soluble oligomeric species are strongly associated with pathological dysfunction, whereas their conversion into stable, β-sheet-rich fibrils represents a critical phase transformation that can mitigate toxicity by sequestering these oligomeric species into less reactive architectures. Lithium ($Li^+$), which has been implicated in modulating amyloid pathology, may influence these assembly pathways, yet the fundamental mechanisms governing $Li^+$-mediated nucleation and growth dynamics remain poorly understood due to the limitations of conventional bulk measurements.

In this study, we utilize time-resolved, quantitative high-speed atomic force microscopy (HS-AFM) to achieve real-time, high-resolution monitoring of Aβ42 self-assembly and phase transformations. This approach enables the direct evaluation of parallel processes including primary nucleation, fibril growth, and the emergence of new assemblies at the organic interface. By studying the evolution of these protein structures in situ at biomimetic peptide and $Li^+$ concentrations, we provide molecular-level evidence of how ionic environments bias the assembly landscape toward specific morphological outcomes.

Our results document a key role for $Li^+$ in modulating the interconversion from disordered oligomers to ordered fibrillar architectures. We identify two distinct mechanisms of assembly modulation in the presence of $Li^+$. First, we observe accelerated secondary nucleation and the association of soluble species into stable, branched fibrillar networks. Second, we characterize the promotion of higher-order organization through the bundling of individual fibrils into thickened, stable morphologies that resist fragmentation. We propose that, under our experimental conditions, $Li^+$ partially screens the negative charges of carboxylate groups on aspartate and glutamate residues exposed on fibril surfaces. This reduction in electrostatic repulsion lowers the energetic barrier for molecular attachment and facilitates the sequestration of monomers and oligomers onto the fibril template.

By defining the biophysical mechanisms that govern these phase transformations, this work advances our understanding of how small-molecule and ionic modulators can control the morphology and stability of protein aggregates. These findings offer a framework for connecting fundamental principles of self-assembly with applications in biomimetic materials and therapeutic design.

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Mesoporous frameworks engineered from crystallizable collagen-mimetic peptide amphiphiles.
Andrea Merg, University of California, Merced

While proteins serve as nature's building block of choice for constructing complex and functional architectures, peptides represent an attractive, synthetically accessible alternative. Peptides can mimic several features of proteins, including common protein folding motifs (e.g., alpha helices, coiled coils, collagen triple helices, etc.) and various biological functions. Moreover, due to their relatively short sequence length, peptides are amenable to a myriad of bioorganic chemical transformations, which affords the ability to incorporate a broad range of nonnatural moieties into the sequence design. These features position peptides as robust, sequence-programmable building blocks for constructing bioinspired materials with properties and functions that extend beyond the proteome. However, despite their advantages, the truncated sequences of peptides often relegate their assembly to forming primarily lower-dimensional architectures with limited structural and functional complexity. Higher dimensional, porous materials are of special interest as their structural features (e.g., high surface area and confined porous channels), play a critical role for a broad range of applications in catalysis, storage, separations, and sensing. Current porous frameworks are, for the most part, restricted to non-biological assembly platforms such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). In this presentation, I will discuss our lab's exploration into the development of 3D mesoporous crystalline frameworks that are assembled from amphiphilic collagen-mimetic peptides (aCMPs). We reveal that the combination of hydrophobic and electrostatic intermolecular interactions directs the assembly of aCMPs into extended crystalline frameworks with porous 1D channels. We demonstrate that the physical features of the porous architectures can be systematically modified via altering the aCMP building block design. From TEM and SAXS data, we propose an assembly model that accounts for the structural features of the assembled structures. These results demonstrate the potential for peptides to serve as an alternative biocompatible and chemically rich building block for creating functional and programmable, porous materials.

