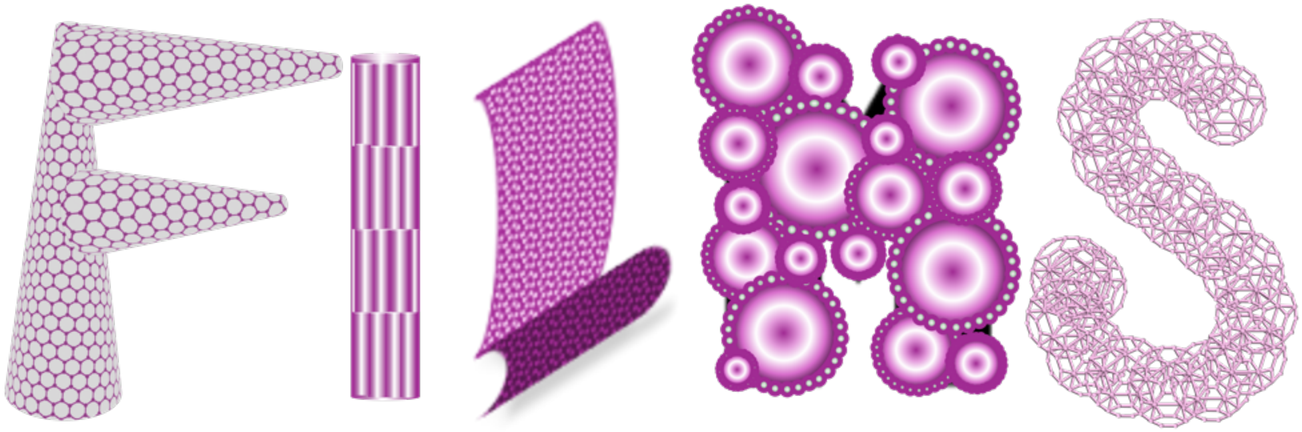

Frontiers
in
Low dimensional
Materials
Symposium

October 31, 2025

CREST iDEALS PHASE II

NSF

CUNY GRADUATE CENTER

ADVANCED SCIENCE RESEARCH CENTER
THE GRADUATE CENTER
CITY UNIVERSITY OF NEW YORK

The City College of New York

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INTRODUCTION

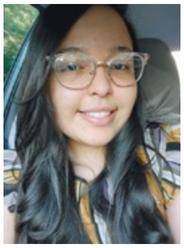
It is a pleasure to introduce the Book of Abstracts for the IDEALS sponsored and student-led Frontiers in Low Dimensional Materials Symposium (FiLMS). This Symposium is intended to depict and showcase the research that takes place in the NSF CREST Center IDEALS at The City College of New York, and to provide networking opportunities to the researchers. The Symposium took place on August 22, 2025 at the CUNY Advance Science Research Center (ASRC). It was fully organized and carried out by IDEALS students, and features the work of three outside Keynote Speakers, world leaders in their fields, each representing an aspect of the research area that is performed in each of the three IDEALS's Subprojects. We thank them for their willingness to share their knowledge, as they inspire us to continue our work in frontier areas of materials research. It also includes a series of interactive networking sessions supported by the viewing of posters presented by IDEALS students and postdocs in which they describe their latest research findings. This Book of Abstracts serves to document the work carried out in the Center and to provide a lasting remembrance of the FiLMS Symposium that can be shared with friends and associates within our university and beyond.

Sincerely,
Maria C. Tamargo, Director
NSF CREST Center IDEALS
CUNY ASRC - October 31, 2025

DEDICATION

This Book of Abstracts is dedicated to the memory of our friend and colleague Professor Kyungwha Park of Virginia Tech, whose untimely passing on August 14, 2025 is deeply felt by the entire IDEALS community

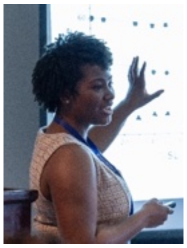
FILMS STUDENT ORGANIZING COMMITTEE



Paola Colon de Leon

Subproject 2

Dr. Rein Ulijn & Dr. Raymond Tu



Candice R. Forrester

Subproject 1

Dr. Maria C. Tamargo

Samhita Kattekola

Subproject 2

Dr. Ilona Kretzschmar & Dr. Alexander Couzis

Eric A. McPherson

Subproject 2

Dr. Ilona Kretzschmar

Justin Pinca

Subproject 2

Dr. Ilona Kretzschmar & Dr. Gustavo Lopez

Patrick K. Yang

Subproject 2

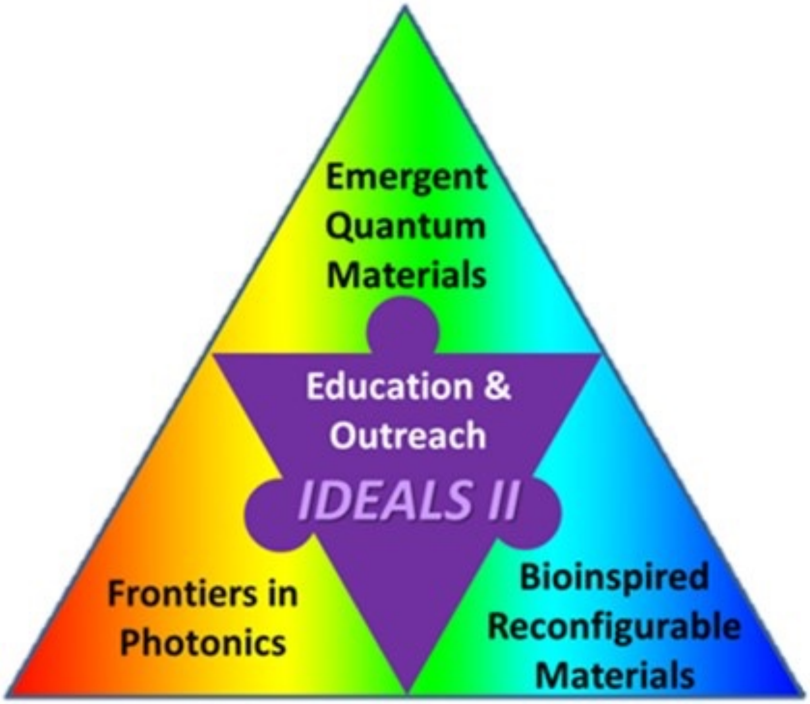
Dr. Stephen O'Brien & Dr. Sanjoy Banerjee

ABOUT CREST IDEALS

Centers of Research Excellence in Science and Technology (CREST) is a National Science Foundation (NSF) program that makes resources available to enhance the research capabilities of minority-serving institutions through the establishment of centers that effectively integrate education and research. Building upon the salient accomplishments of IDEALS I, the Phase II CREST Center for Interface Design and Engineered Assembly of Low-dimensional Systems (IDEALS II) addresses the need to strengthen the nation's leadership in materials capabilities in the frontier areas of quantum materials, bioinspired reconfigurable materials, and photonic materials and technologies.

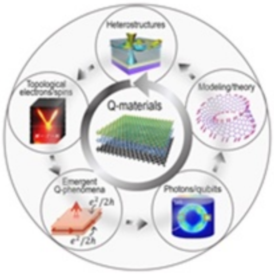
IDEALS I advanced the state of the art in materials research producing over 120 peer-reviewed publications in leading journals and over 200 presentations at national and international conferences. It helped develop the future science and technology leaders by building a highly skilled community of researchers comprising 27 doctoral students, with 11 PhDs awarded, and over fifty undergraduates involved in academic year and summer research.

The innovative IDEALS II research activities are organized into three synergistic interdisciplinary subprojects entitled: (1) Emergent Quantum Materials and Functions; (2) Bioinspired Reconfigurable Materials to Scale; and (3) Frontiers in Photonics: Materials, Phenomena and Devices. IDEALS II researchers are poised to discover and design new materials, develop sophisticated probing techniques, introduce applications and generate intellectual property with profound scientific impact. IDEALS II aims to have far-reaching societal impacts by continuing to educate a community of scientists and engineers that will help transform the materials landscape of the US and the world.



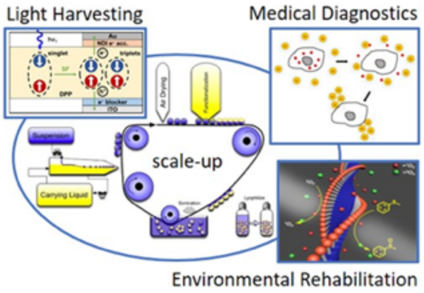
Subproject 1: Emergent Quantum Materials and Functions

Subproject 1 aims to create a core of excellence in Materials Science and Engineering of two-dimensional (2D, surfaces and interfaces) systems where band topology and strong electron correlations emerge, creating new concepts, functions and quantum phenomena for the next-generation quantum technologies. Zero-dimensional (0D, localized defects) systems (rare-earth ions in host matrices) will be utilized as platforms for implementing spin qubits that circumvent the limitations of current schemes. The Subproject research aligns directly with the national priority of "Leading the Next Quantum Revolution".



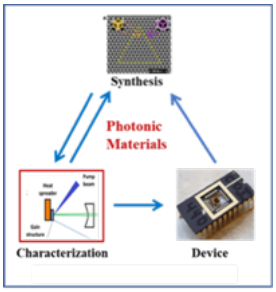
Subproject 2: Bioinspired Reconfigurable Materials to Scale

During IDEALS I, Subproject 2 explored materials with bio-inspired design that change their application-relevant properties by adapting to an external stimulus. IDEALS II research focuses on scalability of reconfigurable materials designed in IDEALS I, and further explores specific applications of new bio-inspired materials in three research clusters drawing on the team's strength and expertise. The efforts address national priorities in energy, health and the environment.



Subproject 3: Frontiers in Photonics: Materials, Phenomena and Devices

Subproject 3 is designed to explore emerging basic ideas, synthesize new materials with unprecedented functionalities, investigate salient properties of the engineered materials, design and test devices based on promising materials, and provide feedback for materials and device design criteria. New in IDEALS II, it will organize this synergistic interplay between bold basic concepts and technological advances in three clusters: (i) Topological photonics and entangled photons; (ii) Photonic phenomena in hybrid materials; and (iii) Semiconductor nanostructures for next-generation photonic devices. The proposed activities align with national priorities of quantum optics, energy sources and sensors.



