2025 EFRC-HUB-CMS-CCS PI MEETING TEAM SCIENCE CONTEST

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INTRODUCTION TO THE TEAM SCIENCE CONTEST AT THE 2025 EFRC-HUB-CMS-CCS PRINCIPAL INVESTIGATORS' MEETING

There are more than 1,700 graduate students and postdoctoral researchers involved in the Energy Frontier Research Centers (EFRC), BES energy storage and fuels from sunlight Energy Innovation Hubs, BES Computational Materials Sciences awards (CMS), and BES Computational Chemical Sciences awards (CCS). To highlight their accomplishments and further the development of the future scientific energy workforce, the Department of Energy's Office of Basic Energy Sciences (BES) sponsored a Team Science Contest as part of the 2025 EFRC-Hub-CMS-CCS Principal Investigators' Meeting in Washington, D.C. on August 11-12, 2025. Each Director was invited to nominate a team of two or more graduate students and/or postdoctoral researchers to present a joint talk about their center research. The DOE EFRC management team selected 22 finalists. At the meeting, teams of DOE program managers selected the top six teams based on how well the research exemplified the opportunities provided by the center funding modality, scientific excellence, and integration of the research. The winners received an award certificate from Bindu Nair, Associate Director of the DOE Office of Basic Energy Sciences, during a ceremony at the end of the meeting.

For more information, visit the EFRC program website: http://science.osti.gov/bes/efrc.

The talk abstracts are listed below in alphabetical order by center acronym. Team members are highlighted in orange; presenters at the meeting are underlined.

TEAM SCIENCE WINNERS

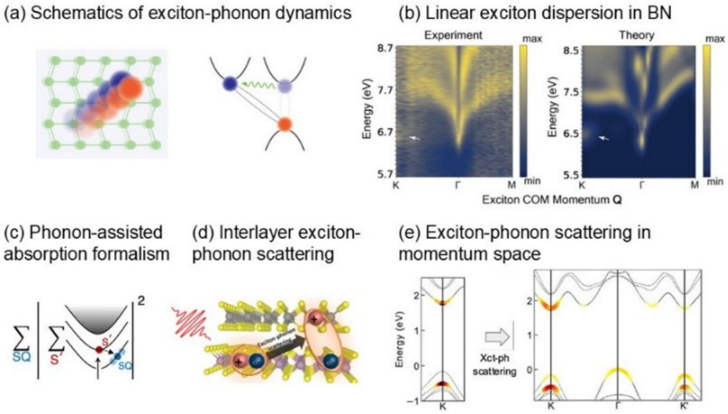
(Top row, from left) Luna Liu, Gurjyot Sethi, Jonah Haber (Bottom row, from left) Jinyuan Wu, Bowen Hou, Zhenfa Zheng

FIRST-PRINCIPLES ANATOMY OF EXCITON DYNAMICS: FROM DISPERSION TO QUANTUM TRANSPORT

[CMS - C2SEPEM] Luna Liu[1], Gurjyot Sethi[2,3], Jonah Haber[4], Jinyuan Wu[1], Bowen Hou[1], Zhenfa Zheng[5], Jeffrey B. Neaton[2,3], Felipe H. da Jornada[4], Zhenglu Li[5], Diana Y. Qiu[1], Steven G. Louie[2,3]

[1]Yale University; [2]Lawrence Berkeley National Laboratory; [3]University of California, Berkeley; [4]Stanford University; [5]University of Southern California

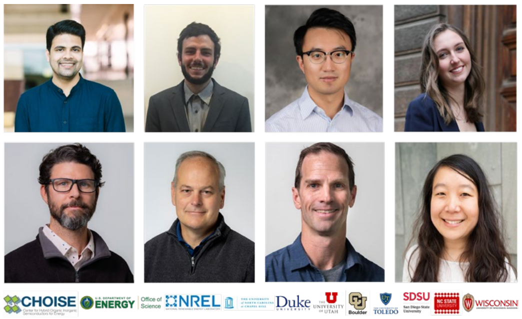
Exciton dynamics underpin the practical realization of light-matter interactions ranging from the efficiency of energy transport in photovoltaics and photocatalysis to the coherence of quantum information and light-driven quantum phase transitions. The first-principles understanding of exciton dynamics requires a few basic building blocks: 1) The full exciton dispersion to capture the phase space of momentum and energy conserving scattering processes, 2) Interaction of excitons with external perturbations such as electromagnetic fields and lattice vibrations, 3) Exciton scattering matrix elements and self-energies, and 4) An equation of motion describing the dynamical processes. In this talk, we highlight our center's multi-modal developments along these directions, which build synergistically to provide a complete first-principles picture of exciton dynamics spanning from the coherent regime through diffusive transport. We begin by calculating exciton dispersion and validating our theoretical predictions against momentum-resolved electron energy loss spectroscopy measurements (Q-EELS), revealing for the first time the emergence of a massless excitons composed of massive electrons and holes [1]. Building on accurate exciton band structures, we include exciton-phonon scattering from first principles, revealing exciton lifetimes [2], diffusion [3], and relaxation processes [4-5]. We develop the first full quantum theory of exciton orbital magnetic moment [6]. Finally, we implement a real-time quantum master equation, going beyond the secular/Lindblad approximation, that explicitly includes the electron-electron and electron-phonon interactions on the same footing across the Brillouin zone [7]. Our developments put calculations of exciton dynamics in real materials, especially reduced-dimensional systems, within reach through the synergistic combination of novel theoretical developments, innovative algorithmic acceleration, and highly-optimized massively-parallel codes for high performance computing.



(a) Schematics of exciton-phonon dynamics (b) Linear exciton dispersion in BN (c) Phonon-assisted absorption formalism (d) Interlayer exciton-phonon scattering (e) Exciton-phonon scattering in momentum space

[1] L. Liu *et al.*, under review, arXiv:2502.20454v2 (2025). [2] Y.-H. Chan *et al.*, Nano Lett., **23**, 3971 (2023). [3] G. Cohen *et al.*, Phys. Rev. Lett., **132**, 126902 (2024). [4] Y.-H. Chan *et al.*, Nano Lett. **24**, 7972 (2024). [5] Y.-H. Chan *et al.*, Phys. Rev. B, **111**, 184305 (2025). [6] G. Sethi *et al*, in preparation (2025). [7] Z. Zheng *et al.*, in preparation (2025).

Contributions: L.L., J.W., and B.H. performed calculations and experiments on hBN. G.S. developed the theory for exciton orbital magnetic moment. J.H. performed calculations on exciton-phonon coupling. Z.Z. developed the nonequilibrium exciton-phonon dynamics implementation. J.B.N., F.H.J., Z.L., D.Y.Q., and S.G.L. supervised and conceived the research.



(Top row, from left) Md Azimul Haque, Andrew Grieder, Yi Xie, Margherita Taddei,

(Bottom row, from left) Joseph M. Luther, Matthew C. Beard, Jeffrey L. Blackburn, Yuan Ping

CHIRALITY TRANSFER AND SPIN SELECTIVITY IN HYBRID METAL HALIDE SEMICONDUCTORS

[EFRC – CHOISE] Md Azimul Haque[1], Andrew Grieder[2], Steven P. Harvey[1], Roman Brunecky[1], Jiselle Y. Ye[1], Bennett Addison[1], Junxiang Zhang[3], Yifan Dong[1], Yi Xie[4], Matthew P. Hautzinger[1], Heshan Hewa Walpitage[5], Ian A. Leahy[1], Jeiwan Tan[1], Margherita Taddei[1], Pius Markus Theiler[1], Aeron McConnell[6], Andrew H. Comstock[6], Kai Zhu[1], Kirstin Alberi[1], Jeffrey L. Blackburn[1], Zeev Valy Vardeny[5], David B. Mitzi[4], Joseph J. Berry[1,3], Seth R. Marder[1,3], Peter Sercel[7], Dali Sun[6], Joseph M. Luther[1], Yuan Ping[2], Matthew C. Beard[1]

[1]National Renewable Energy Laboratory; [2]University of Wisconsin-Madison; [3]University of Colorado Boulder; [4]Duke University; [5]University of Utah; [6]North Carolina State University; [7]Center for Hybrid Organic Inorganic Semiconductors for Energy

Traditionally, chiroptical properties in hybrid metal halide semiconductors (MHS) arise from symmetry breaking by incorporating chiral A-site organic cations, which restricts compositional flexibility. Furthermore, how structural chirality governs the charge and spin transport has been illusive due to the lack of tunability in traditional chiral semiconductors. Here, we present a new strategy for inducing chirality in MHS through remote chirality transfer, where a proximal chiral molecule selectively interacts with divalent metal cations to impose asymmetric distortions deep into the lattice, as revealed by density functional theory calculations, achieving large circular dichroism dissymmetry factors.[1] Exploiting the tunable chirality of MHS, we demonstrate an exceptionally large room-temperature chirality-induced spin selectivity (CISS)-driven magnetoresistance response exceeding 300% in a spin valve device, where the chiral MHS forms a spin-selective tunneling barrier governed by molecular handedness, generating current dissymmetry factors beyond the limits predicted by conventional models.[2] These findings establish a structure-property relationship between CISS and structural chirality, providing new design principles for controlling charge-to-spin interconversion and advancing chiral opto-spintronic semiconductors.

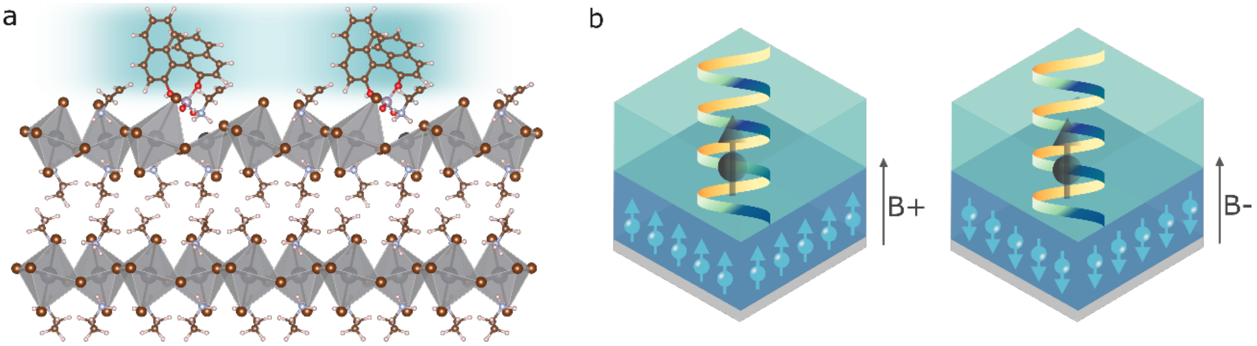


Fig. (a) Schematic showing the structural distortion of CMHS upon interaction with chiral molecules. (b) A low resistance state is observed when the ferromagnet and enantiomorph spins are parallel and high resistance when the spins are antiparallel in a spin valve.

References:

[1] Haque et al., Remote Chirality Transfer in Low-Dimensional Hybrid Metal Halide Semiconductors, Nat. Chem. 17, 29-37, 2025. [2] Haque et al., Chirality-Induced Magnetoresistance in Hybrid Organic-Inorganic Perovskite Semiconductors, Submitted, 2025

Contributions: M.A.H. synthesized the CMHS compositions, fabricated the spin valves and performed characterizations. A.G. developed the chirality transfer model and performed the CCM and DFT calculations.

