User Science Plenary Session: Day 1

Monday, May 5, Afternoon

Session Chair: Stuart Stock, APS Users' Executive Committee Vice-chair (Northwestern University)

1:15 – 1:20	Stuart Stock, Vice-chair, APS Users' Executive Committee (Northwestern University) *Welcome; Announcement of the 2025 Gopal K. Shenoy Excellence in Beamline Science Award Winner (Kamel Fezzaa, Argonne National Laboratory); Announcement and Introduction of the 2025 Rosalind Franklin Young Investigator Award Winner*
1:20 – 2:00	Lin Gao – APS (Argonne National Laboratory) 2025 Rosalind Franklin Young Investigator Award Recipient *Metal Additive Manufacturing: From Printing Mechanisms to Microstructure Control*
2:00 – 2:40	Wei Bao – CNM (Rensselaer Polytechnic Institute) *New Room-temperature Playground for Bose-Einstein Condensates Using Halide Perovskites*
2:40 – 3:20	Daniel Shoemaker – APS (University of Illinois at Urbana-Champaign) *Functional Electronic Materials on the Verge of Stability*
3:20 – 3:40	Break
3:40 – 4:20	Deji Akinwande – CNM (University of Texas at Austin) CNM Keynote Presentation *Atomic Sheets for Nonvolatile Energy-efficient Systems and Hydrogen Clean Energy Materials*
4:20 – 5:00	Karena Chapman (State University of New York, Stony Brook) APS Keynote Presentation *X-ray Visions: Bringing Future Materials into Focus*
5:00	Adjourn

User Science Plenary Session: Day 2

Tuesday, May 6, Morning

Session Chair: Preston Snee, CNM Users' Executive Committee Chair (University of Illinois at Chicago)

8:30 – 8:35	Preston Snee, Chair, CNM Users' Executive Committee (University of Illinois at Chicago) *Welcome and Introduction of the 2025 Arthur H. Compton Award Winner Ian Robinson (University College London)*
8:35 – 9:15	Ian Robinson – APS (University College London) 2025 Arthur H. Compton Award Recipient *Bragg Coherent Diffraction Imaging at the Advanced Photon Source*
9:15 – 9:55	Dmitri Talapin – CNM (University of Chicago) *Advancing Synthetic Frontiers at the Intersection of Solid-state and Molecular Chemistry*
9:55 – 10:15	Break
10:15 – 10:55	Efrain Rodriguez – APS (University of Maryland, College Park) *Solid State Synthesis on the Beamline: What We Gain by Peering into the "Black Box"*
10:55 – 11:35	Su Ying Quek – CNM (National University of Singapore) *Light-matter Interaction in Nanoscale Materials from First Principles*
11:35	Adjourn

Metal Additive Manufacturing: From Printing Mechanisms to Microstructure Control

Lin Gao[1]

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Fusion-based metal additive manufacturing (AM) technologies have garnered considerable attention for their ability to rapidly produce near-net-shape or end-use metallic components, effectively addressing supply chain challenges across various industries. These processes utilize a highly concentrated energy source to rapidly melt feedstock materials, creating a melt pool that scans across the build platform to print specific patterns and deposit materials layer by layer. Compared to traditional manufacturing methods, fusion-based AM processes involve more complex physics, such as the intricate interaction between the heat source and feedstocks, drastic melt flow, and rapid cooling. These events are synergistically influenced by many printing parameters and conditions, which can significantly impact the microstructures and properties of as-fabricated products. Therefore, mechanistic studies on solidification, phase transformation, and microstructure evolution under the non-equilibrium conditions involved in metal AM are critical for advancing industrial adoption and enabling material-process-product co-design. Maintaining a highly stable melt pool has traditionally been considered crucial in the AM community to ensure consistency and prevent structural defects. In this presentation, I will discuss how certain melt pool instabilities can unexpectedly be leveraged to enhance microstructure control without introducing printing defects. The instability can be introduced by (i) applying dynamic thermal conditions, (ii) limiting feedstock melting, and (iii) modulating local melt flow. *Operando* synchrotron x-ray characterization techniques, combined with high-fidelity multi-physics simulations, are employed to accelerate the understanding of these highly dynamic phenomena during printing. Beyond understanding the underlying mechanisms, strategies and insights are developed to gain improved control over various microstructures in metal AM.

New Room-temperature Playground for Bose-Einstein Condensates Using Halide Perovskites

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Strong coupling of the photons with semiconductors' excitons in the high-quality optical cavities can create new quasiparticles called exciton-polaritons and many exotic phenomena, such as Bose-Einstein Condensates and superfluidity. Traditionally exciton-polariton experiments were mainly performed in quantum-well microcavities grown with molecular beam epitaxy (MBE), where liquid helium temperatures must be maintained to prevent exciton autoionization.