THE CREST IDEALS LEADERSHIP TEAM

Maria C. Tamargo

Center Director

Maria Tamargo is a CUNY Distinguished Professor of Chemistry at CCNY and is on the doctoral faculty of Chemistry, Physics and Electrical Engineering. Her research deals with molecular beam epitaxy of low dimensional layered materials and nanostructures of wide band gap semiconductors, topological insulators, and other materials. She is a member of the National Academy of Engineering (2020).

Lia Krusin-Elbaum

Subproject 1 Director

Lia Krusin-Elbaum is a Professor of Physics at CCNY and is on the doctoral faculty of Physics. Her research deals with complex nanostructured materials, topological insulators and other novel quantum materials. She is also the IRG-I co-director of the newly awarded Columbia University-CCNY MRSEC on Precision Assembled Quantum Materials (PAQM).

Ilona Kretzschmar

Subproject 2 Director

Ilona Kretzschmar is a Professor of Chemical Engineering at CCNY's Grove School of Engineering, and is on the doctoral faculty of Chemical Engineering and Chemistry. Her research is based on the study of nano and microparticles, such as Janus and Patchy particles, their directed self-assembly, and their use in energy and sensing applications.

Swapan K. Gayen

Subproject 3 Director

Swapan K. Gayen is a Professor of Physics at CCNY and is on the Physics and Electrical Engineering doctoral faculties. His research is on ultrafast lasers and spectroscopy of nanoscale materials and devices, and its combination with scanning probe techniques, to investigate the physics of novel nanostructures and their applications.

Donna McGregor

Outreach and Education Programs Co-Director

Donna McGregor is an Associate Professor of Chemistry at Lehman College and is on the Chemistry doctoral faculty. Her research interests are in the fields of Chemical Education Pedagogy, the understanding of Tc-99 coordination chemistry, and the use of short peptide building blocks for the intelligent design of chelating systems and nanostructures. She is PI of the IDMinNYC REU Site.

Anthony Richardson

Center Administrator

Anthony Richardson is the IDEALS Center Administrator, responsible for coordinating the management and reporting responsibilities of the Center. He is also the Coordinator of the Research Experience for Undergraduates (REU) program supported by IDEALS.

CURRENT CREST IDEALS II AFFILIATED FACULTY

Elizabeth Biddinger

Subproject 2

Chemical Engineering, The City College of New York

Adam Braunschweig

Subproject 2, 3

Nanoscience Initiative, Advanced Science Research Center
Chemistry and Biochemistry, Hunter College

Ubaldo Cordova

Subproject 2

Executive Vice President for Academic Affairs and Research,
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Interim Dean of Science and Professor, The City College of New York
Chemistry and Biochemistry, The City College of New York
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Kyungwha Park

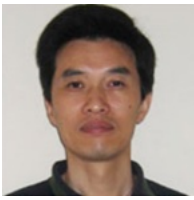
Subproject 1

Physics, Virginia Tech

Matthew Y. Sfeir

Subproject 3

Physics, The City College of New York
Photonics Initiative, Advanced Science Research Center



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Raymond Tu

Subproject 2

Chemical Engineering, The City College of New York
Nanoscience Initiative, Advanced Science Research Center

Rein V. Ulijn

Subproject 2

Nanoscience Initiative, Advanced Science Research Center
Chemistry, Hunter College

AGENDA

Time	Item
8:00 AM	Registration Breakfast, Coffee, and Networking
9:00 AM	Introductory Remarks CREST IDEALS PI **Prof. Maria Tamargo,** FILMS Committee
9:15 AM	Introduction of Keynote Speaker (*Samhita Kattekola, Eric McPherson*) Keynote speech #2 (45 + 10 Q&A) **Prof. Kyle J.M. Bishop** Professor, Chemical Engineering Department, Columbia University
10:15 AM	Group Photo
10:30 AM	**Poster session 1** Coffee, Tea, and Light Snack Break
11:45 AM	Lunch/Networking
1:15 PM	Introduction of Keynote Speaker (*Justin Pinca, Patrick Yang*) Keynote speech #1 (45 + 10 Q&A) **Prof. Andrea Alù** Distinguished Professor, ASRC Photonics Initiative, CUNY
2:15 PM	**Poster session 2** Coffee, Tea, and Light Snack Break
3:15 PM	Greetings from the President **Dr. Vincent Boudreau** President of The City College of New York
3:30 PM	Introduction of Keynote Speaker (*Paola Colon De Leon, Candice Forrester*) Keynote speech #3 (45 + 10 Q&A) **Prof. Tatiana A. Webb** Assistant Professor, Department of Physics & Astronomy, Barnard College
3:30 PM	Closing Remarks & Awards Announcement

KEYNOTE SPEAKERS

Tatiana A. Webb

Assistant Professor, Barnard College

Tatiana Webb is an Assistant Professor in the Department of Physics and Astronomy at Barnard College. She completed her BSc and MSc at McGill University, where she investigated magnetic frustration in amorphous materials in Prof. Dominic Ryan's lab. She earned a PhD Physics from Harvard University, working with Prof. Jenny Hoffman to investigate the electronic structure of high-Tc superconductors. She then completed a postdoc working with Prof. Abhay Pasupathy at Columbia University, where she shifted focus to investigating 2D materials with atomic force microscopy. Tatiana's work focuses on understanding and manipulating novel electronic phenomena. She employs a variety of scanning probe techniques to measure electronic, structural and magnetic properties from the atomic scale through mesoscales. A central theme is to use mesoscale structure as a tool both to explore the complex phase diagrams of materials in which electrons interact strongly, and to manipulate properties of electronic devices.

A cavity-altered superconductor probed via magnetic force microscopy

Tatiana A. Webb[1,2], Itai Keren[2], Shuai Zhang[2], Jikai Xu[2], Dihao Sun[2], Brian S. Y. Kim[2], Dongbin Shin[3,4], Songtian S. Zhang[2], Junhe Zhang[2], Giancarlo Pereira[2], Juntao Yao[5,6], Takuya Okugawa[2,3], Marios H. Michael[3], James H. Edgar[7], Stuart Wolf[8], Matthew Julian[8], Rohit P. Prasankumar[8], Kazuya Miyagawa[9], Kazushi Kanoda[9,10,11], Genda Gu[5], Matthew Cothrine[12], David Mandrus[12], Michele Buzzi[3], Andrea Cavalleri[3,13], Cory R. Dean[2], Dante M. Kennes[3,14], Andrew J. Millis[2,15], Qiang Li[5,16], Michael A. Sentef[17,3], Angel Rubio[3,18], Abhay N. Pasupathy[2,5], and D. N. Basov[2]

[1]*Department of Physics and Astronomy, Barnard College, New York, NY, USA*
[2]*Department of Physics, Columbia University, New York, NY, USA*
[3]*Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*
[4]*Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Gwangju, Republic of Korea*
[5]*Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, NY, USA*
[6]*Department of Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, NY, USA*
[7]*Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, KS, USA*
[8]*Deep Science Fund, Intellectual Ventures, Bellevue, WA, USA*
[9]*Department of Applied Physics, The University of Tokyo, Bunkyo, Tokyo, Japan*
[10]*Max Planck Institute for Solid State Research, Stuttgart, Germany*
[11]*Physics Institute, University of Stuttgart, Stuttgart, Germany*
[12]*Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN, USA*
[13]*Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom*
[14]*Institut für Theorie der Statistischen Physik, Aachen, Germany and JARA - Fundamentals of Future Information Technology*
[15]*Center for Computational Quantum Physics, The Flatiron Institute, New York, NY, USA*
[16]*Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA*
[17]*Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany*
[18]*Initiative for Computational Catalysts, The Flatiron Institute, New York, NY, USA*

Electronic properties arise from phenomena at a multitude of length scales from sub-atomic to macroscopic. Atomic force microscopy (AFM) provides a multimodal lens on the rich mesoscale electronic, magnetic, optical, and mechanical structure of materials to bridge the gap between nanoscale local properties and global device properties. In this talk, I will focus specifically on a materials design route to cavity-engineered electronic ground states.[1]

Enhanced coupling in cavities facilitates modification of the electronic properties of materials through light-matter interactions.[2]. Theories predict that these cavity effects have the potential to not only generate novel excited state phenomena, but also to modify ground state properties, opening the possibility for engineering electronic phases without the need for optical pumping. In particular, multiple proposals suggest that superconductivity could be modified via cavity coupling.[3,4] Thin crystals of 2D materials that naturally act as high-quality cavities allow facile integration of cavity geometries directly into heterostructures.[5,6] Here, we place 2D material hexagonal boron nitride (hBN) on the surface of superconductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br. We demonstrate the resonant coupling of phonon-polaritons of the hBN to phonons within the superconductor. Using the Meissner force measured via magnetic force microscopy to probe superconductivity[7], we observe a reduction of superfluid density near this resonant interface. We discuss experimental constraints on the underlying mechanism for suppressing superconductivity, and the future possibilities for engineering quantum materials.

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[1] Keren, I. et al. (2025).doi:10.48550/arXiv.2505.17378
[2] Schlawin, F., Kennes, D.M. & Sentef, M.A. Applied Physics Reviews 9, 011312 (2022).
[3] Le Dé, B., Eckhardt, C.J., Kennes, D.M. & Sentef, M.A. J. Phys. Mater. 5, 024006 (2022).
[4] Sentef, M.A., Ruggenthaler, M. & Rubio, A. Sci Adv 4, eaau6969 (2018).
[5] Basov, D.N., Fogler, M.M. & García de Abajo, F.J. Science 354, aag1992 (2016).
[6] Berkowitz, M.E. et al. Nano Lett 21, 308–316 (2021).
[7] Luan, L. et al. Phys. Rev. B 81, 100501 (2010).

Kyle J. M. Bishop

Professor, Columbia University

Kyle J. M. Bishop is Professor of Chemical Engineering at Columbia University. He received his BS in Chemical Engineering with highest distinction from the University of Virginia and his PhD from Northwestern University. Prior to joining the Columbia faculty in 2016, he was a post-doctoral fellow with George Whitesides at Harvard University and an Assistant Professor of Chemical Engineering at the Pennsylvania State University. His research seeks to discover, understand, and apply new strategies for organizing and directing the assembly of colloids and other soft materials outside of thermodynamic equilibrium. Bishop is the recipient of the 3M Non-tenured Faculty award and the NSF CAREER award.