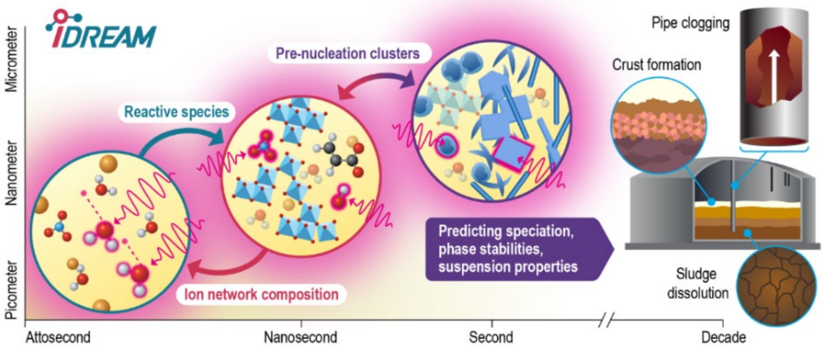
(From left) Ryan Beck, Amita Bedar, Simantini Paul, and Robert Felsted

UNDERSTANDING HOW RADIATION UNIQUELY TRANSFORMS THE PHYSICOCHEMICAL PROPERTIES OF ELECTROLYTES

[EFRC - IDREAM] Ryan Beck[1], Simantini Paul[2], Amita Bedar[3], Greg Felsted[4], Aodong Liu[1], Hemanth Haridas[2], Eleftherios Lambros[1], Maxime Pouvreau[4], Jacob Morton[4], Yifu Feng[4], Pravalika Butreddy[4], Ashley Kennedy[4], William Denman[5], Hossam Elshendidi[6], Shuai Li[7], Emily Nienhuis[4], Trent Graham[4], Xin Zhang[4]

[1]University of Washington; [2]University of Utah; [3]Notre Dame University; [4]Pacific Northwest National Laboratory; [5]Georgia Institute of Technology; [6]Hunter College CUNY; [7]Argonne National Laboratory

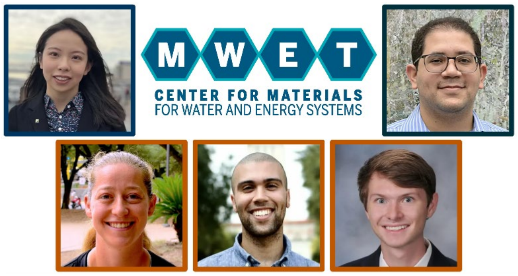
The instantaneous, radiation-induced changes to the electronic structure of concentrated electrolytes is central to the retrieval, transport, and treatment of legacy radioactive waste. Based on our new knowledge of the attosecond electronic response of water molecules to radiation, we used the LCLS through our campaign



suspensions over decades.

proposal to break new ground by measuring single X-ray pulse resonant inelastic X-ray spectra at the oxygen K-edge in aqueous sodium chloride for the first time. We saw that the generation of an outer valence hole, and the subsequent excitation of a core electron into the hole, was different in the presence of cation traps. To isolate these signatures of short-lived species under radiation, we ran high-accuracy density functional theory (DFT) calculations on water-solute ensembles. Ultrafast proton dynamics also play a pivotal role, and we examined the relaxation of an excess solvated electron in water and with solutes using real-time nuclear electronic orbital (NEO) time dependent DFT calculations. We also pushed our understanding of ultrafast dynamics and structure into more complex high-pH solutions using lab-based two-dimensional infrared (2D-IR) spectroscopy, and we now know that hydroxide preferentially forms solute-solute interactions with other dissolved ions. Classical molecular dynamics (CMD) and graph theory show us how this ion clustering affects transport properties, e.g., viscosity. With ab-initio DFT and our new reactive force field, in combination with Raman and NMR spectroscopy, we are now demonstrating how the strength of these ion networks affects oligomerization of key species in radioactive waste (aluminate and pertechnetate) and the nature of precipitated phases. Using electron paramagnetic resonance and electrochemistry, we tracked the distribution of radicals and redox states that result from radiation-induced changes to local solution structure, so that we can predict reduction of redox active species (pertechnetate and nitrate) and nucleation of aluminum-bearing phases. Through our team science, we are coordinating X-ray, gamma-ray, and electron beam irradiation across multiple institutions to unravel how radiation-induced ultrafast processes in the electrolyte cascade to macroscopic effects, including aggregation, dissolution and hydrogen production.

Contributions: R. Beck, A. Liu: DFT assignment of X-ray signatures. E. Lambros: NEO calculations. S. Paul: CMD/graph theory of ion clustering and solvation. A. Bedar: gamma radiation-induced radical species. G. Felsted: 2D-IR for ultrafast solution dynamics. H. Haridas: RFF modelling of dissolution. T. Graham: NMR and muon spectroscopy. M. Pouvreau: Raman/NMR spectra computation. J. Morton: radiation electrochemistry. X. Zhang: particle synthesis. Y. Feng: atomic force microscopy. P. Butreddy: X-ray imaging of dissolution. A. Kennedy, E. Nienhuis: alkaline electrolyte synthesis. W. Denham: laser spectroscopy measuring gas production. H. Elshendidi: technetium chemistry. S. Li: LCLS experiments

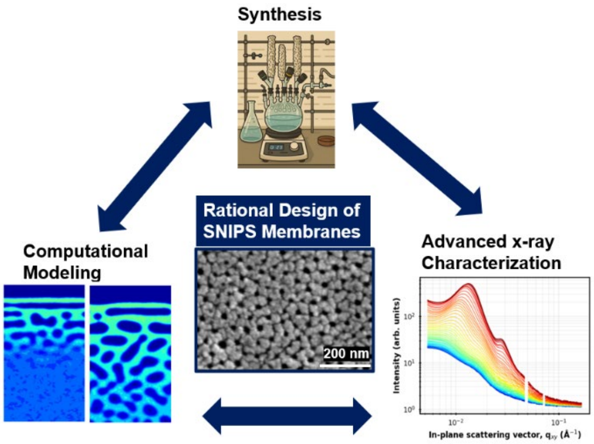


(Top row, from left) Chuqiao (Elise) Chen, José Carlos Diaz
(Bottom row, from left) Louise Kuehster, Adam Mann, Noah Wamble

TOWARDS RATIONAL DESIGN OF TOUGHER SNIPS MEMBRANES FOR WATER AND ENERGY SYSTEMS

[EFRC - M-WET] Noah P. Wamble[1], Chuqiao Chen[2], José Carlos Díaz[1,3], Benjamin J. Pedretti[1], Adam N. Mann[1], Matthew R. Landsman[1,3], Louise Kuehster[1], Mostafa Nassr[1], Lynn E. Katz[1], Nathaniel A. Lynd[1], Glenn H. Fredrickson[2], Gregory M. Su[3], Gabriel E. Sanoja[1], Benny D. Freeman[1]

[1]University of Texas at Austin; [2]University of California, Santa Barbara; [3]Lawrence Berkeley National Laboratory



Ultrafiltration membranes with high selectivity and permeability are essential for reducing the pernicious coupling between water and energy, enabling low-energy routes to clean water. SNIPS (i.e., self-assembly plus nonsolvent-induced phase separation) membranes, which combines block copolymer self-assembly with nonequilibrium membrane manufacturing methods, yields asymmetric, isoporous membranes with a narrow surface pore size distribution and high permeances and selectivities. In this process, a block copolymer is cast into a film from a solution where the polymer has formed micelles. The cast film is evaporated (i.e., the dry step) to preferentially concentrate polymer at the polymer solution/air interface, then placed in a non-solvent (usually water) to bring about nonsolvent-induced phase separation to form a well-ordered membrane having pores of nearly the same size, rather than a broad pore size distribution as is found in conventional membranes. However, the design space for these membranes is vast, and control over membrane morphology (and hence membrane performance) during this nonequilibrium process requires laborious optimization. Additionally, polystyrene-b-poly(4-vinylpyridine) (SV), which works well with SNIPS, has a brittle, polystyrene membrane matrix with poor mechanical properties that limits the utility of these high-performance membranes. In this project, tough, isoporous membranes were cast using an ABAC tetrablock polymer, polystyrene-*b*-polyisoprene-*b*-polystyrene-*b*-poly(4-vinylpyridine) (SISV), synthesized by anionic polymerization. This unique architecture gave membranes with an order of magnitude higher toughness than SV membranes due to rubber toughening. Resonant soft x-ray scattering experiments were used to probe the length scales of these rubbery and glassy domain sizes to understand the impact of nanoscale morphology on membrane performance. Additionally, micelle morphology and evolution during the dry step were investigated via NMR experiments and in situ grazing incidence small angle x-ray scattering experiments to elucidate the connection between casting conditions and membrane performance (i.e., rejection and permeance). To study the impact of solvent blend choice on membrane performance, self-consistent field theory (SCFT) simulations were conducted and revealed that solvent-nonsolvent interactions influence how well-connected the membrane substructure is during diffusion-induced phase separation, which could rationalize membrane performance. Together, these efforts lay the groundwork for rational codesign of SNIPS membranes with high permeability, selectivity and enhanced mechanical toughness.

Contributions: B.J.P. and L.K. synthesized the polymers. N.P.W. cast membranes, performed scattering, NMR, and membrane characterization studies. N.P.W. conducted data analysis, led the project, and wrote the first draft of the manuscript. C.C. performed SCFT simulations. M.R.L., J.C.D., and M.N. helped design and conduct x-ray scattering experiments. A.N.M performed mechanical tests. L.E.K., N.A.L., G.H.F., G.M.S., G.E.S., and B.D.F. secured the resources to conduct this study and provided guidance for the project.

(From left) John Ponis, Kenna Ashen, Michelle Smeation, Jialu Li

Mapping Atomistic Structure to Neuromorphic Function through Single-Crystal Neuronal Oscillators

[EFRC - reMIND] John Ponis[1], Kenna Ashen[1], Michelle Smeaton[2], Jialu Li[3], Fatme Jardali[1], George Agbeworvi[1], Jinghua Guo[3], Xiaofeng Qian[1], Katherine Jungjohann[2], Lance Wheeler[2], Patrick Shamberger[1], Sarbajit Banerjee[1] [1]*Texas A&M University;* [2]*National Renewable Energy Laboratory;* [3]*Lawrence Berkeley National Laboratory*

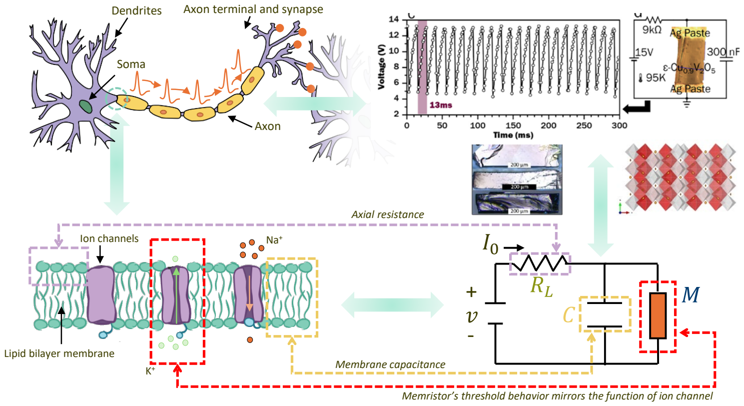


Figure 1. A memristive neuromorphic element is fabricated from an entire single crystal and X-ray crystallography is used as a powerful lens to image structural rearrangements underpinning memristive behavior with sub-Å resolution.

The superexponential increase in demand for computing power accompanying the rise of artificial intelligence, combined with the end of Moore's Law and Dennard's scaling, has spurred intense interest in alternative computing architectures. Neuromorphic computing aims to mimic the human brain by leveraging materials with non-linear conductance to emulate neuron function. However, mechanisms to describe such conductance nonlinearities remain obscure, and have rarely ever been framed in terms of atoms and electrons. As such, strategies for atomistic materials design remain exceedingly empirical. Our collaborative team has addressed critical gap in the field. We have achieved the long-cherished goal of fabricating a memristive neuromorphic element out of an entire single crystal and have used X-ray crystallography as a powerful lens to image structural rearrangements underpinning memristive behavior with sub-Å resolution.[1] We discover interstitial copper-ion migration and reordering in **ε**-$Cu_{0.9}V_2O_5$ and β'-$Cu_xV_2O_5$, mapping ion trajectories with atomic resolution, as the defining structural rearrangement underpinning the structural transformation.[1,2] We further map the nature of charge and spin ordering in the insulating phase. Based on mechanistic understanding, we have devised co-intercalation and topochemical modification as atom-precise methods for broadening the first-order electronic transition, which maps directly to an expanded range of stable and persistent self-sustaining oscillations. The results demonstrate mapping of complex circuit properties to specific features of atomistic and electronic structure in strongly electron correlated materials and are an exemplar for bridging across decades of length and time scales using multimodal characterization, scale-bridging simulations, and iterative materials design and discovery. The results further demonstrate the promise of reMIND's distinctive library of single crystals.

1. J. Ponis, et. al. Atomistic Origins of Conductance Switching in an **ε**-$Cu_{0.9}V_2O_5$ Neuromorphic Single Crystal Oscillator. *Journal of the American Chemical Society* **2024**, 146 (50), 34536-34550.

2. G. Agbeworvi et al. An Atom-Precise Approach for Introducing Weak Disorder in First-Order Phase Transitions to Stabilize Broad-Band Neuromorphic Oscillators, submitted for publication.
3. L. Wheeler et al. Tuning Optical and Electrical Properties of Vanadium Oxide with Topochemical Reduction and Substitutional Tin. *Chemistry of Materials* **2024**, 36, 21, 10483–10495.