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The structural landscape of amyloid-β oligomerization by high-speed AFM.
Nghia D. Nguyen, University of Houston

Amyloid-β (Aβ) aggregates, oligomers in particular, have emerged as the main carrier of neurotoxicity in Alzheimer's dementia and research focus for drug design and discovery. Our understanding of oligomer and fibrils and more complex assemblies of the two thus far have been garnered mostly from bulk analyses, ensemble-averaging, and static techniques, providing limited insights into these aggregates at the single-aggregate level. Although advancements have elucidated fibril structural and dynamics, oligomers and amorphous aggregates studies are still a hurdle because they are small, heterogeneous, and transient. Here, we overcome this obstacle by leveraging high-speed high-resolution atomic force microscopy with image acquisition rate

up to 77 frames per second. The structure and dynamics of the Ab42 oligomers and their assemblies diverge significantly from those of fibrils. As a first step, we show that amorphous aggregates, considered a third outcome of Aβ aggregation, besides oligomers and fibrils, represent clusters of oligomers and not conglomerates with a distinct molecular structure. We demonstrate that the oligomers are heterogeneous, comprised of two to 20 peptide chains, and do not grow. The number of assembled oligomers remains constant after four- and 10-fold Aβ42 concentration increases. The observed zeroth-order kinetics defies the generally accepted nucleation–and–growth scenario of oligomer formation. Our findings are consistent with a mechanism of oligomerization as a chemical reaction yielding products with predefined stoichiometries. The proposed pathway is significantly simpler than the current paradigm. It suggests that oligomers form at any Ab concentration, with no critical threshold, and may guide the rational design of inhibitors of oligomer assembly as potential Alzheimer's drugs.

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Organization and complexation of an extracellular matrix protein with Ca2+ ions.
Jong Seto, Arizona State University

Many biomineralized tissues rapidly organize an organic scaffold accompanied by mineralization processes in their formation processes. In the sea urchin, a similar scheme is observed in the formation of its larval spicules. We investigate the role of the most abundant matrix protein, SM50, and observe that this protein is an active inhibitor of mineral nucleation. By stabilizing a hydrated amorphous calcium carbonate phase, SM50 prevents premature intracellular mineralization—enabling transport across and subsequent, assembly of mineralized tissues in the extracellular space. We demonstrate that SM50 is a vital component in the organization of the initial events of mineral growth and assembly of sea urchin larvae spicules. Specifically, a spicule matrix protein SM50 is observed to assemble into a highly ordered scaffold in the presence of water, forming a scaffold that allows for binding of $CaCO_3$ mineral species. In this work, we demonstrate that through the C-type lectin domain SM50 in its monomeric form can assemble to form a larger, ordered structures. Through a diverse set of in situ methods, we show in real-time the SM50-composed scaffold is a highly organized complex and is essential in the orientation and epitaxial growth of calcite-related spicules.

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Programming Crystal Composition through Polymer-Controlled ACC Transformation.
Stephan Wolf, Friedrich-Alexander University

How can foreign components be incorporated into crystals when direct lattice doping is unfavorable? Biomineralization suggests an alternative route: encode composition first in an amorphous precursor, then transfer, redistribute, or reject components during crystallization. Using calcium carbonate as a model system, we examine amorphous calcium carbonate (ACC) as such a chemically programmable precursor.

Our results show that ACC composition is not dictated simply by bulk solution composition or solubility trends. Instead, carbonato–calcium coordination clusters act as compositional gatekeepers. Their specific interactions with small organic ligands, polycarboxylates, and foreign ions control both nucleation inhibition and incorporation into the amorphous phase, leading to highly ion-specific behavior for Mg, Sr, and Ba.
Polymeric agents provide a second level of control by modulating ACC stability, hydration, mobility, and its pseudomorphic transformation into crystalline calcium carbonate. Thus, pseudomorphic transformation is not merely a morphology-preserving amorphous-to-crystalline pathway, but a chemically active route through which precursor composition and nanoscale organization can be translated into the final crystal.
This precursor-mediated strategy offers a general principle for incorporating otherwise difficult components into crystals under mild conditions and helps explain how biominerals achieve chemical complexity beyond classical growth models.