Active Colloids as Models, Materials, and Machines

Kyle J.M. Bishop
Department of Chemical Engineering, Columbia University, New York, NY, USA

Active colloids use energy input at the particle level to propel persistent motion and direct dynamic assemblies. These microscopic systems provide useful experimental models of nonequilibrium many-body physics in which dissipative currents break time-reversal symmetry. Freed from the constraints of thermodynamic equilibrium, active colloids assemble to form materials that move, reconfigure, heal, and adapt. Colloidal machines based on engineered particles and their assemblies provide a basis for mobile robots with increasing levels of autonomy. This talk surveys our efforts to understand and apply active colloids animated by chemical reactions, time-varying magnetic fields, and electric currents in pursuit of material systems that mimic the functions of living matter. We highlight opportunities for chemical engineers to contribute to this growing field.

Andrea Alù

Distinguished Professor, CUNY ASRC

Andrea Alù is a Distinguished Professor at the City University of New York (CUNY), the Founding Director of the Photonics Initiative at the CUNY Advanced Science Research Center, and the Einstein Professor of Physics at the CUNY Graduate Center. He received his Laurea (2001) and PhD (2007) from the University of Roma Tre, Italy, and, after a postdoc at the University of Pennsylvania, he joined the faculty of the University of Texas at Austin in 2009, where he was the Temple Foundation Endowed Professor until Jan. 2018. Dr. Alù is a Fellow of the National Academy of Inventors (NAI), the American Association for the Advancement of Science (AAAS), the Institute of Electrical and Electronic Engineers (IEEE), the Materials Research Society (MRS), Optica, the International Society for Optics and Photonics (SPIE) and the American Physical Society (APS). He is a Highly Cited Researcher since 2017, a Simons Investigator in Physics, the director of the Simons Collaboration on Extreme Wave Phenomena Based on Symmetries, and the Editor in Chief of Optical Materials Express. He has received several scientific awards, including the NSF Alan T. Waterman award, the Blavatnik National Award for Physical Sciences and Engineering, the IEEE Kiyo Tomiyasu Award, the ICO Prize in Optics, the Optica Max Born Award, the SPIE Mozi Award and the URSI Issac Koga Gold Medal.

Polaritonic Metasurfaces

Andrea Alù
Photonics Initiative, Advanced Science Research Center, City University of New York, New York, NY, USA
Physics Program, Graduate Center, City University of New York, New York, NY, USA
Department of Electrical and Computer Engineering, City College of New York, New York, NY, USA

In this talk, I discuss our recent efforts in the context of nano-optics and photonics, with a special emphasis on strong light-matter interactions enabled by excitonic, phononic, electronic and magnonic 2D material responses coupled to engineered metasurfaces. I will discuss our recent theoretical and experimental results in the context of polariton manipulation in these systems, the role of symmetries in their control, and their opportunities for technological advances. The combination of these features with photonic engineering enables giant optical nonlinearities, efficient nanoscale light manipulation and topological wave phenomena. During the talk, I will discuss the exotic light-matter interactions arising in these systems, and their opportunities for wave physics and photonics technologies.

SUBPROJECT 1:

STUDENT ABSTRACTS

Characterization of defective hBN

Saifa Amin[1,2], Aidan Jimenez[2], John Woods[2], Enrique Mejia[2], Ashok Adhikari[1,2], Jonathan Pelliciari[3] and Gabriele Grosso[1,2]

[1]*Physics Program, Graduate Center, City University of New York, New York, NY, USA*
[2]*Photonics Initiative, Advanced Science Research Center, City University of New York, New York, NY, USA*
[3]*National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA*

Single-photon emitters in hexagonal boron nitride (hBN) arise from defects of the crystal lattice involving excitations of antibonding orbitals of nitrogen atoms. Optical recombination occurs through a donor–acceptor pair (DAP) process, which explains the observed photophysical emission properties in which the charge carrier recombination between donor and acceptor defects results in a very broad spectral distribution of emission. PL spectroscopy was carried out on hBN samples that had been treated by plasma exposure and thermal annealing to induce defect states. Using DAP model and photoluminescence (PL) measurements, we find that nonlocal recombination occurs from distant defects, indicating the presence of defect-mediated quantum emitters in hBN. These results provide insights into engineering defect states in hBN for single photon emission and quantum photonic applications.

Molecular Beam Epitaxy Growth and X-Ray Analysis of α and γ MnTe

Candice R. Forrester,[1] Sina Mohammadi,[1] Aran Barton,[1] Jisoo Moon,[1] Rei Miyazawa,[2] Amy Lopez,[1] Vishnu Vijayakrishnan,[1] Masakazu Kobayashi[2] and Maria C. Tamargo[1]
[1]*City University of New York, New York, NY 10031, USA*
[2]*Waseda University, Shinjuku Tokyo 1698555, Japan*

Recently, α-MnTe has shown to exhibit altermagnetism, a novel class of magnetism that significantly broadens the frontiers for unconventional d-wave superconductivity and for innovative spintronic devices.[1,2] However, the growth of pure, single phase α-MnTe is challenging. Here, we report the growth optimization of MnTe using molecular beam epitaxy (MBE). High resolution X-ray diffraction 2θ-ω scans and pole figure analysis were done to characterize the layers.

Reducing the Te:Mn beam equivalent pressure (BEP) ratio between 180:1 and 5:1 and increasing growth temperatures between 350 and 400°C progressively yields mixed MnTe phases toward predominantly α-MnTe. Furthermore. The intensity of the γ-MnTe peaks in the 2θ-ω scans remains the same while intensity of the α-MnTe signal increases as a function of thickness, suggesting that the mixed phases are formed near the interface, implying that appropriate substrate-layer interfaces may lead to fully single phase materials.

Pole figures indicated that for samples grown on InP(111)B with high BEP ratio, two cubic phases (one for InP substrate and the other for γ-MnTe) could be distinguished, while a single hexagonal phase (α-MnTe) was identified when the layer was grown on InP(111)A. These findings provide key evidence to understand the details of the epitaxial relationship of the structure.

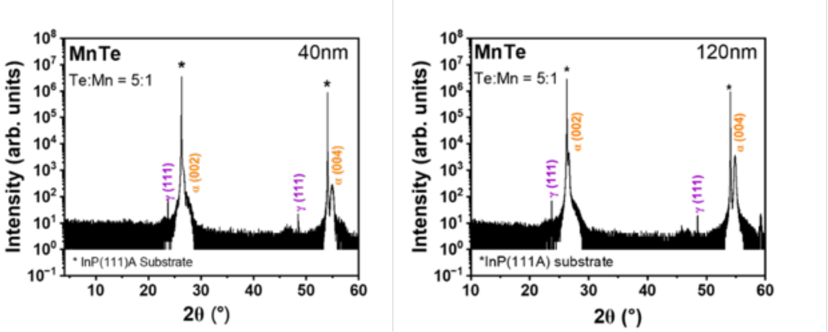

Figure 1: High resolution XRD scans for a 40nm (left) and 120nm (right) MnTe layers grown on InP(111)A.

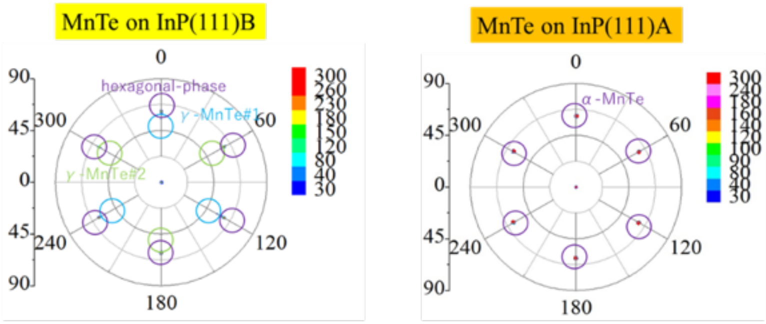

Figure 2: Pole figure images for predominantly γ-MnTe layer on InP(111)B (left) and a predominantly α-MnTe layer on InP(111)A (right). 2θ = 28.12°

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[1] Šmejkal, L., Sinova, J. & Jungwirth, T. Phys. Rev. X 12, 031042 (2022).

[2] Šmejkal, L., Sinova, J. & Jungwirth, T. Phys. Rev. X 12, 040501 (2022).

Advancing Quantum Device Fabrication Through Hybrid Semiconductor-Superconductor Nanowire Platforms

Bo Gao, Colin Wong, Ethan Van Metre
Department of Physics and Astronomy, CUNY Hunter College, NY, USA

Hybrid semiconductor nanowires represent a versatile platform for realizing quantum devices with engineered electronic and superconducting properties. This review highlights recent progress in the fabrication and study of hybrid nanowire systems for quantum technology applications. We summarize advances in nanowire growth, device integration using superconducting materials and low-temperature measurement that reveal key quantum behaviors. Factors that affect the device performance are also discussed. These findings provide important guidance for improving fabrication methods and materials design toward scalable nanowire-based quantum computing and sensing devices.

Highly Tunable Moiré Proximity System in Twisted Hexagonal Boron Nitrides Heterostructure

Kwanghee Han[1,2], Minhyun Cho[1,2], Abhishek Budarapu[2], Taehyung Kim[1], Seung Tae Kim[1], Suk Hyun Kim[1,3], Sang Hwa Park[4], Sang Mo Yang[4], Kenji Watanabe[5], Takashi Taniguchi[6], James Hone[7], Young Duck Kim[1,3,8]* and Vinod Menon[2]
[1] *Department of Physics, Kyung Hee University, Seoul, South Korea*
[2] *Department of Physics, The City College of New York, New York, NY, USA*
[3] *Department of Information Display, Kyung Hee University, Seoul, South Korea*
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[7] *Department of Mechanical Engineering, Columbia University, New York, NY, USA*
[8] *KHU-KIST Department of Converging Science and Technology department, Kyung Hee University, Seoul, South Korea*

Moiré superlattice in twisted van der Waals materials have emerged as a promising platform for emulating strongly correlated physics due to the tunability of many-body interactions via external stimuli such as gate, strain, and twist angle. In the twisted Hexagonal Boron Nitrides (hBN) heterostructure with a small-angle mismatch, nanoscale ferroelectric domains are formed due to their dipole polarization difference and minimize the interlayer configurations energy. Here, we report various types of moiré potentials such as the quasi 1-dimensional moiré structure and cumulative moiré superlattice. In addition, we introduce an approach for programming the moiré potential using femtosecond laser. Furthermore, we confirm the moiré proximity effect using Kelvin Probe Force Microscopy (KPFM) even after transferring monolayer $MoSe_2$. The twisted hBN platform could pave the way for remote engineering of moiré potentials on demand and use it for Hamiltonian simulators.

