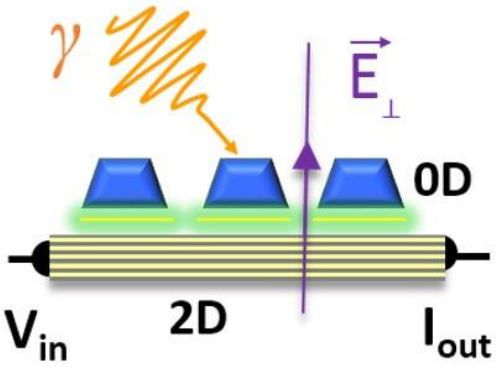
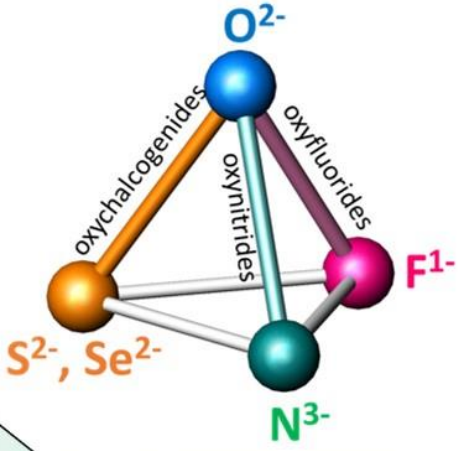
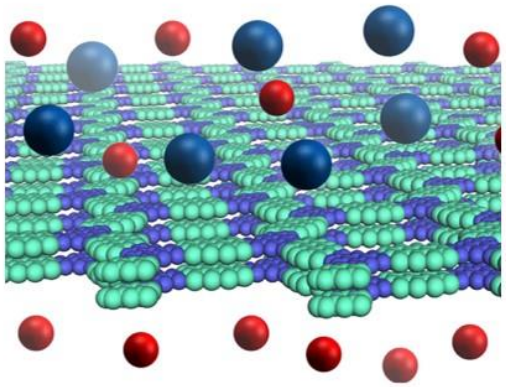
NU-MRSEC Research Overview



IRG-1

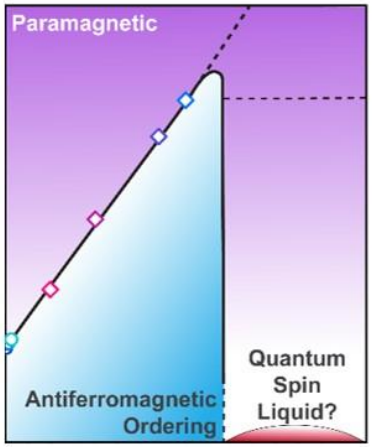
IRG-2





Super-Seed

Seed Projects



Professor Mark C. Hersam
Northwestern University MRSEC
https://mrsec.northwestern.edu/

IRG-1: Reconfigurable Responses in Mixed Dimensional Heterojunctions

Lincoln Lauhon*
MatSci, Appl Phys
Low-D Materials
Imaging

Emily Weiss*
Chem, MatSci, Appl Phys
Quantum Dots
Optical Spectroscopy

Tobin Marks
Chem, MatSci, Appl Phys
Design /Synthesis of Organic Electronic Materials

Mark Hersam
MatSci, Chem, Appl Phys
Elec and Comp. Eng
Low-D Materials/Devices

Nate Stern
Phys, Appl Phys
Magneto-optics,
Photonics

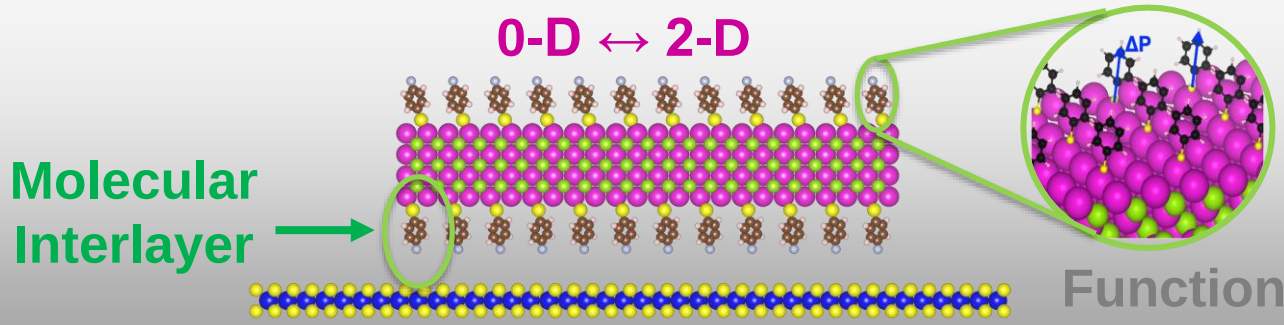
Oluwaseyi Balogun
Mech Eng, Civ Eng
Thermal Transport
Local probes