Contributions: J. P.: design, synthesis, characterization; K.A.: simulations; M.S.: electron micrsocopy; J.L.: RIXS and XAS; F. J.: compact model; G.A.: synthesis, magnetism; J.G. RIXS & XAS; X.Q: first-principles modeling; K. J.: electron microscopy; L.W.: topochemistry; P.S.: compact models; S.B.: design and conceptualization

(From left) Megan Brown, Spencer Yeager, Jude Kpare, Eui Hyun Suh, Henry Kantrow, Arianna Magni, and Yael Tsarfati

UNDERSTANDING AND MANIPULATING THE NANOENVIRONMENT OF RIBBON-LIKE (SOFT) POLYMER SEMICONDUCTORS TO ENABLE PHOTOELECTROCHEMISTRY

[EFRC - SPECS] Henry J. Kantrow[1], Yael Tsarfati[2,3], Spencer Yeager[4], Megan Brown[5], Arianna Magni[2], Eui Hyun Suh[1], Jude Kpare[1], Chad Risko[5], Alberto Salleo[2], Erin Ratcliff[1], Natalie Stingelin[1]
[1]Georgia Institute of Technology; [2]Stanford University; [3]Lawrence Berkeley National Laboratory; [4]University of Arizona; [5]University of Kentucky

Ribbon-like polymer semiconductors, comprised of rigid electron donating/withdrawing groups, have exceptional promise as next-generation energy conversion and storage materials, providing exquisite control over redox properties, high efficiencies in radiation-to-electrical energy conversion, long-lived charge carriers, and ease of large-scale processing.[1,2] In contrast to traditional flexible-chain macromolecules, ribbon-like polymers feature a rich structural landscape that cannot be described solely by the classical picture of amorphous and semicrystalline domains.[3] To enable rational materials design, a holistic understanding of the distribution in local nanoenvironments is needed to control charge transport and transfer across length and time scales. For example, there are contributions from both static and dynamic energetic disorder that vary across 100s of nanometers and femtosecond timescales, which contribute to significant differences in charge transport (Figure 1).

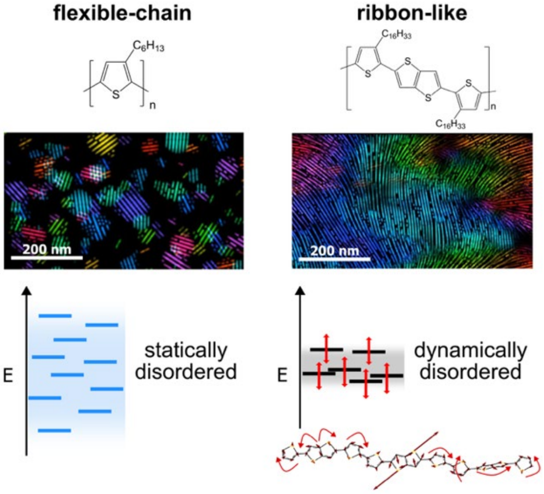


Figure 1: Top: Chemical structures and corresponding 4D-scanning transmission electron microscopy of flexible-chain and ribbon-like polymers. Bottom: Schematic energy level distributions for the two polymers, with a vector schematic of a torsional mode that contributes to dynamic disorder in the ribbon-like polymer.

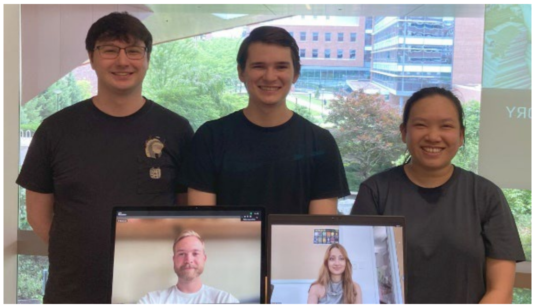
We demonstrate state-of-the-art characterization tool suites developed within the SPECS EFRC to investigate processes at multiple length scales in soft materials. Using prototype polymers, we demonstrate for the first time that ribbon-like polymers feature distinct, dynamically disordered energy landscapes. Combinations of multimodal characterization using spectroelectrochemistry, *operando* X-ray scattering, electron microscopy, and coherent electronic spectroscopy reveal that flexible-chain polymers are often structurally heterogeneous and statically disordered. Ribbon-like polymers, however, display a homogenous structure, leading to narrower distributions in energy levels that are highly dynamic, driven by coupling to torsional vibrational modes. Concurrent modeling across scales reveals that charge carrier (polaron) transport and densities of states (DOS) depend on the local and dynamic nanoenvironments of these complex systems, with polymer morphologies and electrolyte compositions (solvent/ions) impacting polaron signatures and transport. These differences in electronic disorder translate to control of rates of charge transfer in polymer–electrolyte interphase regions. This work paves the way for elucidating the complex multiscale polymer structure across the broad temporal scales (fs to ms) relevant to ion and polaron transport. This dynamic structure ultimately controls charge-transfer reactivity to promote specific redox chemistries, such as H_2 evolution, and is a critical step toward design guidelines for creation of future transducers of light to chemical energy.

Contributions: H.J.K. conducted coherent electronic spectroscopy experiments. Y.T. performed electron microscopy. S.Y. and E.H.S. executed electrochemical measurements and the photoelectrochemistry. M.B. performed DFT and MD simulations. C.R., A.S., E.R., and N.S. helped design the experiments and supervised the project.

References: [1] F. Machui et al. *Energy Environ. Sci* **7** (9), 2014. [2] J. Kosko et al. *Nat Energy* **7** (4), 2022. [3] E. Ratcliff & N. Stingelin *Nat Mater* **24** (1), 2025.

2025 EFRC-HUB-CMS-CCS PI MEETING TEAM SCIENCE CONTEST

TEAM SCIENCE FINALISTS



(Standing, from left) Albert Suceava, Ian Mercer, and Quyen Tran. (On screen, from left) Drew Behrendt and Ece Gunay

FORGING THE FUTURE OF FERROELECTRIC MEMORY

[EFRC - 3DFeM2] Ece Gunay[1], Drew Behrendt[2]; Albert Suceava[3], Ian Mercer[3], Quyen Tran[3], Elizabeth C. Dickey[1], Thomas Jackson[3], Jon-Paul Maria[3], Venkatraman Gopalan[3], Andrew M. Rappe[2], Susan Trolier-McKinstry[3]

[1]Carnegie Mellon University; [2]University of Pennsylvania; [3]The Pennsylvania State University

Breakthroughs in computation technologies are deeply tied to growing demands for energy consumption and large data volumes. To meet these needs and power the future of artificial intelligence and large language models, stepwise advancement of current technology is not enough; a new paradigm of accessible memory capable of performing in-situ computation at the atomic level is required. For low-power compute- in-memory architectures, The Center for Three-Dimensional Ferroelectric Microelectronics Manufacturing (3DFeM2) believes that next generation ferroelectrics, materials with a spontaneous polarization that is reversible with application of external electric field, is the answer. The realization of this revolutionary idea however faces challenges in both the implementation of devices and in the understanding of the underlying behavior of such materials. Here, we present significant advances by our team in (1) the theoretical modeling and experimental characterization of the most interesting candidate materials aimed at improving underlying material properties (2) how these materials can be used in real functional memory devices and (3) how our quest can be augmented by automated machine learning experiments. Through collaborative efforts from across universities and scientific backgrounds, we have managed to discover new ferroelectric materials tailored to our application, unravel how they work at the atomic level, and ultimately leverage these insights to implement

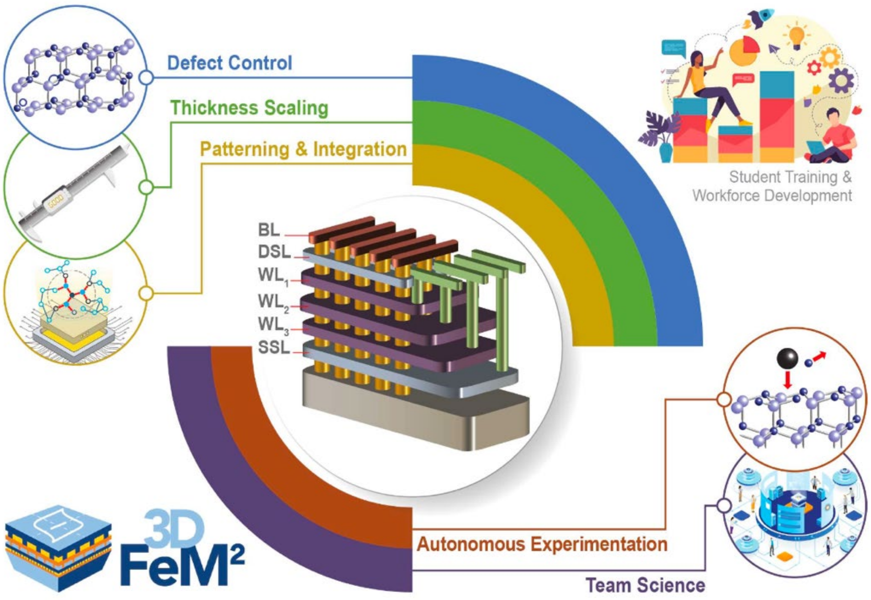


Figure 1: Vision for 3DFeM2 in which fundamental materials science and processing science enable 3D ferroelectric memory for low power computing.

them into electronics that can eventually become the backbone of the next generation of computer memory.

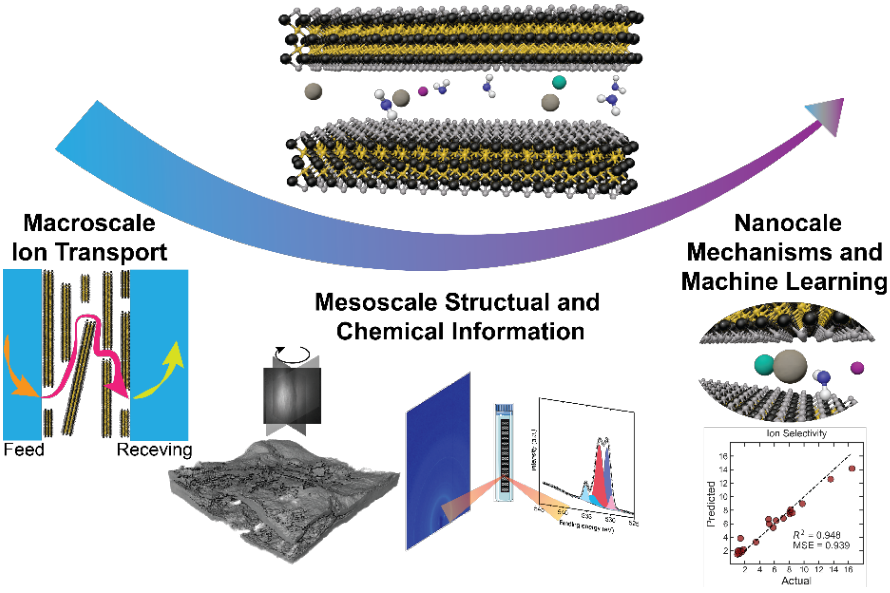
Contributions: E.G., D.B., A.S., I.M., and Q.T. organized and prepared the presentation based on their original research. S.T.M., T.J., J.P.M., V.G., A.M.R., and E.C.D., planned and guided the research as well as supervised and edited the presentation.

(From left) Yaguang Zhu and Qinsi Xiong

MORE THAN A SPECTATOR: CRITICAL ROLE OF WATER IN ION TRANSPORT THROUGH 2D MEMBRANES

[EFRC - AMEWS] Yaguang Zhu[1], Qinsi Xiong[2], George C. Schatz[2], Kelsey B. Hatzell[1]
[1]Princeton University; [2]Northwestern University

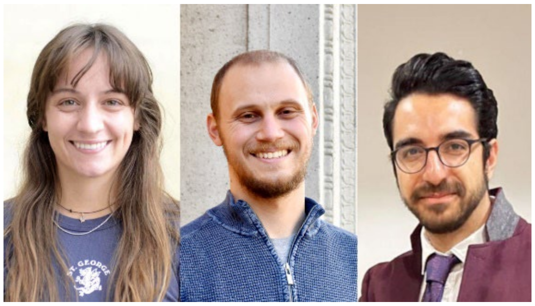
The accelerating depletion of freshwater resources coupled with increasing interest in recovering resources from water underscores an urgent scientific imperative to develop technologies for efficient ion separations in aqueous systems. Understanding solute–interface interactions in membrane systems is a core focus of the Advanced Materials for Energy-Water Systems (AMEWS) Center. Among the most challenging impurities to remove are small, tightly hydrated solutes, which exhibit strong interactions with water. Two-dimensional (2D) membranes, such as those based on transition metal carbides (MXene), show great promise for ion sieving and separation in such contexts. This presentation highlights a close collaboration by the Hatzell and Schatz groups to elucidate the key role of water in ion transport through 2D MXene membranes. First, at the **macroscale**, we discovered that intercalation of chaotropic cesium ions (Cs^+) into the 2D MXene membranes significantly inhibits ion permeation, resulting in enhanced ion sieving performance. Second, **mesoscale** three-dimensional imaging and synchrotron-based characterization revealed that Cs^+–intercalation uniquely reduces water content within the membrane both at the surface and within the membrane, thereby **mitigating membrane swelling**. Third, at the **nanoscale**, all-atom molecular dynamic simulations revealed critical roles of ion hydration and confinement in tuning selectivity. Guided by machine learning, we identified physicochemical



descriptors and developed a predictive model of ion transport under nanoconfinement, which was experimentally validated. This framework enables effective separation of critical resource ions, including Ni^{2+}, Co^{2+}, and Cu^{2+}. By integrating experiments and simulations across scales, this work advances the understanding of solute–interface interactions in 2D membranes and supports the rational design of next-generation ion-selective materials, in alignment with the AMEWS mission.