Computational Methods for Strong Light-Matter Simulations

Mohammad Hassan[1], Fabijan Pavosevic[2], Derek Wang[3], Cankut Tasci[1] and Johannes Flick[1]
[1]Department of Physics, City College of New York, NY, USA
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In polaritonic chemistry, strong light-matter interactions between molecular matter and cavity photons can alter chemical reactions. Recent experimental advances in this field has motivated the development of ab-initio methods for studying these systems. With the advent of the photon Many Body Dispersion (pMBD) method, it became possible to efficiently calculate cavity-modified van der Waals interactions for molecular systems. Currently, we are extending the capabilities of the pMBD method for studying extended materials. The recent advent of quantum algorithms for noisy quantum devices offers a new route toward simulating complex polaritonic systems. Building on previous work that uses the variational quantum eigensolver (VQE) to calculate polaritonic ground state energies[1,2], we extend these methods to compute the excited-state properties of polaritonic systems. Using the polaritonic unitary coupled cluster (PUCC) ansatz with the VQE to obtain the ground state, we use the quantum equation of motion (qEOM)[2] method to calculate excitation energies, transition dipole moments, and Rabi splittings. We explore the robustness of this approach across a diverse set of regimes for the bond length, cavity frequency, and coupling strength of the H_2 molecule in an optical cavity.

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[1] Hassan, M., Pavošević, F., Wang, D.S. & Flick, J. J Phys Chem Lett 15, 1373–1381 (2024).
[2] Ollitrault, P.J. et al. Phys. Rev. Res. 2, 043140 (2020).

Realizing the Half-Integer Quantized In-Plane Anomalous Hall Effect in Magnetic Weyl Semimetal $MnSb_2Te_4$

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Weyl semimetals are topological quantum materials hosting chiral Weyl fermions populating linear non-degenerate band crossings (nodes) in their bulk. This nontrivial band topology is expected to promote exotic transport behaviors, many yet to be uncovered. Here, we report the emergence of a half-integer quantized in-plane anomalous Hall effect (IPAHE) in the magnetic Weyl semimetal $MnSb_2Te_4$, where the in-plane Hall conductivity $\sigma_{yx}(H \parallel ab)$takes values of $\boldsymbol{n}\frac{e^2}{2h}$, with integer $\boldsymbol{n}$ programmable via a post-growth hydrogen intake-and-release technique.[1] This quantized IPAHE, with both the applied field H and magnetization M in the ab-plane, is distinct from the Lorentz force Hall effect or a conventional planar Hall effect –it is a possible realization of an elusive parity anomaly. We have previously shown that hydrogen incorporation modifies the Mn orbitals and tilts M toward the ab-plane, thereby transforming the Weyl phase[2] to reshape out-of-plane Berry curvature, and also inducing hysteresis loop in $\sigma_{yx}(H \parallel ab)$. Here we show how half-quantum steps in σ_{yx}^{IPAHE} emerge and evolve with tunable M-tilt. Angle-dependent transport measurements reveal an unusual $\sigma_{yx}(\varphi) \propto \cos(3\varphi) - \sin(\varphi)$dependence, consistent with mirror symmetry breaking while preserving the three-fold rotational (C_3) symmetry of the crystal, all leading to half-quantization and symmetry-engineered novel quantum states.

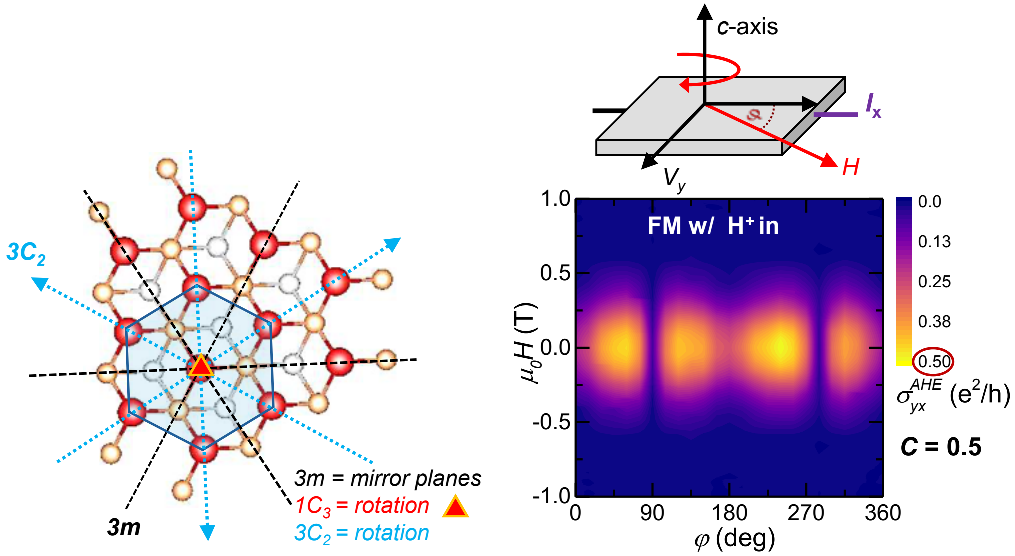

Figure: (*left*) Symmetry axes and planes in the vdW Weyl semimetal $MnSb_2Te_4$.
(*right*) Half-quantization of in-plane anomalous Hall conductivity $\boldsymbol{\sigma_{yx}^{AHE}}$ induced by hydrogen.

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[1] Deng, H. et al. Nat Commun 13, 2308 (2022).

[2] Tamanna, A.N. et al. Nat Commun 15, 9830 (2024).

Exciton-magnon dynamics in layered magnet

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CrSBr is an intriguing 2D semiconductor magnet that hosts multiple excitons coupled to its magnetic order. The exciton -exciton interactions in the material is mediated by magnons in the system unlike the usual exchange interactions or phase space filling mechanism.[1] High dielectric constant of the material provides strong optical confinement leading to the bulk polaritons formation.[2] Here, we report the signatures of magnons on excitons and polaritons in the transient absorption data. We have studied the dependence of the magnon oscillation frequency, decay rate and amplitude on incident photon density and magnetic. The dependence of the magnon dynamics and propagation with the magnon wave vector will also be discussed along with the temperature dependent variations in magnon density and frequency. The interactions between the electronic dynamics and magnetic ordering underpins it's potential for the opto-spintronic and quantum transduction technologies.

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[1] Datta, B. et al. Nature Materials. 24, 1027–1033 (2025)
[2] Dirnberger. F. et al. Nature, 620, 533-537(2023)

Magnetic Doping of Transition Metal Dichalcogenides for Spintronics Applications

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Tin diselenide ($SnSe_2$), a layered transition metal dichalcogenide (TMD), has emerged as a promising two-dimensional semiconductor for applications in optoelectronics and spintronics. In this work, cobalt (Co) was introduced as a dopant to modify the electronic and magnetic properties of $SnSe_2$. Monolayer $SnSe_2$ films were first synthesized via chemical vapor transport and then doped with Co via electron beam evaporation, followed by a thermal annealing.

The presence of Co and its chemical state were confirmed by X-ray photoelectron spectroscopy (XPS). Atomic force microscopy (AFM) revealed changes in surface morphology and formation of wide grain boundaries after doping, and Hall resistance measurements indicated magnetic interactions in the temperature range of 120–150 K. This preliminary study highlights how magnetic doping can enhance the properties of $SnSe_2$ monolayers, making them promising candidates for future spintronic and nanoelectronics technologies.

X-ray characterization techniques for analysis of thin films and nanomaterials.

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X-rays are a common and efficient way of analyzing the crystalline structure of 2D and 3D materials.[1] One of the key advantages of X-ray characterization techniques is that they are non-destructive, allowing researchers to probe material properties without damaging the sample. X-ray diffraction (XRD) is a widely used method for analyzing the crystal structure of thin films and nanomaterials. Depending on the configuration of the X-ray setup, it is possible to extract a variety of information ranging from composition, strain, degree of twinning, and lattice mismatch (via diffraction) to thickness, roughness, and density differences (via reflectivity).

The samples we analyzed in this poster include II-VI compound semiconductors, such as ZnCdSe, III-V compounds, such as GaAlAs, and topological insulators, such as Bi_2Se_3, all grown by molecular beam epitaxy. We examined the twinning defects in Bi_2Se_3 grown on two different substrates and observed that the substrate and the dopant used during growth directly affect the degree of twinning in the sample. We also analyzed three quantum dot (QD) samples and observed a trend in which higher zinc source temperatures during spacer layer growth led to a decrease in strain and lattice mismatch. The insights gained from X-ray characterization inform the crystal grower to better understand and optimize the structural properties of the materials.

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[1] Harrington, G.F. & Santiso, J. J Electroceram 47, 141–163 (2021).

Insights at the diamond-water interface; from charge injection studies to detection of water with nitrogen vacancy centers

Abraham Wolcott [1], Daniela Pagliero[1], Rohma Khan[1,2], Kapila Elkaduwe[2,3], Ankit Bharadwaj[4], Kang Xu[1], Gustavo E. López[2,7], Boya Radha[4,7], Nicolas Giovambattista[2,3], and Carlos A. Meriles[1,2]

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[4]*Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, USA.*
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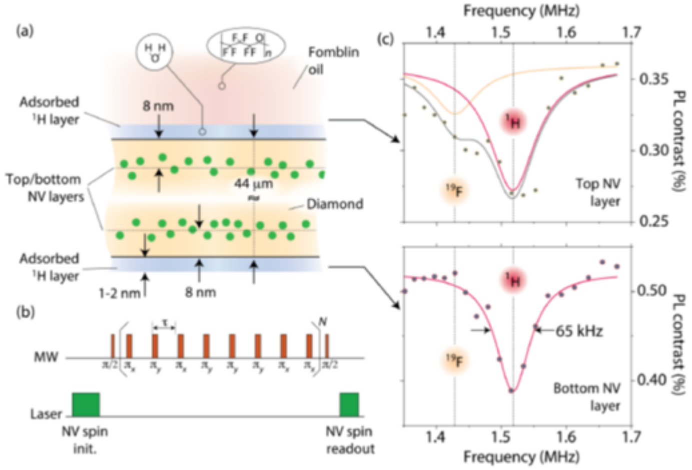
Diamond has excellent physical and optical properties that make it ideal for applications in photonics, biological sensing and chemical transformations. The study of diamond surfaces, its affect on color centers including the nitrogen vacancy (NV) center, are an open avenue of research with the diamond-water interface being especially relevant. Oxidized bulk diamond 100 surfaces are generally understood to be terminated with ethers and ketones and found to be hydrophilic, while leading to a stable negatively charged NV- state. The NV- charge state is a ground state triplet and allows for optical electron-spin readout and NMR-like detection protocols at room temperature. In an electrochemical cell with visible laser illumination we found that NV centers and P1 centers (substitutional nitrogen) generate sustained and photon energy dependent currents. The photocurrents are generated by excitation into the conduction band of diamond via the NV center and P1 centers emission from the diamond-water interface and collected at the electrodes. Additionally, the detection of water via 1H sensing occurs using the quantum sensing capabilities of the NV center. 2 scenarios are explored whereby monolayers of water are detected after oxidative etching of the diamond surface and another in a diamond h-BN nanostructure with a 5 nm gap space. Detection of "slow water" was discovered where the diffusion rates were drastically reduced and spin-spin correlation measurements were used to infer the dynamics of the diamond-water interface. The combination of high sensitivity and nanoscale dynamics provides direct information that is useful to researchers interested in solid-liquid interfaces, photocatalysis and biological systems.