Pierre Darancet
NU-ANL Inst Sci & Eng
Electronic Structure,
Transport

Maria Chan
NU-ANL Inst. Sci & Eng
Data-Driven Approaches,
Defects, Therm. Transport

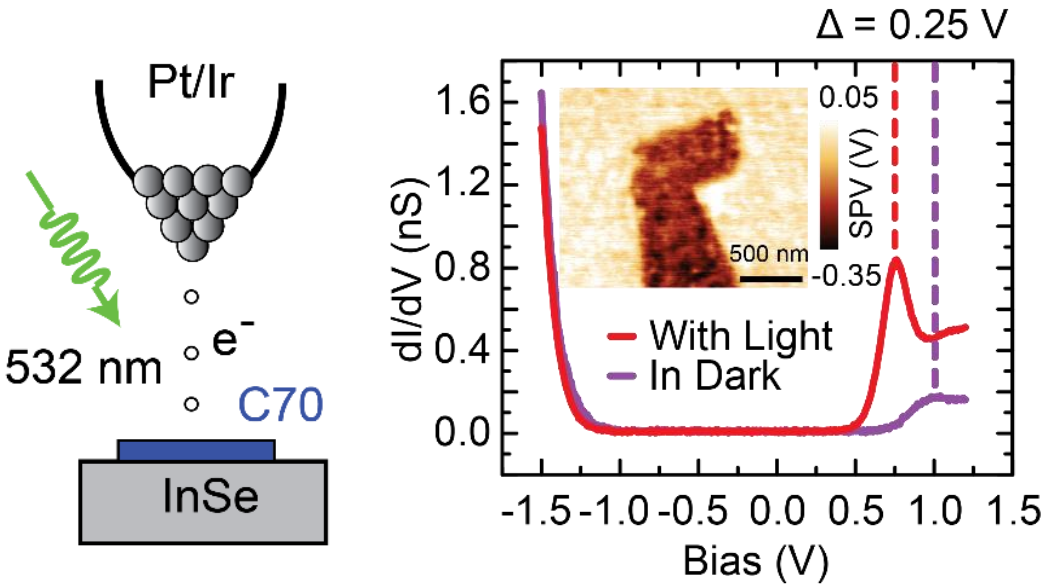
IRG-1 Grand Challenge

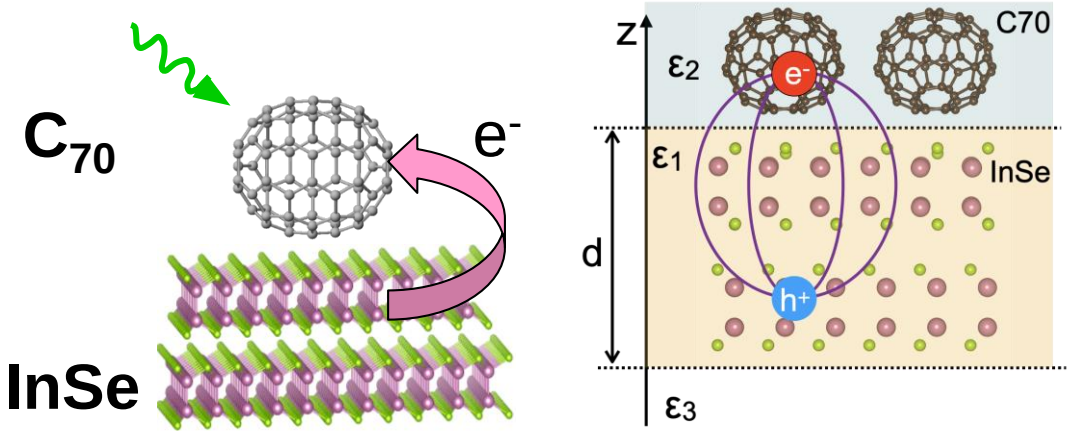
Realize tunable responses to fields and photons in mixed-dimensional heterojunctions



- Inhomogeneous screening of low-dimensional components enables geometric control of the response to external electric fields.
- Hybrid mixed-dimensional ground and excited states enable chemical and electrostatic tuning of electronic and optical properties.
- Dynamics on multiple time scales, from ultrafast electron transfer to long-lived excitons, lead to new properties in assemblies.