Recently, semiconducting lead halide perovskites with a composition of ABX3 (where A is commonly CH3NH3+ (MA+) or Cs+; B is Pb2+; X is Cl−, and Br−) have emerged as contenders to MBE-grown quantum-well microcavities like GaAs for polaritonic but at room temperature, due to their large exciton binding energy, high photoluminescence (PL) quantum yield, tunable bandgap and high room-temperature nonlinear interaction strength.

In this talk, will first highlight recent researchers’ efforts with emergent excitonic materials on room-temperature polaritonic. Then, I will introduce our approaches to obtain various large halide perovskite single crystals inside optical nanocavities. Due to the uniform confined environment, the solution growth approach shows uniformity, comparable to the MBE-grown GaAs quantum well, enabling submillimeter-large single crystals with superb excitonic quality. These crystals with Wannier-Mott excitons allowed us to demonstrate a polaritonic XY spin Hamiltonian with array of Bose-Einstein Condensates at room temperature successfully. Further, we will also our recent two works using halide perovskite on topological valley Hall polariton condensation and polariton superfluidity, critical steps towards the ultimate goal of realizing a room-temperature polaritonic platform on par with other systems at low temperatures.

Functional Electronic Materials on the Verge of Stability

Daniel Shoemaker[1]

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Materials for next-generation electronic and quantum applications are historically sought to have many competing degrees of freedom, meaning their transport or susceptibility has a novel response that relies on a delicate balance of interactions. But those interactions can be surprisingly strong, so disorder and phase instability can become insidious guests. Synchrotron users know this well – with sensitive tools, we find tricky details that can undermine simple interpretations of functional materials. We examine complex responses in charge density wave materials and antiferromagnets for spintronics. In $(TaSe_4)_2I$, the simple explanation is a highly degenerate metallic state. But single-crystal diffuse scattering and photoelectron spectroscopy reveal a highly complex chemical system. Likewise, in antiferromagnetic materials like CuMnAs, a simple cartoon can be drawn of magnetic domains that flip quickly back and forth. Our high-resolution synchrotron data reveals that domain formation is widespread, and any attempt to utilize the transport must contend with how magnetic transitions can move ions in these materials. While domains and disorder may seem to rear their heads at inopportune times, we can plan how to harness them in beneficial ways. I will discuss outstanding problems and opportunities in crystal growth and engineering that should have multiple avenues of success at the Advanced Photon Source.

Atomic Sheets for Nonvolatile Energy-efficient Systems and Hydrogen Clean Energy Materials

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This presentation will cover recent advancements in 2D atomic sheets, emphasizing their potential for both scientific exploration and practical engineering applications. Key topics include defects, single-atom monolayer resistive switching devices/memory, neuromorphic computing, and nonvolatile RF/5G/6G switches. Nonvolatile switching devices based on 2D materials are an application of defects and is a rapidly advancing field with rich physics that can be attributed to metal adsorption into vacancies and other phenomena. Furthermore, recent progress in proton exchange membranes for selective ion transport in fuel cells will be discussed. This progress includes increased understanding of proton transport in atomic sheets and enhanced performance in transport, crossover reduction, and durability.

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X-ray Visions: Bringing Future Materials into Focus

Karena Chapman[1]

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Abstract coming soon.

Bragg Coherent Diffraction Imaging at the Advanced Photon Source

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The arrival of third-generation synchrotron sources, such as the APS, created new opportunities to exploit the high flux of coherent x-rays. The first demonstration of coherent "speckle" effects in hard x-ray diffraction had been demonstrated by Sutton et al. [1] at the end of the second-generation era. In the original build-up of APS, Sector 8 was dedicated to x-ray photon correlation spectroscopy as the first application of coherent diffraction. Our group, then part of UNICAT at the University of Illinois, decided to pursue the structural possibilities of coherent x-ray diffraction, first at ESRF, then at Sector 33. After a few successful demonstration experiments, the UNICAT consortium committed to build a dedicated station at Sector 34 in the second wave of beamline construction. This beamline had the great innovation of splitting the wavefront to provide coherent flux into two stations in parallel, capitalising on the fact that only a few percent of the area of an APS undulator beam was coherent. We built a full 6-circle diffractometer coupled to a sample vacuum chamber dedicated to Bragg coherent diffraction imaging (BCDI) at 34-ID-C. The first major publication was of contact strain imaging in Pb nanocrystals, grown at the beamline [2]. This talk will present the series of technical advances that took place of the following years as BCDI was developed into a mainstream x-ray analytical method at APS.