Nanoscale Color Center Sensing of Adsorbed Water in Contact With Oil

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Understanding the behavior of confined water at liquid–solid interfaces is central to numerous physical, chemical, and biological processes, yet remains experimentally challenging. Here, shallow nitrogen-vacancy (NV) centers in diamond serve as sensors to investigate the nanoscale dynamics of interfacial water confined between the diamond surface and an overlying fluorinated oil droplet. With the help of nuclear magnetic resonance (NMR) protocols selectively sensitive to ^{1}H and ^{19}F, NVs are used to probe water and oil near the interface under ambient conditions. Comparing opposite sides of a doubly-implanted diamond membrane — one exposed to oil, the other not — a slow, multi-day process is uncovered in which the interfacial water layer is gradually depleted. This desorption appears to be driven by sustained interactions with the fluorinated oil and is supported by molecular dynamics simulations and surface-sensitive X-ray spectroscopies. These findings provide molecular-level insight into long-timescale hydration dynamics and underscore the power of NV-NMR for probing liquid–solid heterointerfaces with chemical specificity.

SUBPROJECT 2:

STUDENT ABSTRACTS

Cerenkov Luminescence Imaging Enhancement using a Multimodal Metamaterial Contrast Agent

Natalie Boykoff[1], Samhita Kattekola[2], Anuja Ogirala[3], Ilona Kretzschmar[2], Vinod Menon[2], Stephen O'Brien[2], Jan Grimm[3]
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[3]Memorial Sloan Kettering Cancer Center, New York, NY, USA

In recent clinical trials, Cerenkov Luminescence Imaging (CLI), the luminescent signal produced from a charged supra-relativistic subatomic particle in a dielectric medium, was assessed for multimodal imaging using FDA-approved radiotracers for Positron Emission Tomography (PET).[1,2] Albeit faster imaging speeds, lower service costs, higher resolution, and no incident light source, CLI is emitted as a relatively weak signal, which limits the multimodal imaging to superficial tumors. This poses a need for a CLI contrast agent that would enhance the signal without increasing the radioactive dose for patients.[1] While Cerenkov Radiation Energy Transfer (CRET) has been used to shift the most intense UV-emission into the red/NIR-light region to reduce background signal and tissue absorption[1], an artificial medium, known as hyperbolic metamaterials (HMMs), have been shown to lower the Cerenkov threshold.[3] Here, we report on a novel hyperbolic metamaterial (HMM) contrast agent for amplifying CLI for improved multimodal cancer diagnosis.

So far, these promising findings show that by using our novel contrast agent, we see broad enhancement of CL over wavelengths ranging from 550-750 nm, which overlaps specifically with the biological imaging window with reduced tissue scattering. This novel biocompatible contrast agent can be used to replace toxic dyes/lanthanides and has been shown to apply to other forms of optical enhancement.

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[1] Shaffer, T.M., Pratt, E.C. & Grimm, J. Nature Nanotech 12, 106–117 (2017).
[2] Pratt, E.C. et al. Nat Biomed Eng 6, 559–568 (2022).
[3] Liu, F. et al. Nature Photon 11, 289–292 (2017).

Colloidal Black Gold Janus Particles for Photocatalytic Hydrogen Production

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This report addresses the challenge of high-cost hydrogen production from photocatalysis by proposing a novel Janus particle system to enhance solar energy conversion efficiency. The system pairs a TiO2 base particle with a black gold Au-b cap material, a broadband light absorber. This design significantly increases solar spectrum absorption from 5% to 48% by leveraging the plasmonic properties and engineered nanostructures of the Au-b film. The Au-b cap not only acts as an efficient absorber but also generates heat which is transferred to the core and surrounding fluid, potentially increasing the photocatalytic hydrogen production rate. This approach decouples hydrogen generation from electricity cost and allows for integration with existing thermochemical energy storage using the generated heat. The report discusses the synthesis and properties of Au-b, photocatalytic water splitting, surface plasmons, radiative heat transfer, and the effect of temperature on catalytic rates, assessing the viability of this innovative system for scalable green hydrogen production.

The Influence of pH Changes Via Carbon Dioxide Sparging on Complex Coacervates

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Complex coacervation is a form of liquid-liquid phase separation that can be formed via oppositely charge polyelectrolytes (PEs). They have gained interest for their ability to compartmentalize molecules, which may be controlled via stimuli. The ability of coacervates to reversibly respond to stimuli allows for the engineering of materials that are responsive and controllable. Changes in pH act as a stimulus by protonating or deprotonating weak PEs, thus strengthening or weakening the electrostatic interactions that drive coacervation. We propose a system using cycles of CO_2 and inert gas sparging to reversibly alter pH. This work focuses on the forward reaction of the coacervate system with CO_2. Complex coacervates of the polycation, poly(L-lysine hydrochloride), (Plys), and polyanion poly(D,L-glutamic acid sodium salt), (PGlu), are created. Next, the system is adjusted to an alkaline pH, allowing NaOH to deprotonate the ammonium group on PLys. This newly formed amine reversibly reacts with CO_2 to form bicarbonate and lower the pH. Additionally, NaOH reversibly reacts with CO_2, lowering the pH and producing bicarbonate and carbonic acid. We explore how the reduction in pH from the reaction changes size and charge of coacervates.

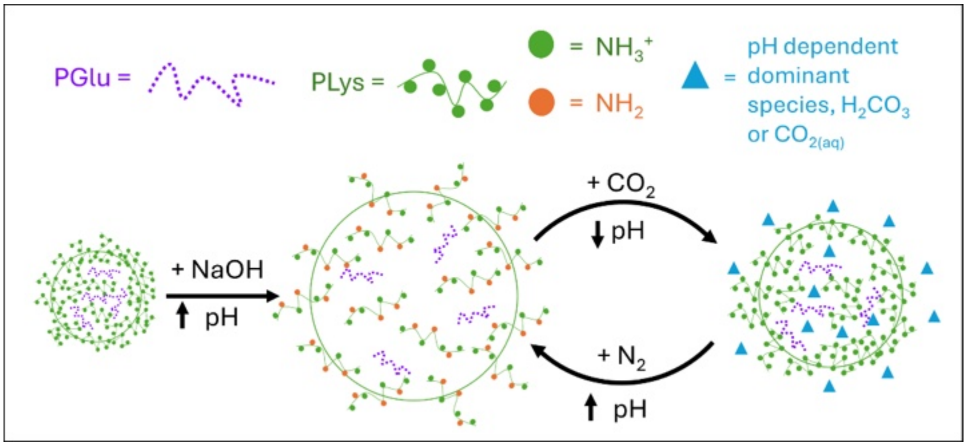

Fig. 1: Reaction of coacervates with sodium hydroxide and subsequent sparging of CO_2

Enhanced Solubility and Stability of Riboflavin (Vitamin VB2) Using Tryptophan-Containing Tripeptide Soluble Dispersions

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Many essential vitamins, including riboflavin (B_2), retinol (A), cholecalciferol (D_3), and ascorbic acid (C), have poor aqueous solubility and are sensitive to light and oxidation, limiting their stability and formulation potential. Tripeptides, short chains of three amino acids, self-assemble via hydrophobic effects, hydrogen bonding, and π–π stacking, making them useful for functional materials. We studied two sequence-isomeric tripeptides, WKY and WYK, selected for their distinct aggregation behaviors. NMR shows WKY assembles through π–π stacking among tryptophan, forming a hydrophobic, electron-rich core, while WYK forms a hydrogen-bonded polar network via lysine, yielding a more electron-poor environment. WKY favors hydrophobic molecules, whereas WYK better stabilizes polar ones. At high concentrations, both form dynamic soluble aggregates and undergo liquid–liquid phase separation upon drying, rigidifying into solid microstructures. These assemblies were used to encapsulate and protect VB_2. Combining molecular dynamics, spectroscopy, LC–MS, circular dichroism, and NMR, we found that the peptides form hydrophobic cages: aromatic residues drive stacking and partitioning, while lysine enhances solubility. VB_2 coated with either peptide retained full stability under UV and visible light in the dry state and showed a ten-fold stability increase in solution. This simple platform offers broad potential for stabilizing light-sensitive molecules in pharmaceutical and nutraceutical applications.