References: Zhu, Y., Xiong, Q.,et al., (2025). Water content modulation enables selective ion transport in 2D MXene membranes. PNAS, under review

Contributions: Y.Z. designed and conducted the experiments. Q.X. developed the computational model and performed the simulations. G.S. and K.H. conceived the presented idea and supervised this work.


(From left) Sophie Gerits, Daniel Weinberg and Nima Karimitari

ACCURATE ELECTROCHEMICAL PREDICTIONS WITH MANY-BODY AND MACHINE-LEARNING METHODS

[CCS - BEAST] Sophie Gerits[1], Daniel Weinberg[2], Nima Karimitari[3], Cooper Tezak[1], Jacob Clary[4], Taylor Aubry[4], Charles Musgrave[1], Mauro Del Ben[2], Christopher Sutton[3], Derek Vigil-Fowler[4], Ravishankar Sundararaman[5]

[1]University of Colorado Boulder; [2]Lawrence Berkeley National Laboratory; [3]University of South Carolina; [4]National Renewable Energy Laboratory; [5]Rensselaer Polytechnic Institute

Manipulating chemical dynamics at complex heterogeneous interfaces requires accurate *ab initio* methods beyond density functional theory (DFT) to design materials such as electrocatalysts. We have developed scalable and efficient algorithms for performing many-body calculations for electrocatalysts using the random-phase approximation (RPA), formulated machine learning (ML) techniques to rapidly predict beyond-DFT outputs from DFT inputs, and created an electrocatalytic database with grand-canonical DFT simulations of electrochemical systems to facilitate combined application of the RPA and ML techniques for rapid, accurate electrochemical predictions. This open-source database, BEAST DB, contains over 20,000 surface calculations at fixed electrode potential, covering a broad set of heterogeneous catalyst materials and electrochemical reactions (Figure 1(a)), with continued expansion leveraging automated high-throughput workflows for grand-canonical DFT.

To facilitate accurate simulation of these electrochemical systems beyond the limitations of DFT, we implemented highly scalable and efficient RPA calculations using the static subspace approximation and a compressed representation of the frequency-dependent polarizability. This technique enables RPA calculations of typical surface slabs within a few hundred GPU-hours (Figure 1(b)), thereby facilitating RPA calculations for hundreds to thousands of prototypical electrochemical systems. Finally, we have developed ML techniques based on graph neural networks that can predict higher-level electronic structure using energies and atomic orbital projections from DFT (Figure 1(c)), including for the highly inhomogeneous electrochemical interface calculations. Training such ML techniques to RPA calculations on a subset of BEAST DB will enable rapid RPA-quality predictions for the entire DB as well as for any additional electrochemical systems with just DFT-level calculations and computational cost.

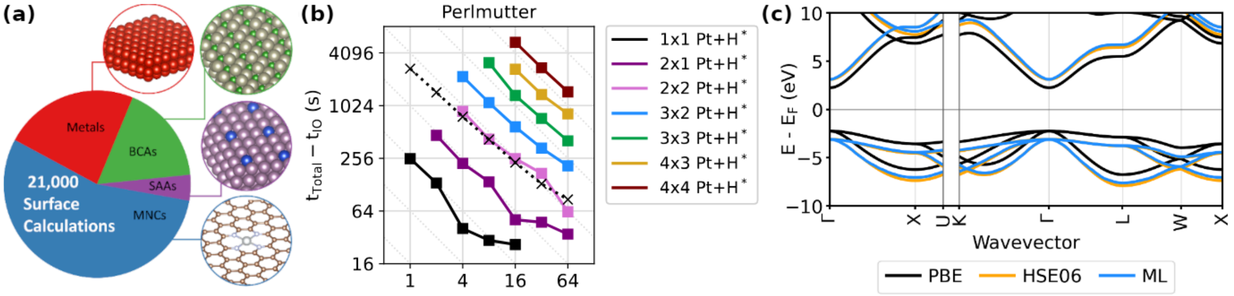


Figure 1. To enable accurate, rapid first-principles predictions for electrochemical reactions, we have (a) established a database (BEAST DB) with >20,000 grand-canonical density functional theory (GC-DFT) calculations, (b) scaled beyond-DFT electrochemical calculations based on the random phase approximation (RPA) to GPU-based supercomputers, and (c) demonstrated machine learning methods to predict higher-level electronic structure from DFT inputs, targeting RPA-quality electrochemical predictions at DFT cost using BEAST DB.

Contributions: Sophie Gerits developed the high-throughput workflow for grand-canonical calculations enabling BEAST DB. Daniel Weinberg implemented the static subspace approximation to optimize RPA calculations on GPU supercomputers. Nima Karimitari developed machine learning methods to predict higher-level electronic structure.

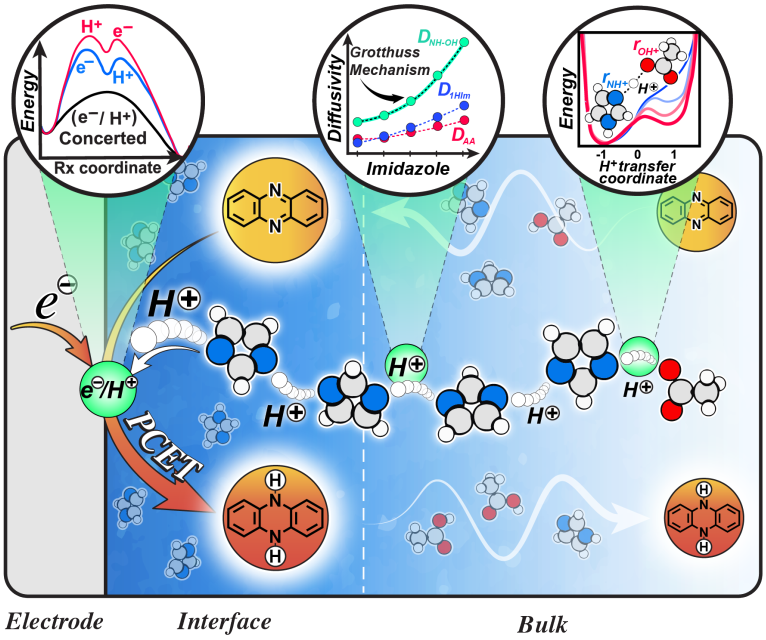
QUANTUM-TUNED CONCENTRATED HYDROGEN-BONDED ELECTROLYTES FOR ENHANCED PROTON TRANSFER

[EFRC - BEES2] Miguel Muñoz[1], Giselle de Araujo Lima e Souza[2], Michael S. Chen[3], Kaylie Glynn[4], Benworth B. Hansen[4], Peisen Qian[5], Thomas Simunovic[6], Mrinlini Kolaprath[6], Mark Dadmun[6], Thomas Zawodzinski[6], Joaquín Rodríguez-López[5], Steve G. Greenbaum[2], Mark Tuckerman[3], Joshua R. Sangoro[4], and Burcu Gurkan[1]

[1]Case Western Reserve University; [2]Hunter College-CUNY; [3]New York University; [4]The Ohio State University; [5]University of Illinois Urbana-Champaign; [6]University of Tennessee-Knoxvill

(Top Row) Giselle de Araujo Lima e Souza, Benworth B. Hansen, Mrinlini Kolaprath (Middle Row) Miguel Muñoz and Thomas Simunovic (Bottom Row) Peisen Qian, Michael S. Chen, and Kaylie Glyn

Concentrated hydrogen-bonded electrolytes (CoHBEs) are electrochemically stable and less-volatile alternatives to conventional electrolytes that present heterogeneous liquid structure. While the species diffusivity via vehicular transport, where species move with their solvation shell is hindered in viscous structured electrolytes like CoHBEs, Grotthuss transport where hopping occurs through the dynamic reorganization of the solvating species, is fast and hypothesized to enhance electrokinetics. This work presents a fundamental understanding of the proton conduction mechanism in CoHBEs where the dynamic hydrogen-bond networks in mixtures of acids and amphoteric azoles were leveraged to probe the hypothesis for proton coupled electron transfer (PCET) reactions that are relevant to energy storage and conversion processes. In particular, the analysis of proton transfer energy barriers calculated by path integral molecular dynamics (PIMD) simulations showed a reduction at specific compositions with a shift in proton localization toward azole driven tunneling when nuclear quantum effects were incorporated. Broadband Dielectric Spectroscopy (BDS) and Pulsed Field Gradient (PFG) NMR studies, in complement to FTIR and small-angle neutron scattering (SANS) further provided evidence to the decoupling of viscosity and conductivity in protic CoHBEs as the acid dimers are disrupted by the azole and as the extended azole chains enable virtually barrierless proton hopping. For example, despite its high viscosity (55 cP at room temperature), 1H-imidazole (1HIm) and acetic acid (AA) at 70:30 (1HIm:AA) molar mixture exhibit unexpectedly fast PCET kinetics for phenazines (rate constant of 10^{-4} cm/s) that is comparable to conventional electrolytes, as confirmed by rotating disk electrode (RDE) and scanning electrochemical microscopy (SECM) measurements. This is particularly unexpected when compared to the analogous mixture of 1-methyl-imidazole (1MIm) and AA that present lower viscosity (15 cP), however slower PCET reaction rates. Therefore, promoting hydrogen-bonded chain formation among amphoteric species in protic CoHBEs without steric hindrances for proton conduction is shown to enhance PCET kinetics.



Contributions: M. Muñoz - development of CoHBEs, physical property and RDE kinetic measurements; G. de Araujo Lima e Souza - PFG NMR; M. Chen - PIMD simulations; K Glynn and B. B. Hansen - BDS and dynamic measurements; P. Qian - SECM capability development for kinetics; T. Simunovic - relaxation NMR; M. Kolaprath - SANS

(From left) Sheilah Cherono, Cassius Boyd, Jennifer Sormberger, Shay McBride, Maritza Lang, Luka Mitrovic

PHOTO-ELECTROCHEMISTRY OF TITANIUM OXIDES: A PLATFORM FOR ASSIGNING VISIBLE SPECTRA TO OXYGEN EVOLUTION INTERMEDIATES

[EFRC - CEDARS] C. Boyd[1], S. McBride[2], S. Cherono[3], M. Lang[1], L. Mitrovic[4], J. Sormberger[1], D. Schlom[4], D. Jonas[1], D. Kumar[3], G. Hautier[2], T. Cuk[1]

[1]University of Colorado Boulder; [2]Dartmouth College; [3]North Carolina A&T State University; [4]Cornell University

Oxygen evolution intermediates that arise from the electron and proton transfer from water on heterogeneous surfaces inform catalytic mechanism, but their experimental validation by spectroscopy has been challenging. In addition to their efficiency in driving the oxygen evolution reaction (OER), titanium oxides have been a focus of (photo)-electrochemical mechanisms due to an electronic structure that allows for the separation of states associated with electron deficient oxygen configurations (*e.g.* terminal $TiO^{\bullet-}$, lateral $Ti2O^{\bullet-}$).

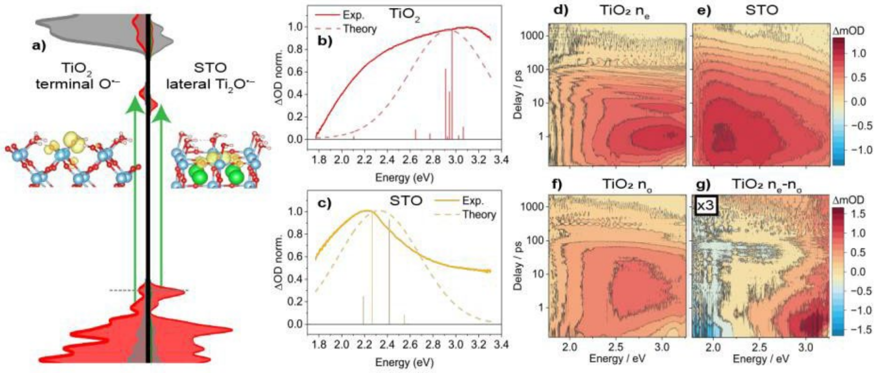


Figure 1 Excited state absorption in titanium oxides a) ESA: transition of valence band electron to unoccupied hole-polaron mid-gap state (yellow orbitals), b) and c) theoretical and experimental spectra compared for rutile TiO_2 100 and perovskite $SrTiO_3$ 100 (STO) respectively, d) and e), corresponding time-spectral contour plots of the transient optical data, f) rutile TiO_2 contour plots for the probe orientated along the ordinary axis, g) the difference between the extraordinary (n_e, d) and ordinary contour plots (n_0, f).