Inhomogeneous Screening Influences Charge Transfer State Formation in 0D/2D Junction

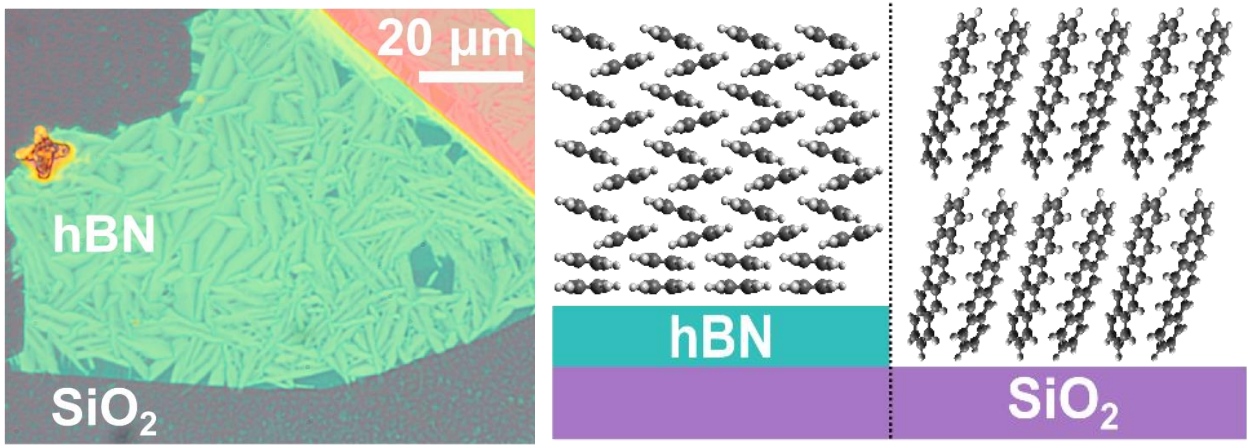




- C_{70}/InSe is a previously unstudied 0D/2D Type-II heterojunction
- Laser-excited scanning tunneling spectroscopy reveals a distinct peak that cannot be explained with a simple band alignment model
- Computational modeling of the inhomogeneous screening across the mixed-dimensional heterointerface is necessary to describe the observed charge transfer state

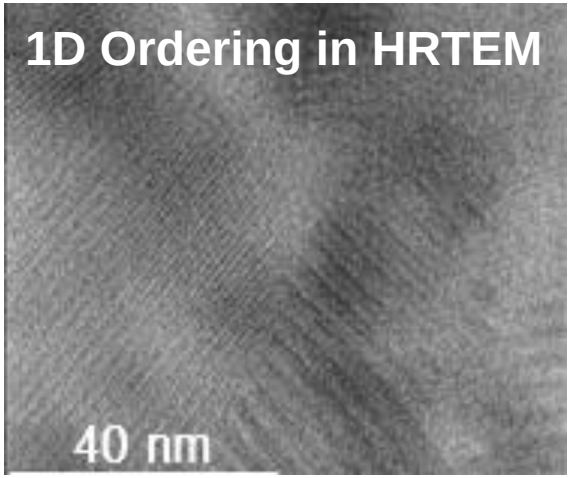
Substrate Interactions Control Assembly of Mixed-Dimensional Heterostructures

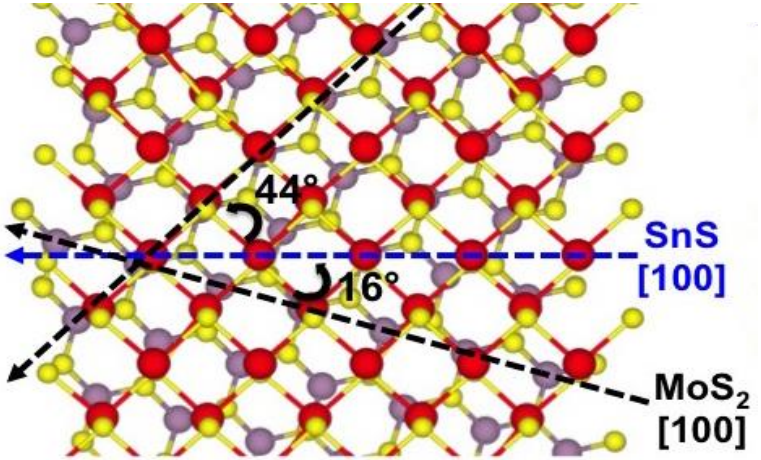
Molecular Orientation Control via Templated Assembly on van der Waals Solids



Weiss, Marks, Hersam, Stern *et al.* *J. Phys. Chem. Lett.* **12**, 26-31 (2021).