Figure 1: Tripeptide Structure

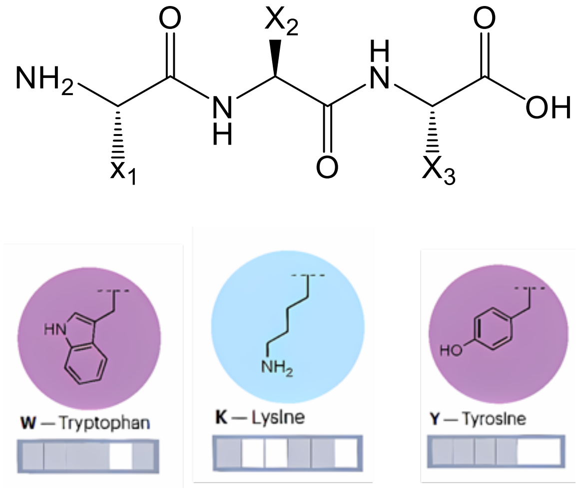
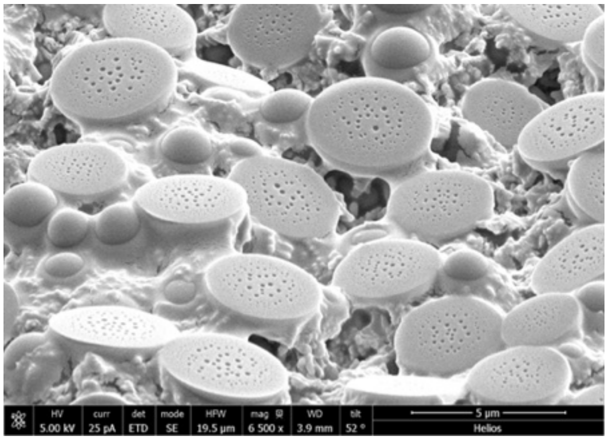


Figure 2: SEM image showing a mixture of porous spheres and half-dome particles at the interface and also showing surface pores.



Tuning optical properties using colloidal hyperbolic metamaterials: design and characterization

Samhita Kattekola, Alexander Couzis, and Ilona Kretzschmar
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Metamaterials made of alternating layers of metals and dielectrics, known as hyperbolic metamaterials, have been shown to enhance emissions, which is of interest in biomedical imaging and detection. The utilization of such materials has been limited due to difficulty in characterization and scale up. In this research, we propose a simplified characterization strategy using ellipsometry to identify unique design parameters for hyperbolic metamaterials. Additionally, we propose creating a dispersible metamaterial using Janus particles. Here, Janus particles with hyperbolic metamaterial cap are fabricated by coating one half of 4 mm diameter silica spheres with alternating layers of metal and dielectric. Analysis using Focused Ion Beam Scanning Electron Microscopy (FIB-SEM), reveals how optical properties of a system can be tuned using hyperbolic metamaterial Janus particles.

Inspired by Nature: Amino Acids for Robust Hierarchical Supramolecular Assembly

Seda Kelestemur[1,3], Ahamed Jubair[2,4], Joshua D. Pagan[1], Vladimir Kartazaev[4], Genesis Fermin[1], Nazifa Meher[1], Brandon Hu[1], Miriam Ramirez Ramos[1], Aeneas Merchant[1], Lillian Engber[1], Riston Vesotsky[1], Omar Green[1], Elisabetta Collini[6], Stephen O'Brien[1,2], Swapan K. Gayen[4,5], and Dorthe M. Eisele[1,2]
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[6]*Department of Chemical Sciences, University of Padova, Padova, Italy.*

Hierarchical supramolecular self-assembly into ordered structures is one of nature's most successful design principles for generating robust functional systems capable of producing ordered materials across multiple length scales. Translating nature's successful design principle to broad applications, ranging from renewable energy and information technology to biomedical applications—requires (1) control over the hierarchical self-assembly process and (2) robust supramolecular structures. While the main forces that drive, supramolecular self-assembling process are known—for example, hydrophobicity—understanding the intimate correlation between the specific self-assembling conditions and the resulting structural properties, to further studies critical in effectively producing supramolecular structures.

Using a well-characterized artificial model system, supramolecular nanotubes (NTs) self-assembled in aqueous solution from amphiphilic cyanine dye molecules, we show how nature's protein building blocks, the amino acids, can control the hierarchical self-assembly process to provide structurally and optoelectronically robust supramolecular assemblies. Steady-state absorption and fluorescence spectroscopy, cryogenic microscopy, time-resolved fluorescence spectroscopy, and atomic force microcopy revealed that the supramolecular NTs stabilized via arginine interactions remain robust under extreme environmental conditions such as heat stress and upon drying on a solid substrate. Our bioinspired approach elegantly employs arginine to control and stabilize solution-based hierarchical supramolecular assemblies, illustrating a promising basis for efficient and stable next generation organic devices.

Using Differential Evolution to Predict Magnetic Janus and Multi-Patch Particle Assembly

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Magnetic Janus particles assemble into a variety of complex structures that can lead to magnetorheological (MR) fluids with interesting macroscopic properties. The structures that form must be characterized to understand the connection between the Janus particle design and macroscopic characteristics. However, the large design space that is possible for Janus and patchy particles –different particle and cap materials and geometries, applied external fields, mixtures of particles, etc. – makes it difficult to explore and therefore design MR fluids with specific properties. A proof-of-concept simulation method based on differential evolution (DE) has been used to explore the directed and nondirected self-assembly of laterally- and radially-shifted magnetic Janus particles.[1] Initial two-dimensional DE simulations without out-of-plane rotation quantitatively reproduced published particle orientations and cluster morphologies. However, observations based on cluster reorientation and multi-particle rearrangement were less well reproduced. Here, the DE simulation is expanded to include multi-patch particles and their impact on cluster structure and aggregation, which are then compared to experimental results.

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[1] McPherson, E.A., Kroenlein, K. & Kretzschmar, I. J. Chem. Phys. 163, 024906 (2025).

Mechanistic Insight into the Reduction of Surface Tension from the Nanostructure of Chemically Modified Janus Particles

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Mixtures of particles and surfactants act synergistically to stabilize fluid interfaces relevant to manufacturing, formulations, and waste remediation. However, some applications have challenges in adopting these mixtures, such as the environmental fate of molecular surfactants. We present a Janus silica microparticle capable of harnessing the advantages of both particles and surfactants when chemically modifying a region on the surface of microparticles with gold nanoparticles. Here, we characterize the particles throughout the fabrication process. We also report the results of the Janus particles reducing the surface tension of the air-water interface. It is hypothesized that the nanostructure on the surface of each Janus particle is the source of the surface tension reduction. Therefore, we provide a systematic study into understanding the underlying mechanism behind the surface tension reduction. By understanding the mechanism, the findings will be utilized to develop new Janus particles, capable of impacting surface tension and being retrievable for particle reuse or disposal, or for purposefully destabilizing an emulsion.

Histidine-Containing Tri-Peptide Hydrogels as Alternative Proton Transfer Materials for Fuel Cell Applications

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[2]*Department of Chemistry at CUNY Hunter College, New York, NY, USA*

Proton exchange membrane fuel cells (PEMFCs) utilize the Grotthuss shuttling mechanism to do proton transfer in relatively low temperatures and highly humidified environments. The most common proton exchange membrane (PEM) used in PEMFCs, known as Nafion, does proton transfer through water, but is toxic to the environment. At high temperatures, water evaporates from the membrane, which inhibits proton transfer and limits fuel cell operation. Histidine (His) containing tripeptides can participate in proton transfer via Grotthuss shuttling through the imidazole group on the His. Long chain peptides containing His and alanine have been shown computationally to coil at the right angle to align the imidazole subunits to form hydrogen bonds. Protons can translocate along these bonds. Unfortunately, synthesis of long chain peptides with the correct angles is difficult. As an alternative, we focus on the synthesis of His-containing tripeptides that are short and can be self-assembled into hydrogels. In this presentation, we discuss our results showing that the Fmoc-HHH hydrogel forms fibers that are capable of proton transfer and that this increases with increased humidity. We will highlight how the incorporation of other amino acids (aspartic acid, glutamic acid, phenylalanine and lysine) in positions 1, 2 and 3 affect the secondary structure of the hydrogel and thus its proton transfer capabilities.

Investigating Cycling and Degradation Pathways of Rechargeable Alkaline Calcium Zincate ($CaZn_2(OH)_6{\cdot}2H_2O$) Anodes

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[4]Department of Chemical Engineering, The City College of New York, New York, NY, USA
[5]Department of Photovoltaics and Materials Technology, Sandia National Laboratories, Albuquerque, NM, USA
[6]Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM, USA

Modern society is strongly dependent on a reliable and resilient electrical grid, with increasing energy demand and aging infrastructure. Battery energy storage systems (BESS) are a key solution necessary to enhance grid resilience, enabling peak demand shaving, and ensuring backup power for critical infrastructure. However, most commercial BESS relies on lithium-ion chemistries with flammable electrolytes, making large installations not safe or suitable for indoor use. Zinc (Zn) anodes are an attractive alternative due to their high theoretical capacity, relative abundance, non-toxic, easily recycled, and non-flammable nature. Zn anodes have been produced industrially for use in primary, single-discharge, alkaline cells, (e.g., in AA, AAA, C and D configurations) for a variety of applications but making such batteries rechargeable has proved difficult. Zn in alkaline electrolytes have poor reversibility at high Zn utilization due to passivation, shape change/redistribution, dendrite formation, hydrogen evolution, and the crossover of zincate ion ($Zn(OH)_4^{2-}$) into the cathode.

Despite recent advances in improving Zn utilization in Zn-MnO_2 and Ni-Zn batteries for commercial applications, utilization of Zn in affordable MnO_2 remains low (~10 - 20%) in favor of high cycle life (1000^+). Zinc oxide (ZnO) anodes with additives such as calcium hydroxide ($Ca(OH)_2$) have shown improvements in cyclability compared to metallic Zn anodes due to the in-situ formation of lower solubility calcium zincate (CaZn, ($CaZn_2(OH)_6{\cdot}2H_2O$). Ex-situ synthesized CaZn[2] has been cycled vs nickel under alkaline conditions vs sintered nickel[3] showing great improvement in cyclability but to be economically feasible, it must be paired with MnO_2. Due to a charge in balance between the “discharged” CaZn and “charged” MnO_2, practical anode recipes will include a higher percentage of charged Zn to prevent the requirement of additional formation steps.

To try and improve CaZn cycle life at high Zn utilization, a detailed understanding of the cycling and failure mechanisms of pure CaZn anodes is required[1]. We conducted a careful investigation of CaZn anodes vs sintered nickel at high 50% Zn utilization, both at “charged” and “discharged” states, over cycle life as the cells begin to capacity fade. What we uncover is that even though CaZn shows great cycling performance at high Zn utilizations, it does not immobilize the Zn to the same extent previously theorized, and Zn remains mobile during electrochemical cycling. Over time, due to the poor conductivity of CaZn, the Zn and Ca ions segregate which exacerbates the reformation of CaZn. Further studies uncover the effect of c-rate on CaZn battery cycling and how at longer (C/5:C/5 and C/10:C/100) durational c-rates, zincate ions can escape the calcium matrix and plate Zn outside of the electrode, lowering the batteries coulombic and energy efficiency. We can achieve 400+ cycles with 70% capacity retention of pure CaZn anodes at high 50% Zn utilization with trace amounts of Bi_2O_3. Additionally other factors that affect the cycling performance of CaZn will be discussed and will lead to future improvements in CaZn electrode design.