However, while these local electronic states have long been predicted theoretically, matching them to experimental spectra has been challenging. Here, we use an excited state absorption (ESA) that arises in the visible regime (Fig. 1a-1c) ultrafast time scales to connect experiment to theory. The data are taken by a broad-band white light probe in reflectance after above bandgap excitation in a pump-probe setup. To obtain the optical dipoles, the calculations use a hybrid functional (PBE0) and time-dependent density functional theory (TD-DFT). The essential challenge is that the optical transitions are broad both intrinsically (due to vibronic transitions and multiple sites hosting the intermediate configurations) and extrinsically (due to sample structural and chemical heterogeneity). It is therefore imperative to use multiple crystal structures of titanium oxide (rutile, perovskite, and anatase) and several material forms (bulk crystals, epitaxial thin films) to correlate calculated and measured spectra with fidelity. A recently published highlight[1] is rationalizing the ~1 eV change in the ESA between rutile TiO_2 (Fig. 1d) and perovskite $SrTiO_3$ (Fig. 1e). We also analyze the polarization dependence of the ESA in uniaxial rutile TiO_2 (Fig. 1d, 1f, 1g) and the coherent acoustic waves that result from an ultrafast strain associated with the ESA formation. Here we present our progress to date, which involves four CEDARS institutions across single crystalline thin film growth (pulsed laser deposition, molecular beam epitaxy), theory, and optical spectroscopy.

Contributions: C. Boyd, M. Lang took the transient optical data and analyzed the results, guided by T. Cuk. S. McBride performed the DFT calculations, guided by G. Hautier. S. Cherono grew epitaxial films of doped rutile TiO_2, guided by D. Kumar. L. Mitrovic grew epitaxial films of anatase TiO_2, guided by D. Schlom. J. Sormberger orientated the rutile polarization axis at the suggestion of D. Jonas.

1. Boyd, C.; McBride, S.; Paolino, M.; Lang, M.; Hautier, G.; Cuk, T., Assigning Surface Hole Polaron Configurations of Titanium Oxide Materials to Excited-State Optical Absorptions. *Journal of the American Chemical Society* **2025,** *147* (13), 10981-10991.

CMQT
CENTER FOR MOLECULAR QUANTUM TRANSDUCTION

(From left) Iqbal B. Utama, Robert Claassen, Srishti Pal, Hannah Christianson

ENABLING AMBIENT STABILITY AND QUANTUM INTEGRATION OF ORGANOMETALLIC MAGNONIC FERRIMAGNETS VIA ATOMIC LAYER ENCAPSULATION

[EFRC - CMQT] Iqbal B. Utama[1], Robert Claassen[2], Srishti Pal[3], Hannah Christianson[4], Donley S. Cormode[2], Dmitry Lebedev[1], Subhajyoti Chaudhuri[1], Qin Xu[3], George C. Schatz[1], Jeffrey R. Long[4], Gregory D. Fuchs[3], Ezekiel Johnston-Halperin[2], and Mark C. Hersam[1]

[1]Northwestern University; [2]The Ohio State University; [3]Cornell University; [4]University of California, Berkeley

Molecule-based spin and magnonic materials are promising for next-generation quantum technologies, offering synthetic tunability beyond what is achievable with fully inorganic counterparts. Magnons, the quanta of spin waves in magnetic materials, are particularly useful in hybrid quantum systems since they bridge electromagnetic and spin degrees of freedom. The magnetic molecular coordination compound vanadium tetracyanoethylene ($V[TCNE]_x$) possesses exceptional magnonic properties but degrades rapidly when exposed to air, limiting its practical use. In this work, we demonstrate a breakthrough in stabilizing $V[TCNE]_x$ by encapsulating it with a sub-100 nm layer of aluminum oxide using atomic layer deposition. This encapsulation substantially enhances the air stability of $V[TCNE]_x$ while preserving its quantum and magnetic properties, thus increasing its viability for practical quantum information technologies. The sub-100 nm thickness of the encapsulation layer enables spectroscopic and surface-sensitive characterization techniques to probe the intrinsic properties of $V[TCNE]_x$ including spatially-resolved magnetometry measurements. Leveraging the optical transparency of the encapsulation layer over a broad electromagnetic spectral range, we performed detailed

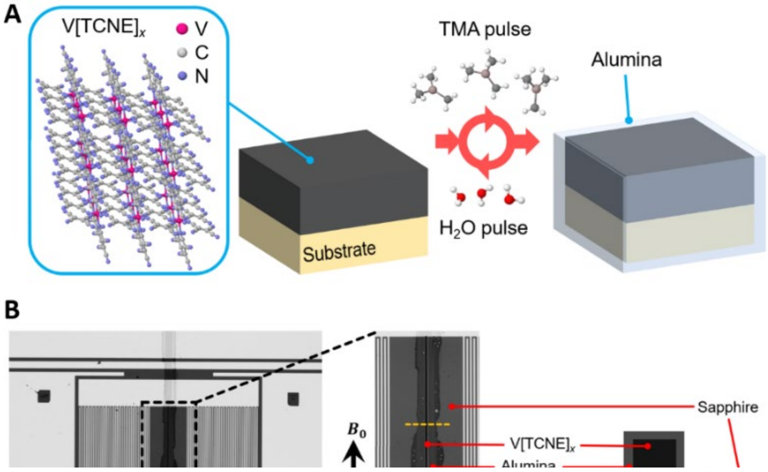


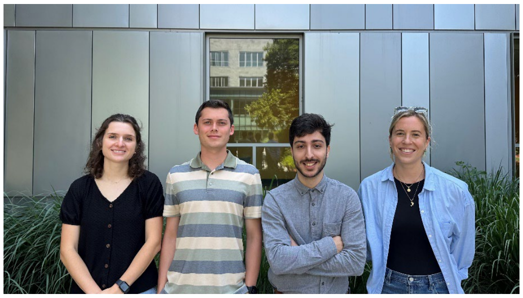
Figure 1. (A) Schematic of ALD alumina encapsulation. (B) Integration of alumina-encapsulated $V[TCNE]_x$ with a microwave resonator.

optical spectroscopy of V[TCNE]$_x$ from deep ultraviolet to mid-infrared energies to resolve the electronic and vibrational excitations of the material. In addition, this encapsulation scheme is compatible with thermal cycling, which allows repeated access to cryogenic temperatures for cavity magnonics, where we observed magnon-photon hybridization at milli-Kelvin temperatures with minimal interference from strain-induced anisotropy effects. Overall, this effective encapsulation scheme enables seamless integration of V[TCNE]$_x$ into advanced quantum devices.

Contributions: M.I.B.U. performed ALD encapsulation, AFM, magnetometry in PPMS, MFM, XPS, UV-vis-NIR, FTIR, ellipsometry, and Raman spectroscopy measurements. R.C. performed CVD growth of V[TCNE]$_x$ and cavity FMR measurements. S.P. fabricated the microwave resonator and performed the cavity magnonics experiments. H.C. performed electrodeposition of V[TCNE]$_x$. M.C.H., E.J.H., G.D.F., J.R.L., and G.C.S. supervised the project.

ENGINEERING SOLUTIONS FOR COMPLEX PLASTICS WASTE USING POLYMER SCIENCE AND CATALYSIS

[EFRC - CPI] Zoé O. G. Schyns, Pedro A. R. Moura, Christine M. Oberhausen, Alex W. Hawkins, Dionisios G. Vlachos, LaShanda T. J. Korley
University of Delaware



(From left) Christine M. Oberhausen, Alex W. Hawkins, Pedro A. R. Moura, and Zoé O. G. Schyns

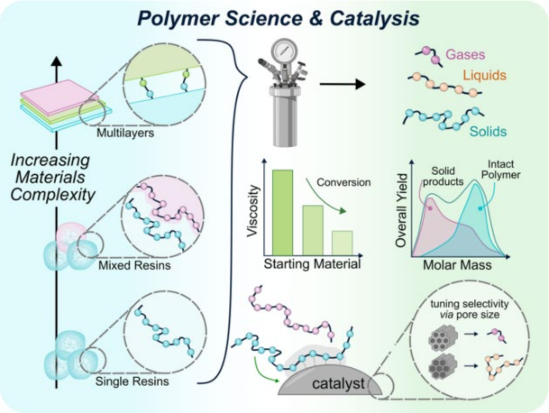


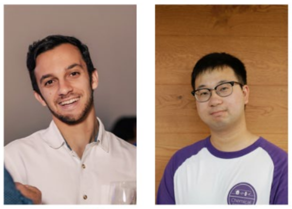
Figure 1 – Schematic representation of polymer science and catalysis concepts used to develop deconstruction strategies for increasingly complex plastic materials.

Most plastics valorization research has focused on single-component systems,[2,3] with limited attention to multicomponent, real-world waste. Overlooking the complexities associated with real-life waste streams (additives, contaminants, multiple resin codes, etc.) can reduce the efficacy of a valorization strategy and hinder sustainable process development.[1-4] By leveraging the multidisciplinary environment within CPI, we integrated catalysis and polymer science to develop robust processes for valorizing structurally complex multilayer plastics. Initially, we explored the deconstruction of key polymer components in multilayer plastic wastes, including heat-sealing and moisture-barrier layers, such as ethylene vinyl acetate (EVA)[5] and ethylene vinyl alcohol (EVOH)[6], and structural outer layers, such as low-density polyethylene (LDPE), and linear-LDPE (LLDPE). We focused on hydrogenolysis over ruthenium-supported catalysts (*e.g.*, Ru/ZrO_2) and hydrocracking over platinum-supported acid zeolite catalysts (*e.g.*, Pt/HY) to produce valuable lubricants and precursors for specialty chemicals, respectively, from the pure resins. We then examined the catalytic activity in physical mixtures of these polymers relevant to multilayer films (LDPE/EVOH or LDPE/EVA). Results showed that pure EVOH and EVA resins and physical mixtures with LDPE (LDPE/EVA and LDPE/EVOH) are slower to deconstruct *via* hydrogenolysis than pure

LDPE, resulting in lower conversion and higher methane selectivity. Hydrocracking showed no such limitations, achieving full conversion and yielding valuable (naphtha-range) products. Further investigation of these catalytic findings using polymer characterization (rheology) revealed thermal degradation, which led to cross-linking (EVA) or conjugated aromatic molecule formation (EVOH), both of which favor hydrogenolysis deactivation mechanisms and support hydrocracking as a promising valorization strategy. Finally, our team utilized these deconstruction strategies to investigate real-world, industrial multilayer films. Initial experiments showed that tie-layer bonds within 5-layer films (LLDPE/LLDPE-gMAH/EVOH/LLDPE-gMAH/LLDPE) inhibited deconstruction. To further explore the effects of tie-layer content, we synthesized maleic-anhydride-based tie layers (LLDPE-gMAH) *via* reactive extrusion to quantitatively assess tie-layer chemistry on deconstruction. Through this sequential work, we aimed to uncover how the complexities of waste-representative materials impacted emerging hydrogenolysis/hydrocracking techniques with the overarching aim of developing plastics valorization strategies more tolerant of difficult-to-recycle materials, as an alternative to landfilling.

References:
[1] Nixon, K. D., *et al.*, *Nat. Chem. Eng.*, 2024, 1, 615–626; **[2]** Nakaji, Y., *et al., Appl. Catal., B*, 2021, 285, 119805; **[3]** Tennakoon, A., *et al.*, *Nature,* 2020, 3; **[4]** Hinton, Z. R., *et al., Green Chem.*, 2022, 24, 7332–7339; **[5]** Moura, P., *et al. ACS Sustain. Chem. Eng.*, 2024, 12, 8717–8728; **[6]** Oberhausen, C. M., *et al.*, *ChemSusChem*, 2024, 17, e202400238.

Contributions: P.R.M. and C.M.O. performed catalytic deconstruction experiments. Z.O.G.S. and A.W.H. performed polymer characterizations and generated polymeric materials. Z.O.G.S. and P.R.M. wrote the abstract.



(From left) Alex Berlaga and Renyu Zheng

From Force-Field Parameters to Programmable Nanostructures: Integrated Simulation, Active Learning, and Experiment for Peptoid-Based Hierarchical Materials

[EFRC - CSSAS] Alex Berlaga[1], Renyu Zheng[2,3], Kaylyn Torkelson[2], Xin Qi[2], Christopher D. Lowe[4], Helen Larson[4], Brandi M. Cossairt[4], Jim Pfaendtner[5], Chun-Long Chen[2,3], Andrew L. Ferguson[1]
[1]University of Chicago; [2]University of Washington; [3]Pacific Northwest National Laboratory; [4]North Carolina State University

In CSSAS, we use sequence-defined peptoids to extrapolate principles from complex biomacromolecules to simplified sequence-defined molecular building blocks and precisely predict and control their assembly into hierarchical materials. We first introduce MoSiC-CGenFF-NTOID, a modular, CHARMM-compatible force field that ports 20 natural and 13 synthetic peptoid sidechains without bespoke parameterization, enabling routine all-atom molecular-dynamics (MD) studies of peptoids and hybrid systems at microsecond time scales (**Fig. A**). Building on this platform, we deploy an active-learning loop that couples MD-derived stability metrics with Gaussian-process regression and Bayesian optimization to identify sequences that mimic known self-assembling peptides (e.g., collagen-mimetic peptides) but whose peptoid substitutions raise triple-helical melting temperatures beyond natural Pro-Pro-Gly analogues. Results establish a hierarchical design framework to provide transferable force fields that furnish reliable energetics, promote active learning that accelerates sequence exploration for peptoids, and demonstrate multiscale simulations to bridge molecular chemistry to higher-order assembly and tertiary and quaternary structure engineering. In a parallel effort, we use DFT and MD calculations, along with experimentally derived design principles, to understand the molecular level peptoid interactions that give rise to the emergence of order, and to synthesize supramolecular hybrid nanostructures. Guided by simulation, we design a series of amphiphilic peptoid regulators that co-assemble with oleate-coated CdS quantum dots (QDs) to precisely tune the formation of peptoid-QD superlattices in non-aqueous solvents (**Fig. B**). We also manipulate the intramolecular folding of multiblock peptoids to control their assembly into Janus 2D nanosheets that template the growth of silica nanoparticles (**Fig. C**). In summary, we use peptoids to unravel the principles that orchestrate the self-assembly of high-information-content molecular building blocks across scales, from the molecular-level emergence of order to supramolecular hybrid hierarchies.