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**Wednesday, June 10, 2026**
**19:30 – 21:10 Epitaxial Crystal Growth II**

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Modeling SiGe quantum dot variability induced by interface disorder reconstructed from multi-perspective microscopy.
Ezra Bussmann, Sandia National Laboratories

Nano-scale quantum dot (QD) qubits in SiGe exhibit competitive quantum characteristics, e.g. long coherence times, required of future quantum information technologies. A challenge in developing the SiGe platform lies in understanding relationships between interface structure and quantum electronic properties.
For example, atomic disorder at Si/SiGe interfaces is theoretically predicted to strongly modulate the conduction band valley spitting (VS). This atomic-scale interface structure-to-electronic-function relationship may be a determining factor in manufacturability of SiGe qubits. Yet, to simply measure, deconvolve, and visualize solid-embedded few-atomic-layer interface structures spanning any appreciable volume is extremely challenging. Interfacial atomic disorder descriptions that span over application relevant ensembles are only partially tractable with post-synthesis microscopy (transmission electron microscopy) or tomography (atom-probe tomography), owing to issues such as image convolution and limited sampling volumes. To yield more comprehensive multiscale yet atomistic heterointerface descriptions, we use a multimodal microscopy approach. By convolving data from scanning tunneling microscopy and high-angle annular dark field scanning transmission electron microscopy, we reconstruct 3D interfacial atomic structure and employ an atomistic multi-valley effective mass theory to quantify qubit spectral variability. The results indicate (1) appreciable VS variability of ~50%

owing to alloy disorder and (2) roughness-induced double-dot detuning bias energy variability of order 1–10 meV depending on well thickness. For measured intermixing, atomic steps have negligible influence on VS, and uncorrelated roughness causes spatially fluctuating energy biases in double-dot detunings, potentially incorrectly attributed to charge disorder. Our approach yields atomic structure spanning orders of magnitude larger areas than post-growth microscopy or tomography alone, enabling more holistic predictions of disorder induced qubit variability and of significance for understanding performance limits in quantum electronics applications. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

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Oxide thin films for electronic and optical applications.
Wilfrid Prellier, Centre National de la Recherche Scientifique (CNRS)

Transition metal oxides with perovskite structures are a compelling and technologically vital class of materials, renowned for their rich array of ordering phenomena—including ferromagnetic, orbital, and charge ordering. These phenomena often interact and coexist in intricate, dynamic ways, giving rise to multifunctional properties such as piezoelectricity and magnetoelasticity, which can be tuned through external stimuli like electric, magnetic, or mechanical fields.
This presentation focuses on the growth of vanadium oxide thin films using pulsed laser deposition, examining their synthesis on both single-crystal and unconventional substrates, such as glass templates. We will discuss how key parameters, such as growth temperature and film thickness, influence the structural and functional properties of these films. Finally, we will explore the promising applications of these materials in fields such as electronics and optics, highlighting their potential for next-generation technologies.

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Analytical x-ray solutions for thin film and wafer analysis.
Destiny Lopez, Malvern Panalytical

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Correlating epitaxial growth and electronic properties of crystalline high-k metal oxides on 2D materials.
Rishabh Kothari, Massachusetts Institute of Technology

Reliably forming heterostructures and controlling the properties of interfaces between 2D materials (mainly semiconductors) and 3D materials (dielectrics and metals, is essential to enable the integration of 2D materials into future highly scaled microelectronics. High-k gate dielectrics – primarily hafnia (HfO2) and related oxides – are required to maintain low leakage current and excellent control of gate electrostatics for ultrathin channels. Atomic layer deposition (ALD) is a well-established for forming dielectric oxides on Si transistor channels, but has issues in applications involving 2D materials due to incompatibility between van der Waals materials and the chemistry and mechanisms of ALD. To overcome this challenge, we explore a two-step process nicknamed EpiOx: (1, Epi) the growth of ultrathin films of a metal with epitaxial relationship and atomically-sharp interface with the 2D substrate followed by (2, Ox) well-controlled oxidation to form a continuous ultrathin dielectric layer. This process allows microstructure and phase control of the resulting oxide, which can act as a seed layer for subsequent ALD. It also provides a means to engineer the 2D/ 3D dielectric interface for lower defect densities. In this presentation, we show studies of controlled oxidation of ultra-thin Hf metal on graphene and MoS2, including wafer-scale processing and transmission electron microscopy (TEM) of phase transformations with atomic resolution.