SUBPROJECT 3:

STUDENT ABSTRACTS

Growth, Characterization, and Optimization of Epitaxially Grown II-VI Type II-Quantum Dots for Application in an Intermediate Band Solar Cell Device

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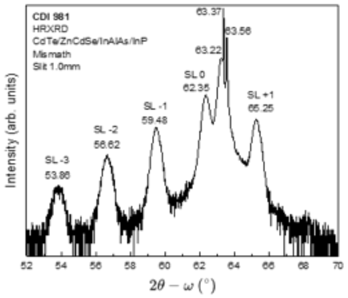
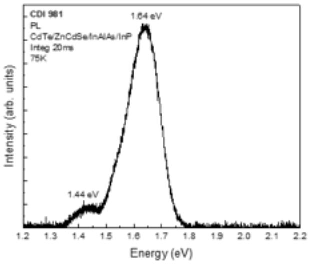
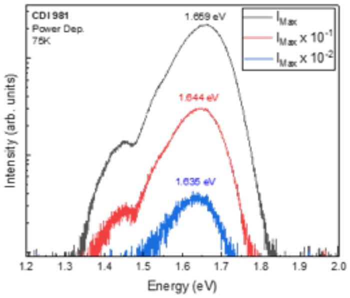
Quantum Dots (QDs) have been utilized for a variety of applications, such as displays, imaging, etc., due to their tunable emission/absorption spectra. We explore the growth and characterization of CdTe-based type-II QDs grown by molecular beam epitaxy (MBE) for application in an intermediate band solar cell (IBSC) device. CdTe QDs embedded in a ZnCdSe matrix are promising candidates due to their band gap energies and large valence band offset (VBO) which can be tuned with strain[1]. These QDs are composed of alternating ultra-thin CdTe layers (sub-monolayers) embedded in ZnCdSe spacer layers, forming a superlattice structure of 50 periods. Previous superlattice structures were grown on InP substrates using an InGaAs III-V buffer layer, which interfered with the absorption of photons at the intermediate band. To avoid this unwanted absorption, the buffer layer was replaced with InAlAs, a III-V material of similar lattice constant and a higher band gap. Growth parameters have been optimized to meet material conditions proposed for a highly efficient IBSC[2]. Samples are analyzed by high resolution X-ray diffraction (XRD) and power-dependent photoluminescent (PL) spectroscopy to determine crystal quality, lattice mismatch, composition, absorption, and type-II QD behavior.







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[1] Deligiannakis, V., Ranepura, G., Kuskovsky, I.L. & Tamargo, M.C. J. Appl. Phys. 126, 235302 (2019).
[2] Luque, A. & Martí, A. Phys. Rev. Lett. 78, 5014–5017 (1997).

PECVD Stacking of Metasurfaces

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Compact, multi-layered metalenses offer a promising path toward miniaturized optical systems with high focusing performance. This project focuses on fabricating stacked metalens structures separated by silicon dioxide (SiO_2) spacers. The primary objective is to determine the optimal SiO_2 spacer thickness that ensures smooth surface morphology and reliable integration between layers. Thin spacers can lead to surface irregularities that degrade optical quality, while thicker layers may increase device size and complexity. To address this, we systematically deposit SiO_2 layers of varying thicknesses and characterize their surface profiles and optical performance. The goal is to identify the minimum thickness required to maintain surface uniformity without compromising lens functionality. The findings will contribute to improving the fabrication reliability of multi-layered metalenses for compact photonic applications.

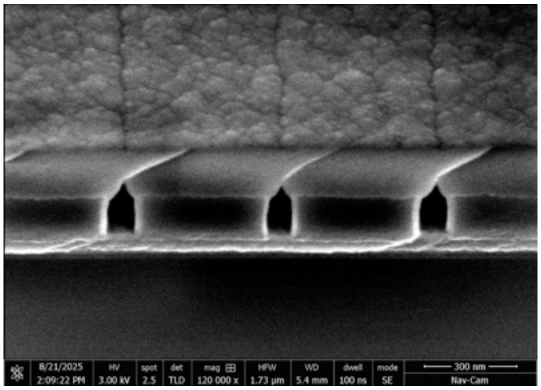

Fig 1. SEM image of Sid186b sample showing a 250nm SiO_2 deposition with 100nm feature width and 400nm

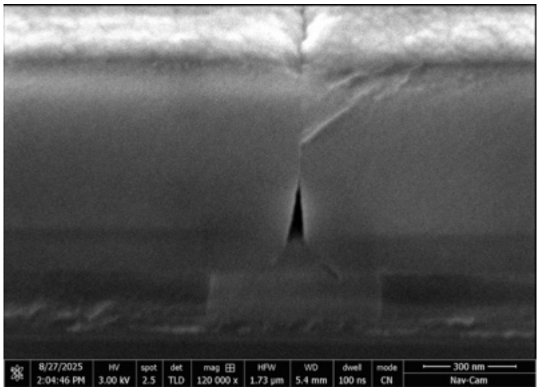

Fig 2. SEM image of Sid186d sample showing a 1000nm SiO_2 deposition with 500nm feature width and2000nm

Erbium implanted 2D materials with Room-Temperature Photon Emission at Telecom Wavelengths

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Optically addressable spin impurities in crystals along with device engineering provide an attractive route to realizing quantum technologies in the solid state but reconciling disparate emitter and host material constraints for a given target application is often challenging. Rare-earth ions in two-dimensional (2D) materials could mitigate this problem given the atomic-like transitions of the emitters and the versatile nature of van der Waals systems. Here we combine ion implantation, confocal microscopy, and ab initio calculations to examine the photon emission of Er-doped WS_2 flakes. Optical spectroscopy reveals narrow, long-lived photoluminescence lines in the telecom band, which we activate after low-temperature thermal annealing. Spectroscopic and polarization-selective measurements show a uniform response across the ensemble, while the fluorescence brightness remains mostly unchanged with temperature, suggesting nonradiative relaxation channels are inefficient. Our results create opportunities for novel solid-state devices coupling 2D-hosted, telecom-band emitters to photonic heterostructures separately optimized for photon manipulation[1,2,3]

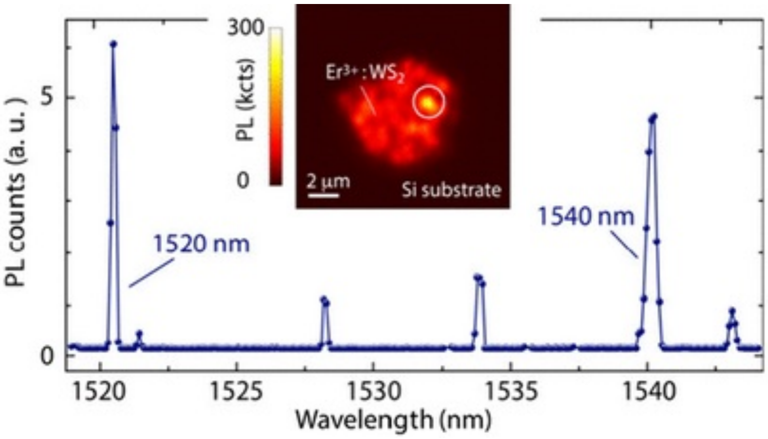

Fig. 1: Telecom emission of an erbium implanted WS2 flake at room temperature and corresponding spectroscopy in the telecom band. [1]

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Exciton dynamics of layered materials in the ultra-low excitation density regime

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The confinement properties of layered materials make them attractive candidates for quantum technologies. These materials are often subjected to relatively high excitation fluences to induce nonlinear processes, such as harmonic generation and two-photon absorption. However, a comprehensive time-resolved study of layered materials perturbed with ultra-low excitation densities remains unexplored. Here we present phenomena after optically exciting these materials with < 1 uJ/cm2. Highly sensitive, broadband, ultrafast spectroscopy and steady-state photoluminescence spectroscopy are employed to probe the fluence dependence of quasi-particle dynamics. Intrinsic optical properties are observable in this regime due to the reduction of many-body effects. We explore low-fluence photophysics for the enhanced design and functionality of optoelectronic devices.

Ultrafast Optical Processes in II-VI Semiconductor ZnCdSe/ZnCdMgSe Heterostructures with Time-resolved Photoluminescence and Transient Absorption Spectroscopy

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Epitaxial II–VI semiconductor $Zn_xCd_{1-x}Se$/ $Zn_xCd_yMg_{1-x-y}Se$ heterostructures grown lattice matched to InP substrates are currently being explored as active material for semiconductor disk lasers (SDLs) operational in the 480-650 nm spectral range.[1] Here, we present the growth, structural properties, photoluminescence (PL), stimulated emission, and carrier dynamics in two ZnCdSe/ZnCdMgSe multiple quantum well (MQW) samples designed for peak PL emission around 540 nm. The room-temperature PL of the samples peak around 556 nm. Excitation intensity dependent time-resolved PL measurements provide a PL lifetime of 1355 ±13ps, and a stimulated emission lifetime of ~ 82 ±2 ps at excitation intensities above 5 GW/cm.[2] Femtosecond time-resolved transient absorption spectroscopy[2] measurements reveal time and excitation intensity dependent amplification, ultrafast photo-pumped carrier dynamics, high material gain at the band edge, and transient phenomenon such as optical Stark effect. The samples exhibit substantial edge-emitting laser emission centered on 568 nm.