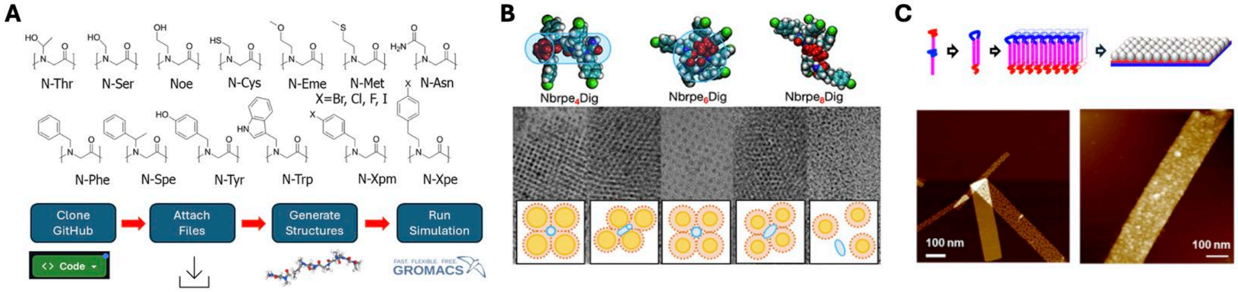


Figure (A) Force field models peptoid-specific interactions. (**B**) Peptoid-control of QD superlattice formation in chloroform. (C) Janus nanosheet formed by multiblock peptoids templates silicification.

Contributions: A.B. and K.T. developed the peptoid force field. A.B. developed the active learning framework. R.Z. synthesized peptoids, characterized their assembly, and developed the Janus nanosheet system. X.Q. conducted DFT and MD calculations of peptoid structure in non-aqueous solvents. C.D.L. and H.L. co-assembled peptoids and QDs into superlattices.

(From upper left) Olivia F. Bird, Faith A. Flinkingshelt, Sophia M. Click (From lower left) Della Hagemann, Hyuna Kwon, Kenneth M. Drbohlav, Evan K. Gowdy

EXTENDING CHARGE-SEPARATED-STATE LIFETIME IN NANOCRYSTAL–MOLECULE HYBRIDS VIA RATIONAL MOLECULAR DESIGN

[EFRC - EPN] Olivia F. Bird[1], Faith A. Flinkingshelt[2], Sophia M. Click[1], Hyuna Kwon[3], Della Hagemann[4], Kenneth M. Drbohlav[4], Evan K. Gowdy[4], Yisrael M. L. Lamb[4], Tadashi Ogitsu[3], Jenny Y. Yang[2], Kenneth A. Miller[4], Gordana Dukovic[1]

[1]University of Colorado Boulder; [2]University of California, Irvine; [3]Lawrence Livermore National Laboratory; [4]Fort Lewis College

Most reactions of practical importance — including those that constitute water splitting — require that multiple charges be accumulated at a single reaction site. Nanocrystal–molecule hybrids are attractive systems for driving such reactions with light. They benefit from the remarkable light-harvesting properties of semiconductor nanocrystals and the synthetic tunability of molecular catalysts. Such systems have previously been demonstrated to achieve near-unity quantum yields for charge separation, but subsequent catalytic yields remain low due to the short lifetimes (~10s of nanoseconds) of charge-separated states. Here, we report the synthesis of a suite of rationally designed molecular charge acceptors, including electron acceptors[1], hole acceptors[2], and hydrogen evolution electrocatalysts[3], for binding to nanocrystals with different anionic donor linker groups to tune rates of charge transfer and recombination. The energetics and thermodynamics of nanocrystal–molecule binding were rigorously evaluated using isothermal titration calorimetry[1] and density functional theory calculations.[3] Transient absorption spectroscopy revealed that our molecular acceptors extend the charge-separated-state lifetime by multiple orders of magnitude, from nanoseconds to microseconds, while maintaining high yields for charge separation.[1,2] We demonstrated hydrogen evolution activity from our catalysts, both electrocatalytically and photocatalytically.[3] We also conducted kinetic Monte Carlo simulations to predict the effects that the charge-transfer dynamics observed in these new systems will have on reactivity.[1] Simulations identified conditions where significant lifetime extension could improve overall photocatalytic yield, providing guidance on new molecular targets. This work represents a step forward in using rational molecular design, and particularly tunable binding, to control charge-separation dynamics.

Contributions: Molecular and materials syntheses were conducted by F.A.F, D.H., K.M.D., E.K.G., K.A.M., and S.M.C. Electrochemical experiments were conducted by F.A.F. Spectroelectrochemical experiments were conducted by F.A.F and Y.M.L.L. Transient absorption spectroscopy experiments were conducted by S.M.C. and O.F.B. Isothermal titration calorimetry experiments and kinetic Monte Carlo simulations were conducted by O.F.B. Density functional theory calculations were performed by H.K. All authors contributed to experimental design and conception.

References: **(1)** Bird, *et al.*, *The Journal of Physical Chemistry C*, **2025**, *129*, 5556, DOI: 10.1021/acs.jpcc.5c00740. **(2)** Click, *et al.*, **2025**, *under review*. **(3)** Flinkingshelt, *et al.*, *Energy & Fuels*, **2025**, *39*, 2196, DOI: 10.1021/acs.energyfuels.4c05559.

ESRA
Energy Storage
Research Alliance

(From left) Alae Eddine Lakraychi, Harshan Reddy Gopidi, Jiaqi Wang, Zeqian (Francis) Zhang, Yu Chen

STRUCTURE–PROPERTY RELATIONSHIPS FOR MULTI-ELECTRON ORGANIC POSITIVE ELECTRODE MATERIALS

[Hub - ESRA] Alae Eddine Lakraychi[1], Harshan Reddy Gopidi[1], Jiaqi Wang[2], Zeqian Zhang[3], Yu Chen[4], Ying Chen[3], Kamila Magdalena Wiaderek[2], Mary C. Scott[4], Pieremanuele Canepa[1], Yan Yao[1]
[1]University of Houston; [2]Argonne National Laboratory; [3]Pacific Northwest National Laboratory; [4]Lawrence Berkeley National Laboratory

Soft organic materials offer a promising platform for solid-state batteries due to their design flexibility and ability to create conformal interfaces with solid electrolyte. However, their design has traditionally focused on molecular-level attributes while neglecting structure, limiting their implementation in energy storage. *Here, we aim to bridge this knowledge gap by understanding structure–property relationships underlying the performance of soft organic electrode materials.* Our research strategy combines expertise in materials design, synthesis, operando characterization, and theoretical modeling through collaboration among various institutions. This integrated approach enables a comprehensive understanding of redox events, structural evolution, and coupled ion–electron transport dynamics as a function of the state of charge.

We have selected *bis*-tetraaminobenzoquinone (TAQ) as a model compound, due to its layered crystal structure and high intrinsic room-temperature electrical conductivity ~10^{-4} S cm^{-1}. To date, we have synthesized all relevant Li_xTAQ (x = 0, 2, and 4) intermediates and independently characterized their physicochemical and electrochemical properties to elucidate the complete reaction pathway. *Ex-situ* and *operando* X-ray diffraction analysis revealed that TAQ undergoes a reversible expansion of the interlayer spacing upon Li intercalation within TAQ layers. The preferred Li-ion insertion sites were accurately predicted using two distinct computational algorithms developed within ESRA.

We investigated the mixed ionic–electronic conduction (MIEC) properties using electrochemical and spectroscopic characterizations. The electrical conductivity was found to be proportional to the concentration of radical species within the material, peaking at ~10^{-2} S cm^{-1} for Li_2TAQ. In contrast, the ionic conductivity increased with lithium content in Li_xTAQ, reaching ~10^{-6} S cm^{-1} for Li_4TAQ. By exploiting the inherent MIEC properties of LixTAQ, we demonstrated solid-state cells operating with a high cathode fraction (~70 wt%) and at low stack pressures (~1 MPa).

These initial exciting findings from ESRA offer fundamental insights into the structure–property relationships of TAQ system, providing a foundational framework for designing novel multi-electron conformal organic electrode materials for durable energy storage systems.

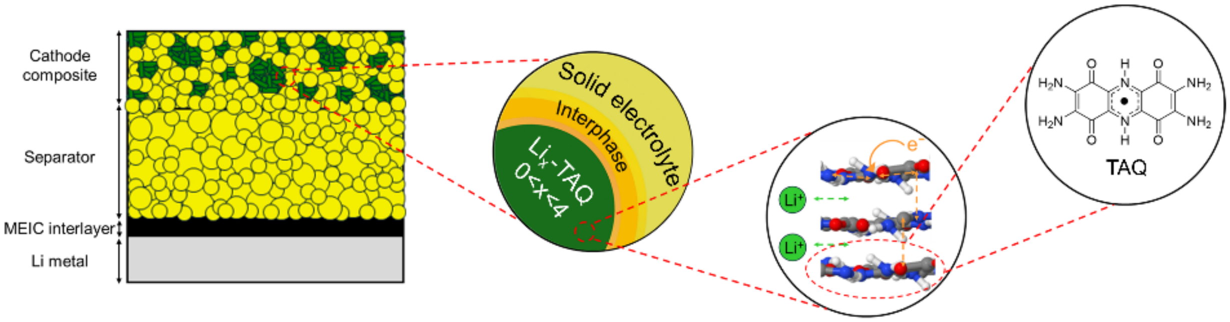


Figure 1: Interdisciplinary research strategy to investigate structure-property relationships in soft organic materials.

Contributions: A.E.L performed material synthesis and characterization, H.R.G carried out theoretical modeling, Y.C micro-electronic diffraction, Z.Z. operando electron paramagnetic resonance, and J.W. X-ray diffraction and pair distribution function.

(From left): Ji-young Ock, Lauren B. Shepard, and Amit Bhattacharya

Unlocking High Conductivity in Composite Electrolytes for Next Generation Energy Storage

[EFRC - FaCT] Ji-young Ock[1], Amit Bhattacharya[2], Lauren B. Shepard[3], Tao Wang[1], Miaofang Chi[1], Sheng Dai[1,4], Susan B. Sinnott[3], Alexei P. Sokolov[1,4], Raphaële J. Clément[2], Xi Chelsea Chen[1]

[1]Oak Ridge National Laboratory; [2]University of California, Santa Barbara; [3]The Pennsylvania State University; [4]University of Tennessee-Knoxville

To accelerate advancements in energy storage and conversion technologies, the FACT-EFRC integrates advanced characterization and computation, bridging atomic and mesoscale processes. Our goal is to uncover ion transport mechanisms in polymer-ceramic composites, which combine robust mechanical strength with high ionic conductivity. A key focus is understanding how ions move along and across polymer–ceramic interfaces and how this influences transport properties, ultimately enabling the rational design of next-generation, high-performance energy storage devices.