In prior work, we showed that EpiOx can produce atomically-sharp epitaxial graphene-HfO2 interfaces and can stabilize less-common HfOx phases. Here, we reveal the dynamics of this process using in situ environmental TEM (ETEM) to study metal oxidation. This provides a view into the kinetics and corresponding temperature regimes relevant for different stages of hafnium oxidation. We find that the range of 300-400$^{o}$C produces metastable (possible novel) hexagonal oxide phase. Further oxidation leads to the equilibrium monoclinic phase that is remarkably stable during heating and ETEM imaging, both in vacuum and under oxygen flow. We further describe how the details of preparing TEM sample grids compatible with in situ heating that has led to additional findings: (1) the impact of cleaning surfaces proximate to the sample within the UHV deposition chamber and (2) an amorphous-to-epitaxial oxide transformation similar to solid state epitaxy.

We then extend these insights to the device and wafer scales using a deposition chamber that achieves the essential cleanliness of ultra-high vacuum (UHV) conditions required for metallic Hf deposition. Finally, we present the dielectric properties of the HfO2 layer and interface trap densities measured via impedance spectroscopy using metal-insulator-metal capacitors (MIMs) to explore correlations between electrical properties and processing conditions. Our results encourage continued research on 2D-3D heteroepitaxial film processing to address a range of challenges with 2D materials integration with specific focus on the “EpiOx” process for forming highly reliable, high-performance semiconductor-dielectric interfaces.

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**Thursday, June 11, 2026**
**9:00 – 12:00 Fundamentals of Crystallization II**

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From colloidal nano building blocks to higher order architectures.
Ou Chen, Brown University

Organization of colloidal nanocrystals into larger scale superstructures is a promising approach for integrating the intriguing microscopic properties of single nanocrystals into macroscopic forms relevant in technology. Especially, continuous developments and optimizations in nanocrystal synthesis and characterization have allowed the production of nanocrystals with exquisitely controlled size, shape, composition, and surface states. Analogous to atoms/molecules, these high-quality nanocrystals can be used as artificial building blocks for constructing higher-order architectures with unique advantages. In particular, when utilizing in assembly, designed nanocrystals can display directional, asymmetric interactions induced by their shape, composition, and anisotropic patchiness, which may complicate the formation of ordered structures compared to the conventional assemblies. In this talk, I will use several different types of colloidal quantum dots and metallic nanocrystals created in my lab as examples to demonstrate how we assemble them into unprecedented superstructures through asymmetric interactions among the building blocks. Importantly, the obtained nanocrystal superstructural materials possess both particle translational ordering and atomic orientational alignment. Examples include conventional crystalline superlattices, aperiodic quasicrystalline and quasicrystalline-approximant and Martensitic in-transition superlattices. The dominating driving forces lead to the obtained architectures are identified through both experimental results and computer simulations/computations.

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The Impact of Wadsley defects and cation disorder on improving MoNb12O33 diffusion.
CJ Sturgill, University of South Carolina

Wadsley-Roth (WR) niobates are promising battery materials due to how their crystal structure accommodates electronic and ionic transport. The WR structure contains (n×m) blocks of corner sharing ReO3-type octahedra connected along shear planes with edge sharing. Here the block region is associated with rapid ionic transport down the open channels whereas the orbital overlap along the shear plan is associated with electronic transport. The roles of defects in such structures remain poorly understood where several prior reports correlated crystallographic defects with enhanced transport characteristics. One under scrutinized aspects is how many WR defects are fundamentally coupled with each other and rarely are capable of forming as a singular defect type. This study examines how each likely defect type affects transport in these materials using a combination of experimental and computational methods. Defect-rich

MoNb12O33 (MNO) samples were compared with order-rich ones prepared different crystallization temperatures. The atomic structure was characterized using a combination of X-ray techniques such as XRD, XANES, and EXAFS, along with atom-resolved STEM. X-ray adsorption spectroscopy identified different local Mo environments in the two samples, confirming cation disorder, while STEM revealed numerous Wadsley defects in the disorder-rich sample. Battery measurements confirmed substantially enhanced transport characteristics in the defect-rich sample, including the ability to cycle 10k times with ~74% capacity retention. Measurements of solid-state lithium diffusivity suggested variation of the progressive lithium ordering for the defect-rich vs order-rich samples. Molecular dynamics with machine-learning interatomic potential (MLIP-MD) were used to investigate numerous defect models to understand the roles of each candidate defect type. In contrast to the order-rich model, it was observed that both defect types led Li to populate fast diffusion paths (window sites) at lower lithiation levels.