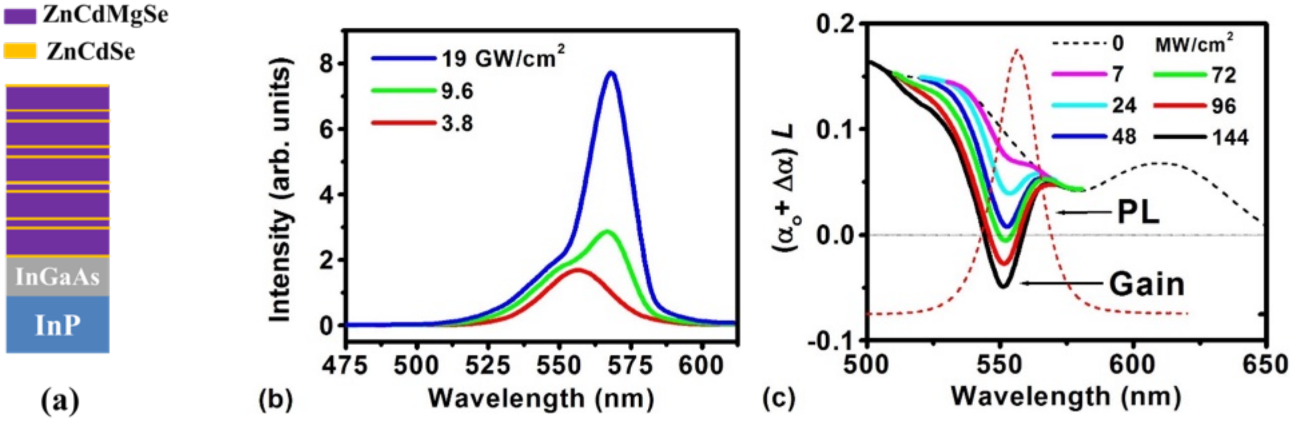

Fig. 1: (a) Schematics of a ZnCdSe/ZnCdMgSe MQW sample, ((b) excitation intensity dependent time resolved PL spectra, (c) transient absorption spectra at different excitation intensities at an optimal pump-probe delay of ~100 ps.

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[1] Jesus, J.D. et al. Phys. Status Solidi A 212, 382–389 (2015).
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Advanced Nanofabrication for Room-Temperature Polariton Condensate Lattices and Energy Transfer

Rishabh Kaurav[1,2], Ravindra Kumar Yadav[1,5],Sitakanta Satapathy[1], Prathmesh Deshmukh[1,2],Biswajit Datta[1], Addhyaya Sharma[1], Andrew Olsson[4], Amar H. Flood[4], Vinod M. Menon[1,2]

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This study investigates exciton–polariton systems with a focus on nanofabrication of polariton lattices and excitonic energy transfer in organic materials. We examine a host–guest system of Rhodamine 3B (R3B) and Nile Blue (NB) dyes embedded in small-molecule ionic isolation lattices (SMILES)[1], which enhances photoluminescence and mitigates aggregationinduced quenching, leading to efficient R3B-to-NB energy transfer. The influence of the donor's condensate phase[2] on transfer dynamics is studied using steady-state, time-resolved, and momentum-resolved spectroscopy.

We also fabricate polariton condensate lattices via a top-down Focused Ion Beam (FIB) approach, enabling precise control of periodic, quasi-periodic, and disordered geometries in planar microcavities with SMILES dyes.[3] Momentum-resolved measurements reveal band structures and condensation behavior. Together, these results integrate enhanced excitonic energy transfer with scalable FIB-based lattice fabrication, advancing the design and control of exciton–polariton platforms.

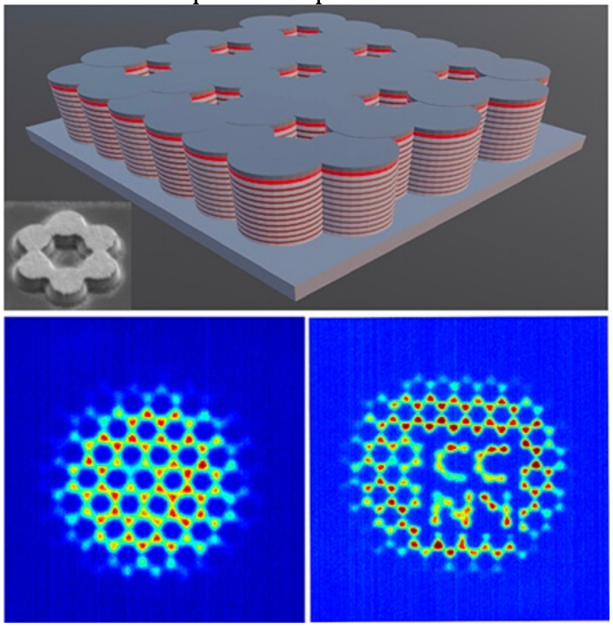

Figure 1. Schematic for patterned honeycomb organic exciton-polariton lattice (top). Room temperature polariton condensate lattice (bottom).

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[1] Benson, Christopher R., et al. Chem 6.8 1978-1997 (2020):
[2] Deshmukh, Prathmesh, et al. ACS Photonics 11.2348-355 (2024)
[3] Yadav, Ravindra Kumar, et al Nano Letters 24.16 4945-4950 (2024)

Nuclear Quantum Effects on Glassy water and Hexagonal Ice under pressure: Vitrification and Pressure-Induced Transformations

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Water's complex phase behavior, particularly the role of nuclear quantum effects (NQE) on its amorphous and crystalline phases, remains poorly understood with its unique properties playing a fundamental role in numerous scientific and engineering applications[1,2,3]. This study investigates the impact of NQE on the vitrification of H_2O and D_2O under isobaric cooling, as well as pressure-induced transformations between low-density amorphous ice (LDA), high-density amorphous ice (HDA), and hexagonal ice (Ih). These insights are essential for understanding water's anomalous properties and their implications for fields such as cryopreservation, material science, and high-pressure physics.[4] Classical molecular dynamics (MD) and path-integral MD (PIMD) simulations were performed on H_2O and D_2O over a wide range of pressures and temperatures to explore their structural and thermodynamic properties.

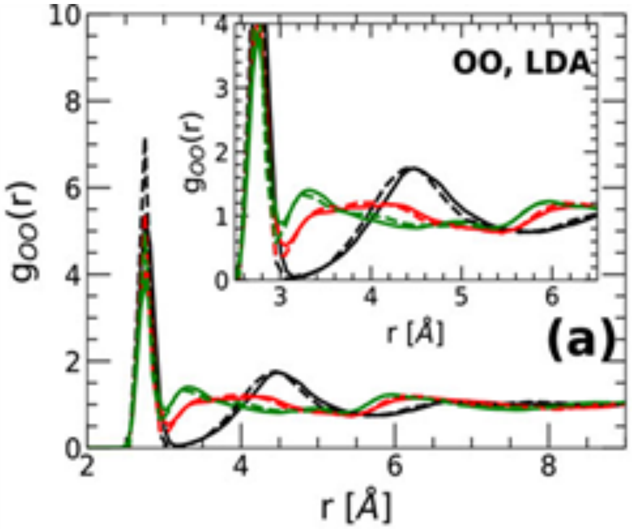

Fig. 1: The oxygen–oxygen (OO), radial distribution functions (RDFs) for LDA at P = 0.1 (BLACK), IA in red at 400 MPa , and HDA in green at 1000 MPa and T = 80 K.

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[1] P. G. Debenedetti, Metastable liquids: concepts and principles, Princeton University Press,(1996).

[2] F. Franks, Royal Society of Chemistry (2007)

[3] L. G. M. Pettersson et al, Chemical Reviews 116 7459-7462 (2016)

[4] Rosu-Finsen, A et al, Science 379, 474 (2023)

Slow Water in Engineered Nanochannels Revealed by Color-Center-Enabled Sensing

Rohma Khan

Daniela Pagliero[1], Rohma Khan[1],Kapila Ekladuwe[2,3], Ankit Bhardwaj[4], Kang Xu[1], Gustavo E Lopéz[2,6], Boya Radha[4,7], Nicolas Giovambattista[2,3], Carlos A Meriles[1,2]

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Characterization of nanoscale confinement of liquids via quantum sensing can overcome the sensitivity, spatial, and temporal limitations of other measurement techniques, allowing deeper understanding of dynamics central to areas spanning geophysics, tribology, catalysis, polymer science, and biology. Using shallow nitrogen vacancy (NV) centers as our quantum sensors we probe the molecular dynamics of water molecules confined within engineered ~5-nm-tall channels formed by a hexagonal boron nitride (hBN) structure on the diamond surface. Our resultant NV-enabled nuclear magnetic resonance spectra of confined water protons reveal a reduced H2O self-diffusivity, orders of magnitude lower than that in bulk water. Correlation measurements show us long lasting nuclear spin coherences, indicative of molecular dynamics intermediate between bulk water and ice. Molecular dynamics modeling indicate cluster formations may arise from accumulation of surface charge and carrier injection into the fluid under laser illumination.

Real-Time Spatial Frequency Filtering with GaAs/AlAs Multilayers Grown by MBE

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We demonstrate a GaAs/AlAs multilayer structure, grown by molecular beam epitaxy (MBE), and optimized for multi-wavelength optical edge detection. This 20-layer aperiodic stack is engineered to manipulate the spatial frequency content of incident light—enhancing high-frequency edges while suppressing low-frequency background variations. Precise control over layer thickness and interface quality is achieved through MBE growth, ensuring close match to the designed profile. Simulated and experimental angle-resolved reflectance measurements reveal a strong reflectance transition dependent on numerical aperture (NA), enabling high-contrast edge enhancement. The multilayer design offers a real-time, energy-efficient solution for optical image processing, scalable for advanced imaging and computational optics. These results highlight the potential of MBE-grown multilayers as compact, hardware-based alternatives to traditional digital and metasurface-based edge detection methods.

Probing Polymorph and Chirality Dependent Singlet Fission Dynamics in Dipyrrolonaphthyridinedione (DPND) Crystal Via Transient Absorption Microscopy

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Dipyrrolonaphthyridinedione (DPND) is a promising organic semiconductor capable of singlet fission (SF) which holds the potential to increase the power conversion efficiency of solar cells by splitting high-energy singlet excitons into two triplets. This study investigates how polymorphism and chirality in DPND crystals influences excited state dynamics, particularly triplet formation. Using Transient Absorption spectroscopy, we compare two distinct crystalline polymorphs; including novel twisted (chiral) phases to spatially and spectrally resolve SF behavior at the microscale. Our goal is to identify which polymorph exhibits faster or more efficient triplet formation, and to determine how molecular packing impacts exciton coupling and spin conversion. We are investigating the role of chirality on carrier dynamics, focusing on spin conversion, exciton diffusion, and polaron transport. We further aim to elucidate emergent features imparted by the chiral nature of the films, such as changes in intermolecular electronic coupling and chiral-induced spin selectivity (CISS). These insights support the rational design of next generation organic semiconductors with tailored photophysics for high performance optoelectronic devices.