We have developed a flux strategy to synthesize 1D $Li_{0.11}Na_{0.24}K_{0.02}La_{0.43}TiO_{2.82}$ (LMTO) single-crystal nanorods with an A-site disordered cubic perovskite phase, overcoming the challenge of achieving cubic symmetry in LMTO. These LMTO nanorods were incorporated into a vinyl ethylene carbonate (VEC)-based single-ion conducting (SIC) polymer electrolyte. Notably, the composite containing 50 wt. % LMTO exhibited a two-fold increase in ionic conductivity, while micron-sized commercial $Li_{0.33}La_{0.55}TiO_3$ (LLTO) showed no enhancement. To elucidate the underlying conduction mechanism, we employed a combination of experimental techniques, including solid-state nuclear magnetic resonance (NMR), in conjunction with density functional theory (DFT) calculations. We hypothesized that the conductivity enhancement originates from the formation of a thin interfacial polymer layer around the LMTO nanorods with enhanced Li^+ mobility. We tracked ion transport pathways in the composite electrolyte using tracer exchange NMR and probed Li exchange at the polymer-ceramic interface using 2D ^6Li exchange spectroscopy measurements and a new $^6Li/^7Li$ isotope exchange method to probe 'ultra-slow' chemical exchange processes occurring on timescales of hours to days. Our experiments confirm that LMTO nanorods function as passive fillers and likely enhance conductivity by reducing electrostatic interactions between Li^+ and the polyanion matrix. Complementary DFT calculations quantify the Li-ion binding energy at the polymer–ceramic interface and show that the Li-ion is less strongly bound to the anion at the LMTO interface compared to the LLTO interface, suggesting that the LMTO composition can also enhance interfacial Li^+ transport. Our experiments suggest that the formation of a percolation pathway and fast ion exchange at the polymer–ceramic interface are key to achieving ultra-high conductivity, as further supported by Li binding energies from DFT calculations. Overall, this work illustrates the interdisciplinary capabilities of FaCT for unveiling interfacial ion transport in polymer-ceramic composite electrolytes for next generation energy storage materials.

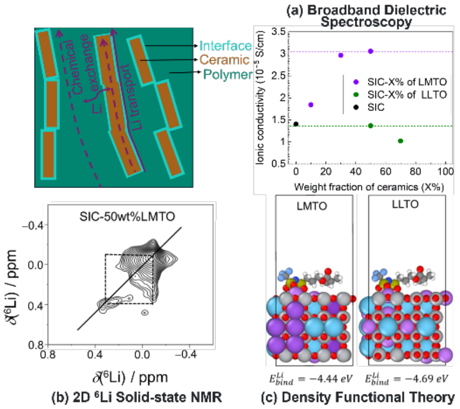


Fig 1. (top-left) Schematic of Li-ion transport in polymer–ceramic composite. (a) Conductivity enhancement with LMTO nanorods. (b) No observable Li-ion exchange between SIC and LMTO (NMR). (c) DFT confirms reduced Li–anion binding at the LMTO interface.

References: [1]Ock, J., et al. *Macromolecules* **2024**, *57*, 7489.; [2]T. Wang, et al., *Adv. Sci.* **2025**, 12, 2408805.; [3]Ock, J., et al. *(under review)* **2025**.*;* [4]Bhattacharya, A.; et al. *(under revision)* **2025**.

Contributions: A.B. performed the NMR spectroscopy characterizations, J.O. synthesized the composite electrolytes and performed electrochemical measurements, L.B.S. conducted the DFT calculations, T.W. synthesized the LMTO ceramic, M.C. performed the TEM. S.D, S.B.S, A.P.S, R.J.C, X.C.C supervised.

METAL CORROSION UNDER IRRADIATION – EXPLAINING IN SITU X-RAY SPECTROSCOPY WITH EX SITU MICROSCOPY AND ATOM PROBE TOMOGRAPHY

[EFRC - FUTURE] Franziska Schmidt[1], Saikumaran Ayyappan[2], Kayla Yano[3], Matthew Chancey[1], Hyosim Kim[1], Djamel Kaoumi[2], Peter Hosemann[4], Blas Uberuaga[1], Yongqiang Wang[1]

[1]Los Alamos National Laboratory; [2]North Carolina State University; [3]Pacific Northwest National Laboratory; [4]University of California, Berkeley

(From left) Franziska Schmidt and Saikumaran Ayyappan

The FUTURE EFRC targets the behavior of solids under environmental extremes. One aspect of this work is the exposure of simple model systems, such as pure Fe, to the extremes of radiation and corrosion simultaneously in the Irradiation-Corrosion Experiment (ICE III) at LANL. ICE III uses proton irradiation and heavy liquid metals like lead bismuth eutectic (LBE) or molten salts to study the effects of radiation on the corrosion process in these environments. During the experiment, particle-induced x-ray emission spectroscopy (PIXE, from protons hitting the target) provides in situ information about pure Fe corrosion in LBE. The PIXE signal indicates a consistent thinning of the sample that is accelerated by proton irradiation [1]. However, ex situ microscopy images (see Figure 3b) and c)) obtained at NC State and atom probe tomography (APT) results from PNNL paint a more complicated picture. This talk focuses on the Fe-LBE system under proton irradiation, the mechanisms of oxide layer formation and degradation, and the importance of applying a host of analysis tools to unravel the complexities of seemingly simple systems.

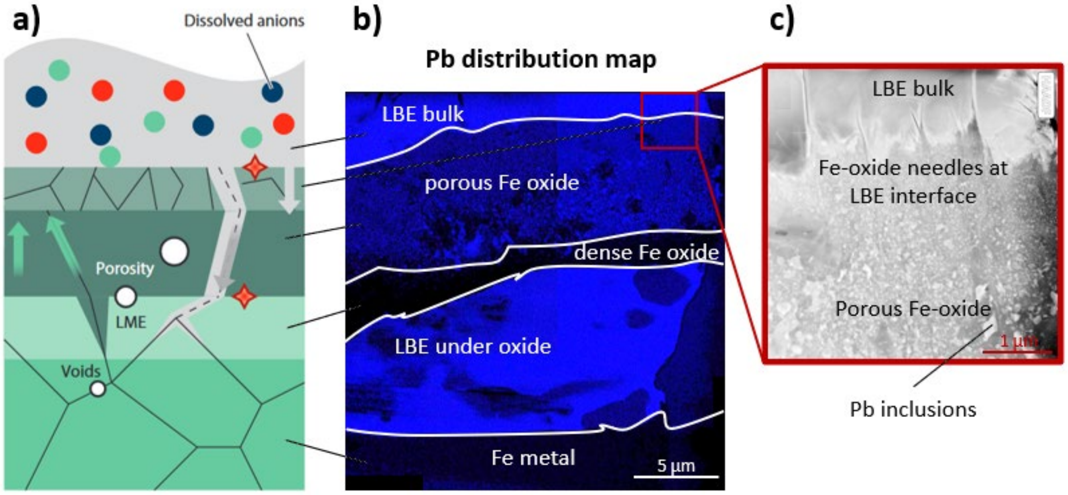


Figure 1 – a) Schematic of corrosion behavior in LBE environments from [2]: In the presence of dissolved O, multiple corrosion layers with varying levels of porosity will form between the LBE (top, grey) and the base metal

(green, bottom), which is also affected by liquid metal embrittlement (LME). b) Pb map of broken-off multilayered Fe-oxide floating in LBE near Fe base metal (unpublished). c) Detailed view of Fe-oxide/LBE interface showing mode of oxide growth (needles) into the liquid (unpublished).

Contributions:

PH, YW, BU conceptualized the study; PH contributed the methodology; FS, SA, KY performed formal analysis; FS, MC, HK, YW conducted the investigation; YW provided resources; FS curated data; FS, SA, KY performed visualization; YW, BU, PH, DK supervised the study; BU, PH obtained funding

References

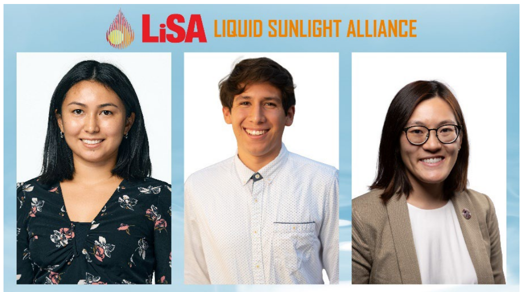
[1] Schmidt, Franziska, et al. "Continuous Monitoring of Pure Fe Corrosion in Lead-Bismuth Eutectic Under Irradiation with Proton-Induced X-ray Emission Spectroscopy." *JOM* 73 (2021): 4041-4050.

[2] Schmidt, Franziska, et al. "Effects of radiation-induced defects on corrosion." Annual Review of Materials Research 51.1 (2021): 293-328.

A Solar-Driven Electrochemical/Photothermocatalytic Process for CO_2 Conversion to C_6 Oxygenates: An Assembly of Coupled Microenvironments

[Hub - LiSA] Matthew Salazar[1,2], Aisulu Aitbekova[1,2], Katherine Yan[1,3], Jonas C. Peters[1,2], Thomas F. Jaramillo[1,3], Harry A. Atwater[1,2], Theodor Agapie[1,2], Alexis T. Bell[1,4]

[1]Liquid Sunlight Alliance; [2]California Institute of Technology; [3]SLAC National Accelerator Laboratory; [4]Lawrence Berkeley National Laboratory



(From left) Aisulu Aitbekova, Matthew Salazar, and Katherine Yan

Coupling CO_2 electrolysis to a thermocatalytic process is a promising approach to convert CO_2 into products beyond C_2 hydrocarbons. Herein, we demonstrate the use of a co-design approach to coupled microenvironments to generate sustainable liquid fuels, advancing LiSA's mission. Specifically, we present a solar-driven, two-step process that converts CO_2 into 2-Methyl-2-pentenal, a C6 oxygenate and food additive, and a flavoring additive (***Figure 1***). In the first step, a photovoltaic-driven membrane electrode assembly (MEA) with a catalyst area of 5 cm^2 converts CO_2 and water into a mixture of carbon monoxide, hydrogen, and ethylene. In the second step, the MEA outlet stream is sent to a photothermocatalytic reactor where it is converted into 2-Methyl-2-pentenal. To obtain the desired product distribution from the CO_2 electrolyzer, we designed a copper/silver (Cu/Ag) tandem electrode. CO_2 is first reduced to CO

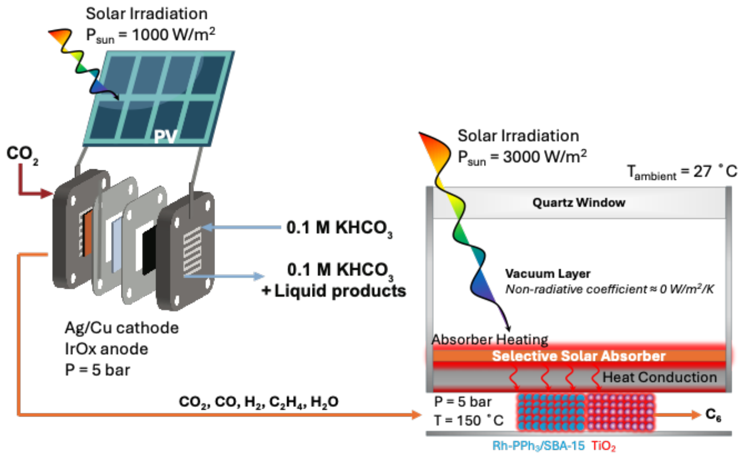


Figure 1. A solar-driven tandem system converts CO_2 into a C_6 oxygenate.

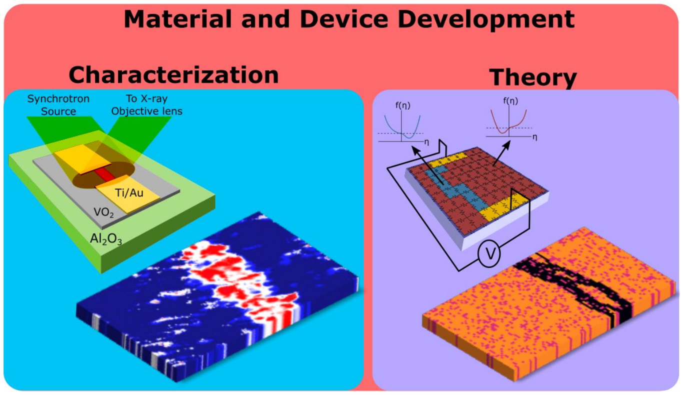
on Ag, and CO is subsequently reduced further on Cu to C_2H_4. From the CO2RR coupled assembly, factors such as varying Ag and Cu ratios and operating parameters (e.g., membrane type, cell compression, and cell pressure) were considered. To perform the photothermocatalytic step, we developed a dual-bed catalyst consisting of phosphine ligand functionalized rhodium (Rh) on SBA-15 and titania (TiO_2). The Rh catalyst converts ethylene, carbon monoxide, and hydrogen to propanal via ethylene hydroformylation. Different co-impregnation hydroformylation catalysts were screened under simulated MEA outlet streams to maximize ethylene conversion to propanal. The best-performing ligand suppresses the formation of undesired ethane and yields an average ethylene-to-propanal conversion of 15 % with propanal selectivity > 95 % (< 5 % selectivity to ethane). The TiO_2 catalyst converts propanal to 2-Methyl-2-pentenal with an average yield of 3.2 %. The development of the photothermocatalytic microenvironment involved tailoring catalyst architectures to match operating pressure and temperature. Our team has successfully demonstrated the solar-driven operation of such a system. To increase the production of 2-methyl-2-pentenal, a larger production of ethylene is needed. As such, we scaled up the MEA area from 5 cm^2 to 25 cm^2. With this larger cathode area, issues such as pressurization and anode degradation were more evident than in the 5 cm^2 MEA. More investigation is needed to address challenges with scale-up within the context of taking a co-design approach to couple electrocatalytic and thermocatalytic processes.