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Solvent-dependent relative stability of crystal forms.
Rohith Pulluri, University of Houston

Polymorphism, the ability of a molecule to exist in different crystalline forms with distinct physical properties, is a phenomenon of critical importance in chemical industry, particularly in the production of active pharmaceutical ingredients. Mefenamic acid (MFA), a non-steroidal anti-inflammatory drug, exhibits at least three neat polymorphs (I, II, III) with distinct MFA conformations. Under ambient conditions, the order of stability of the first two polymorphs is I > II. Numerous recent studies have claimed that solvents only affect the kinetics of polymorphic transformations and do not modify the relative thermodynamic stability of polymorphs. Here we challenge this notion. We demonstrate that the relative stability of MFA Forms I and II is dependent on the solvent in which the crystals grow. To identify and characterize the polymorphs, we employ Raman spectroscopy, solid-state nuclear magnetic resonance (SS-NMR), powder X-ray diffraction (PXRD), microcrystal electron diffraction (microED), and differential scanning calorimetry. We find that the relative differences in Gibbs free energy, enthalpy, and entropy of crystallization of MFA Forms I and II strongly depend on the solvent and that at low temperature in formamide there is a reversal in stability (II > I). This finding is supported by a competition slurry along with Raman, SS-NMR, PXRD, and microED characterizations of the competing forms. All-atom molecular dynamics simulations reveal that the transformations between MFA solution conformations and those in Form I and II crystals take longer times than MFA ingress into crystal growth sites, creating a population of growth-incompetent molecules that are incapable of joining a crystal. These times are solvent- and temperature- dependent and their balance favors crystallization of Form II at lower temperatures in formamide, whereas Form I is preferred at the other three sets of conditions. The found solvent-dependent polymorph stability via the balance of growth-competent and incompetent solute conformations enables additional pathways for polymorph control.

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Coupling catalyst activity and degradation: modeling oxygen evolution reaction with surface dissolution on IrO2(110).
Rhys Bunting, LLNL

Modeling the coupling of surface reactions with dissolution is considered for IrO2(110) using graph Kinetic Monte Carlo. Elementary steps, including oxygen evolution reaction and iridium dissolution is considered using density functional theory. The mechanism for surface dissolution is identified along with the reactivity of intermediate surface states between fully dissolved layers. Partially dissolved layers are found to be more active for oxygen evolution reaction, yet their residence time compared to the pristine surface is marginal, causing the reactivity of the pristine surface to be a good approximation of overall surface reactivity.
With both a TOF and rate of dissolution calculated, a catalyst TON is also presented. The presented methodology is general and can be applied to other reactive systems, such as corrosion.

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Atomic-scale insights into calcite dissolution kinetics in nonstoichiometric solutions and the role of $Mg^{2+}$ ions.
Shuhong Song, PNNL