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[2] M. A. Pfeifer, G. J. Williams, I. A. Vartanyants, R. Harder and I. K. Robinson, "Three-dimensional Mapping of a Deformation Field inside a Nanocrystal ", Nature 442 63 (2006)

Advancing Synthetic Frontiers at the Intersection of Solid-state and Molecular Chemistry

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Low-dimensional materials, including nanocrystals and atomically thin two-dimensional sheets, effectively bridge the gap between bulk solids and molecules. These materials have advanced significantly in recent years, largely due to their potential for real-world applications. In this presentation, I will discuss the development of novel functional materials through the integration of concepts from solid-state chemistry, molecular chemistry, and nanotechnology.

For example, we expanded the range of synthesizable nanomaterials by developing a new class of colloidal systems—colloids in molten inorganic salts. Using molten salts, we successfully synthesized the first colloidal GaAs quantum dots, as well as various other functional nanomaterials previously considered impossible to synthesize via colloidal methods.

In another example, we combined principles from solid-state and molecular chemistry to advance two-dimensional transition metal carbides and nitrides, known as MXenes. These materials combine the electronic and mechanical properties characteristic of inorganic 2D crystals with nearly limitless opportunities to tailor their surface chemistry. Understanding MXene surfaces requires concepts from coordination chemistry, self-assembled monolayers, and surface science. We demonstrate that MXene surface groups actively contribute to the materials' conductivity, superconductivity, and catalytic activity.

Solid State Synthesis on the Beamline: What We Gain by Peering into the "Black Box"

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In-situ powder diffraction experiments allow solid state chemists to 'peer' into relevant reactions at high temperatures and gain useful information on a material's thermal stability and phase transitions driven by their chemistry. In this talk, I will present our work on *in-situ* experiments at the Advanced Photon Source (APS). We performed several solid-state metathesis reactions for the preparation of transition metal chalcophosphates along with hydrothermal and solvothermal synthesis of metal chalcogenides relevant for iron-based superconductivity. First, we present an ion exchange metathesis methodology to synthesize the thiophosphate $CoPS_3$ [1]. On the 11-BM-B beamline at the APS, we take rapid powder x-ray diffraction (PXRD) patterns while reacting isostructural $MgPS_3$ with $CoCl_2$. Through sequential Rietveld refinements for thousands of PXRD patterns, we comprehensively elucidate this solid-state reaction by uncovering a two-step progression in the metathesis reaction – 1) ion diffusion kinetics followed by 2) grain boundary melting and reactions. Second, we perform a series of hydrothermal reactions of iron metal in basic aqueous media above 120 C for the synthesis of superconducting phases such as (LiOH)FeS [2]. Through sequential Rietveld refinements, we find that the amount of iron in the different layers is dynamic during the hydrothermal process. Overall, the insights we gain through beamline solid state chemistry enhances our understanding of reaction dynamics and paves the way for optimizing the synthesis of functional inorganic materials.

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Light-matter Interaction in Nanoscale Materials from First Principles

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First principles calculations – calculations based on quantum physics without the use of empirical parameters – enable us to make predictions about the electronic and optical properties of materials and identify structure-property relations. In this talk, I will share some of our recent predictions on the light-matter interactions in nanoscale materials which are relevant to my work in CNM.

The first part of the talk will focus on properties of quantum defects in 2D materials. Defects in 2D materials are of interest as qubits and as single photon emitters. The holy grail in the field is to be able to controllably introduce defects with desired properties. In recent years, substitutional transition metal defects have been introduced into transition metal dichalcogenide (TMD) monolayers using controllable and scalable approaches. Using a high-throughput approach, we predict that a few of such defect systems are potentially useful as quantum defects in the terahertz (THz) regime. In particular, we identify spin triplet qubitsx, with a zero-field splitting in the THz range, that can be controlled by light-matter interactions for qubit operations using resonant optical excitations. Such qubits have the potential to be operated with higher fidelities at higher temperatures. We also predict the properties of a new class of experimentally relevant defects in hexagonal boron nitride (a wide-band gap layered material); these are defect complexes involving boron interstitials, which can be created by ion bombardment, and stabilised by binding to an existing intrinsic defect [1].

In the second part of the talk, I discuss the effects of many-body excitonic interactions on the non-linear optical response of layered materials. We show that excitonic interactions can dramatically increase the non-linear response as well as change the qualitative features of the observed second harmonic generation spectra [2]. We also discuss the origins of the shift current in the excitonic picture, identifying a new geometric term [3]. This will lay the groundwork for our work in CNM on orbital and spin shift currents in layered materials.

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