Contributions: M.S., A.A., and K.Y. contributed equally to this work.

(From left) Elliot Kisiel, David Alspaugh, Pavel Salev

INHOMOGENEITIES OF ELECTRICALLY TRIGGERED METAL-INSULATOR TRANSITIONS IN NEUROMORPHIC DEVICES

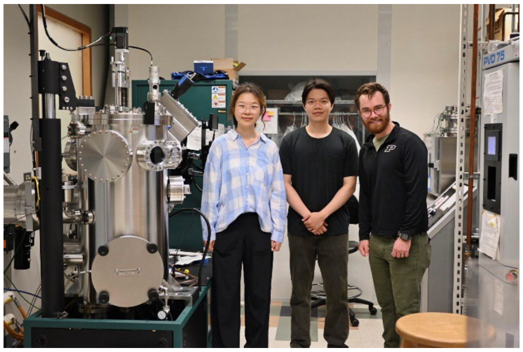
[EFRC - Q-MEEN-C] Pavel Salev[1], Elliot Kisiel[1], David Alspaugh[1], Oleg Shpryko[1], Marcelo J. Rozenberg[1], Yayoi Takamura[2], Zahir Islam[3], Alex Frano[1], Ivan K. Schuller[1]
[1]University of California, San Diego; [2]University of California, Davis; [3]Argonne National Laboratory



Maximizing the number of operations per energy input in neuromorphic hardware requires taking the full advantage of every functionality offered by materials, which in turn necessitates gaining the comprehensive understanding of the material response to external stimuli. In metal-insulator transition (MIT) quantum materials, applying an above-threshold voltage drives a large resistance change, which can mimic the basic neuronal activation [1,2]. MIT electrical triggering can also be accompanied by transient memory, exhibit pronounced stochasticity and show anomalous magnetic responses [3-5]. These subtle properties accompanying the MIT triggering can offer new exciting opportunities to implement advanced neuronal behaviors, such as adaptation and multimodal spiking, and allow processing and storing information leveraging both charge and spin degrees of freedom. Gaining the basic understanding of such properties, however, is a formidable challenge because of the need for advanced *in-operando* micro- and mesoscale characterization and development of nonequilibrium theoretical frameworks. In our recent works [6,7], we demonstrate that electrical MIT triggering is accompanied by a complex structural response resulting in local lattice states that do not emerge when slowly varying equilibrium control parameters such as temperature or pressure. Utilizing advanced synchrotron x-ray techniques, x-ray microdiffraction and dark-field x-ray microscopy, we observed that driving the electronic MIT by external voltage produces spatially inhomogeneous lattice distortions, including nanoscale monoclinic clusters inside the voltage-induced rutile filament in VO_2 and crystal lattice twinning in $(La,Sr)MnO_3$. We showed that the nominally volatile electrically MIT triggering in VO_2 is accompanied by medium-term memory, which is mediated by local lattice sites that tend to undergo the phase transition at significantly lower threshold voltages after performing electrical cycling. This memory persists even through a brief low-temperature thermal cycle and vanishes after the device relaxes for ~30 minutes. Based on experimental observations, we developed an interacting Mott resistor network model, which showed that point defects can lead to spatially extended phase distribution inhomogeneities and lock the local sites in the low-switching voltage state, leading to the medium-term memory. Overall, our collaborative full-cycle research approach incorporating material synthesis and fabrication, advanced characterization, and theoretical modeling allowed an unprecedented insight into the structural evolution in electrical MIT switches and can lead to the development of novel functionalities in quantum materials neuromorphic electronics.

Contributions: P.S. synthesized materials and fabricated devices, E.K. And P.S. performed the x-ray microscopy measurements, D.A. developed the Mott resistor network analysis.

References: [1] Sci Rep **10**, 4292 (2020), [2] Nat Nanotechnol **16**, 680 (2021), [3] Nature **569**, 388 (2019), [4] PNAS **120**, e2303765120 (2023), [5] Phys Rev B **107**, 054415 (2023), [6] ACS Nano **19**, 15385 (2025), [7] PNAS **121**, e2317944121 (2024).



(From left) Zhaoyun Zheng, Hanyu Hong and Jonas Mark Peterson

STRONG LIGHT–MATTER INTERACTION IN PLASMONIC ARRAYS ENABLES COHERENT QUANTUM EMISSION

[EFRC - QuPIDC] Zhaoyuan Zheng[1], Jonas Peterson[2], Hanyu Hong[3], Jiwoong Park[3], Libai Huang[2], and Teri Odom[1]

[1]Northwestern University; [2]Purdue University; [3]University of Chicago

Two-dimensional transition metal dichalcogenides (TMDCs) are promising materials platform for scalable quantum emitters due to their strong excitonic resonances and spin-valley physics. However, their photoluminescence is often weak—particularly in multilayer systems—posing challenges for integration into quantum photonic devices. Here, we demonstrate that plasmonic lattices offer a programable photonic platform to enhance and control light emission from TMDCs (Fig.1 a-g). By coupling single and multilayer TMDCs to engineered plasmonic arrays composed of periodically arranged metallic nanoparticles we hybridize localized surface plasmons with diffractive modes to generate surface lattice resonances (SLRs). Through spectral alignment of single-layer WS_2 excitonic transitions with SLR modes, we achieve up to 36-fold Purcell enhancement in radiative rates of excitons at room temperature. Notably, we observe dramatic brightening of multilayer WS_2, with photoluminescence enhanced by more than 3 orders of magnitude. Ultrafast pump-probe microscopy further uncovers the momentum-resolved dynamics of exciton–polariton modes in these hybrid systems, revealing signatures of coherent light–matter interaction. Together, these results highlight plasmonic arrays as a versatile and scalable platform for enhancing emission and coherence in quantum emitters, directly supporting QuPIDC mission to develop room-temperature quantum photonic technologies.

Contributions: Zhaoyuan Zheng fabricated the plasmonic arrays and conducted simulations of light–matter interactions within the system. Jonas Peterson performed the ultrafast optical spectroscopy measurements and carried out kinetic modeling of the data. Hanyu Hong synthesized the two-dimensional materials.

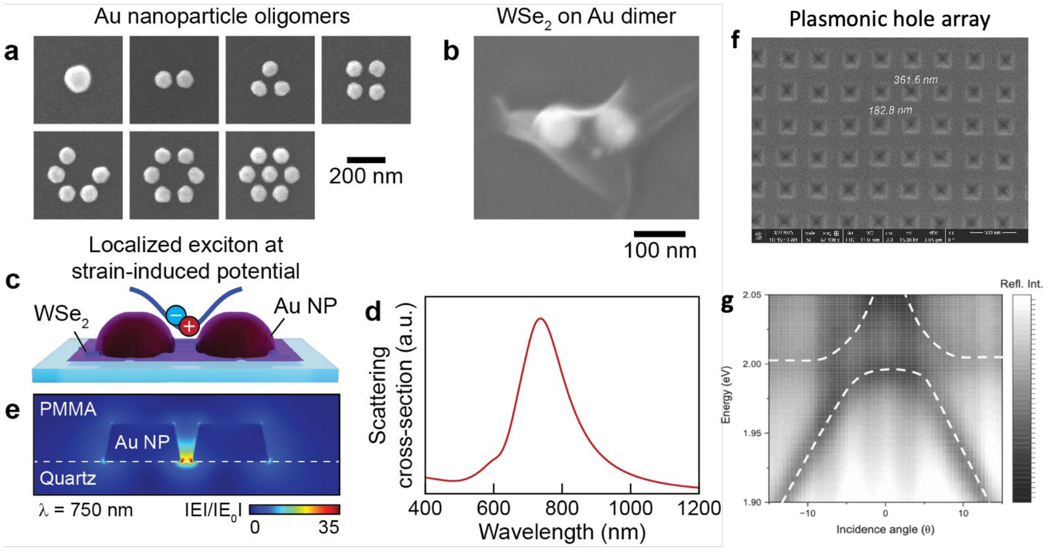


Figure 1: Integration of TMDCs on plasmonic nanoparticle arrays. (a) SEM images of Au oligomers fabricated using soft lithography and reactive ion etching. (b) SEM image of WSe_2 transferred on a Au dimer. (c) Schematics of a TMDC sheet placed on a Au dimer and its exciton trapped in a strain-induced potential. (d-e) Calculated normal scattering spectrum and electric near-field distribution of localized surface plasmon of Au dimer. (f). A SEM image of a plasmonic lattice that can support lattice plasmon. (g) Experimental measured angle-resolved reflectance spectrum showing strong light matter coupling between monolayer WS_2 and lattice plasmon.

(From left) Brandon R. Clarke, Pranav Krishnan, and Yun Seong Kim

MULTI-MATERIAL 3D PRINTING WITH FRONTALLY POLYMERIZABLE RESINS

[EFRC - REMAT] Brandon R. Clarke[1], Pranav Krishnan[2], Connor D. Armstrong[2], Yun Seong Kim[2], Ignacio Arretche[2], Derrick Sanders[2], Jeffrey S. Moore[2], Sameh H. Tawfick[2], Nancy S. Sottos[2], Jennifer A. Lewis[1]
[1]Harvard University; [2]University of Illinois Urbana-Champaign

This work is part of the U.S. Department of Energy's Energy Frontier Research Center (EFRC) for Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials (REMAT), a cross-institutional initiative aimed at revolutionizing the production, performance, and end-of-life management of thermoset polymers. Our collaborative research unites experts in mechanical engineering, polymer chemistry, and polymer physics at Harvard University and the University of Illinois Urbana-Champaign to develop next-generation additive manufacturing (AM) materials and platforms.

Our AM research is driven by the design and deployment of frontally polymerizable (FP) resins, particularly those incorporating dicyclopentadiene (DCPD) and cyclooctadiene (COD), which form low-energy, rapid-curing thermoset systems. These materials polymerize through self-sustaining reaction fronts which require a small thermal activation energy to initiate, significantly reducing cure energy consumption compared to traditional thermoset manufacturing. However, this resin system poses challenges for AM, including short working time and spontaneous polymerization. We address these hurdles through precise control of polymerization kinetics, catalyst/inhibitor ratios, and gelation behavior. Our team leverages copolymer chemistries to modulate network structure, achieving extended pot lives and printable gel states suitable for extrusion-based AM processes.

Our copolymer resin systems have been utilized in three novel multi-material AM platforms: Rotational Direct Ink Writing (DIW), Active Mixing DIW, and Morphogenic Growth Printing (**Figure 1a-c**). These FP AM techniques are capable of efficiently forming complex geometries with orders of magnitude thermomechanical property tunability (*e.g.* glass transition temperature, Young's modulus, and elongation at break) over multiple length scales through a single stream process. Multi-material FP AM offers a promising avenue for fabrication of functional, gradient-rich structures such as tendon-like hinges for soft robotic actuation and shape-memory components for biomedical devices, demonstrating performance tailored by design.

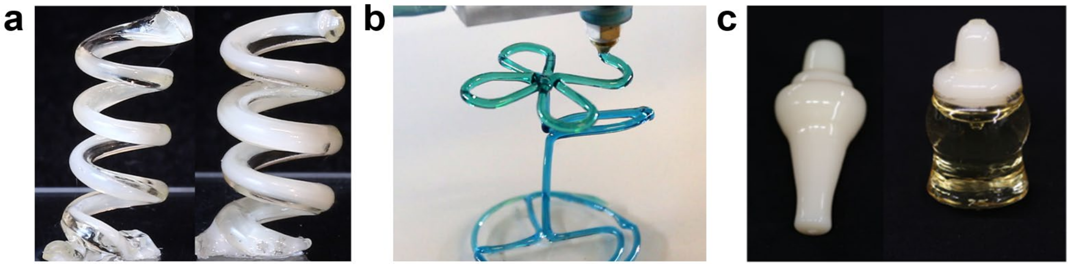


Figure 1. Multi-material parts fabricated using copolymer resin chemistries and additive manufacturing systems developed in REMAT. **(a)** Rotational DIW (R-DIW), **(b)** Active mixing DIW, **(c)** Multimaterial morphogenic growth printing (MMGP). Each manufacturing method allows varied modes of FP resin printing, providing access to a wide variety of possible structures using the same chemistries.

Contributions*:* J.A.L., S.H.T, N.R.S., and J.S.M. supervised the research. B.R.C., P.K., C.D.A., J.A.L., S.H.T., and N.R.S. conceptualized this work. B.R.C., P.K., C.D.A., Y.S.K., I.A., and D.S. conducted all experiments. All worked to draft figures and presentation of the work. J.A.L, S.H.T., N.R.S., and J.S.M. provided funding to graduate students and postdoctoral researchers.

2025 EFRC-HUB-CMS-CCS PI MEETING TEAM SCIENCE CONTEST

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Started: 2016

[CCS – BEAST] Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques
Ravishankar Sundararaman, Rensselaer Polytechnic Institute
Started: 2021