Calcite is a key model system for understanding crystal growth and dissolution. Calcite dissolution has attracted extensive attention due to its environmental and industrial importance. Despite extensive studies of calcite dissolution across a wide range of undersaturation conditions, current rate laws largely neglect the role of solution stoichiometry, particularly calcium-to-carbonate activity ratios (a[Ca^(2+)]/a[CO_3^(2-)]). Because this ratio directly governs the relative availability of Ca^(2+) and CO_3^(2-) at calcite step edges, it provides a powerful handle to probe the molecular processes of calcite dissolution. In particular, the distinct atomic structures of acute and obtuse steps are expected to lead to different sensitivities to a[Ca^(2+)]/a[CO_3^(2-)] ratio. Furthermore, establishing this framework provides a basis for understanding how external ions, such as $Mg^{2+}$, modify these fundamental processes. Here, in situ atomic force microscopy (AFM) was used to investigate dissolution on calcite $\{10\bar{1}4\}$ surfaces under systematically varied a[Ca^(2+)]/a[CO_3^(2-)] ratios and Mg^(2+) concentrations. Dissolution anisotropy, defined here as the relative retreat rates of acute and obtuse steps, is shown to be strongly controlled by solution stoichiometry. Acute steps exhibit maximum rates at a[Ca^(2+)]/a[CO_3^(2-)] ≈ 1, whereas obtuse steps remain suppressed at low ratios and become active under Ca-rich conditions. Mg^(2+) introduces a threshold-like inhibition, strongly suppressing obtuse steps in a ratio-dependent manner. Kinetic Monte Carlo (KMC) modeling enables full utilization of the experimental datasets, including both pit morphology and step velocity trends, to elucidate the underlying mechanisms. The results reveal that dissolution anisotropy arises from the competition between carbonate-mediated suppression of kink propagation at obtuse-related sites and Mg^(2+)-induced site-specific inhibition that progressively modifies propagation pathways. Car-

bonate ions effectively block obtuse-step retreat, whereas Mg^(2+) exhibits weaker but threshold-dependent effects, primarily affecting the most open step configurations without fully suppressing dissolution.

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Crystallization entropy: constituents and contributions to crystal form stability.
Alejandro C Veliz, University of Houston

Crystal polymorphism arises from the ability of a solid-state to adopt at least two distinct crystal forms due to differing arrangements of the molecules. This common phenomenon largely impacts the pharmaceutical industry as each polymorph has different properties that include the solubility, dissolution rate, and overall bioavailability of a drug. Due to these differing properties, the focus in the field of polymorphism is to find ways of predicting different polymorphs using mostly computational methods. This is typically done by determining the crystal form stability via the free energy of crystallization, ∆G_cryst^°. Most models treat ∆G_cryst^° to be equivalent to the enthalpy of crystallization (∆H_cryst^°) and consider the entropic contributions (∆S_cryst^°) to be negligible. However, from our experimental results of mefenamic acid (MFA) Form I and Form II we display that they are not. Solubility measurements of MFA Form I in multiple solvents demonstrate that ∆G_cryst^° deviates from ∆H_cryst^° indicating a non-negligible entropic contribution to polymorph stability. Using all-atom molecular dynamics simulations, we show that positive deviations in ∆S_cryst^° relative to the entropy of the melt are attributed to the binding of solute and solvent, while negative deviations arise from the disruption of solvent structure. Experimental data has also shown that for MFA Form II, ∆S_cryst^° is significantly more negative than that of MFA Form I in both formamide and toluene. To resolve the origins of these entropy differences, enhanced sampling molecular dynamics simulations, including multithermal and multithermal-multiumbrella on-the-fly probability enhanced sampling, were employed to observe if differences in the conformational entropy change occurs between the two forms. The simulations indicate that the conformational entropy changes are equivalent between the two forms, eliminating the conformational flexibility as the driver for the observed differences in ∆S_cryst^°. Analysis based on MFA crystal slabs and corresponding distance maps, however, show that the entropy differences between the two forms correlates with differences in crystal compactness.

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Morphological Stability of Recrystallization Fronts in Polycrystals: Impurity Effects.
Moneesh Upmanyu, Northeastern University

The kinetics of recrystallized nuclei into a deformed matrix is of critical importance for engineering polycrystalline microstructures. These recrystallization fronts are marked with serrations that are usually attributed to an inhomogeneous distribution of stored energy of deformation that manifests as an organized dislocation substructure. Current understanding is based on continuum description of the elastocapillary intrinsic motion of the high angle grain boundary that forms

the font. In this study, we show that impurities fundamentally modify the stability of these recrystallization fronts. Guided by a linear stability analysis, we show that the stability of the front is controlled by an interplay between solute-drag and the segregation of impurities within the deformed sub-grains. As confirmation, a simple Ising model with segregating impurities shows spatial inhomogeneities in motion of the recrystallization front that is consistent with the theoretical predictions. The theoretical framework allows for development an AI-complete strategy for engineering alloys with controlled recrystallization rates and microstructures through spatio-temporal control over the morphology of recrystallization fronts.

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