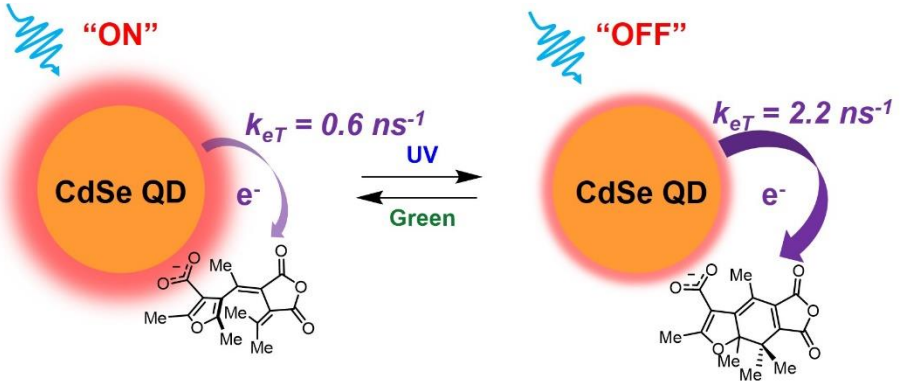
Emergent 1D/2D Mixed-Dimensional Heterostructure via SnS Growth on MoS_2

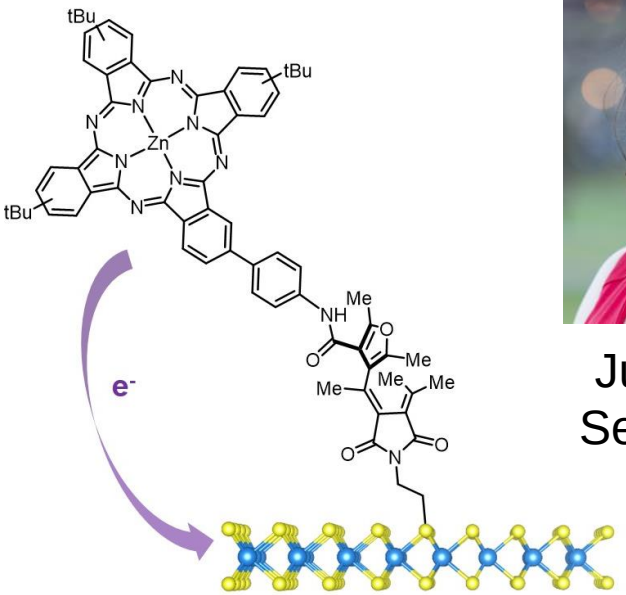




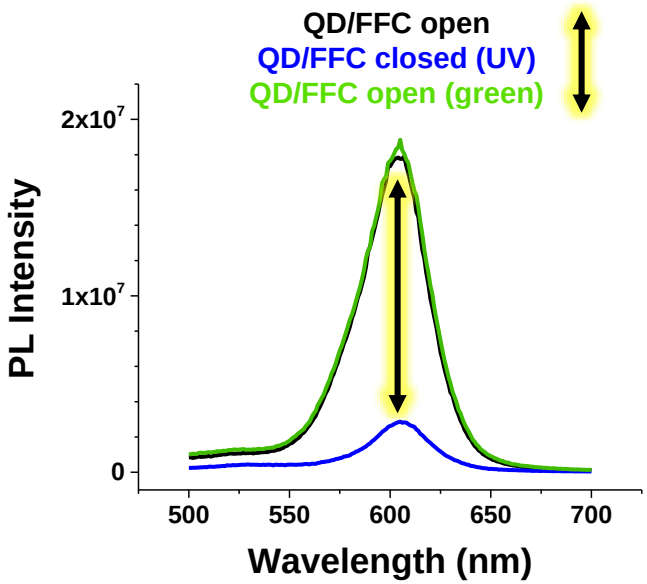
Lauhon, Weiss, Darancet *et al.* *ACS AMI* **43**, 40543 (2019).

Ultrafast Reconfigurability via Fulgide Coupled Mixed-Dimensional Heterojunctions





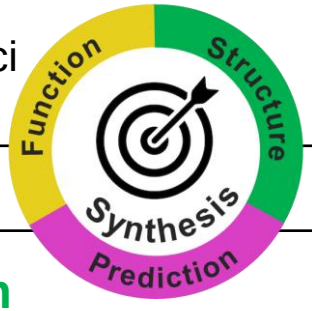
Julia Kalow
Seed Project



Fulgide photoisomerization occurs on sub-picosecond timescales, allowing for ultrafast reconfigurability of mixed-dimensional heterostructures

IRG-2: Functional Heteroanionic Materials via the Science of Synthesis

System	Bulk Synthesis	Film Synthesis
O-S, O-Se	 Co-Lead: Kanatzidis Chemistry, MatSci	 Lead: Haile MatSci, Applied Physics
O-F	 Poeppelmeier Chemistry, MatSci	 Marks Chemistry, MatSci Applied Physics
O-N	Poeppelmeier	Haile, Marks



Property/Function Characterization

Structural Characterization


Bedzyk
MatSci, Physics
Applied Physics


Dravid
MatSci
Applied Physics


González Avilés
Physics
DePaul Univ


Hu
Chemistry
FSU

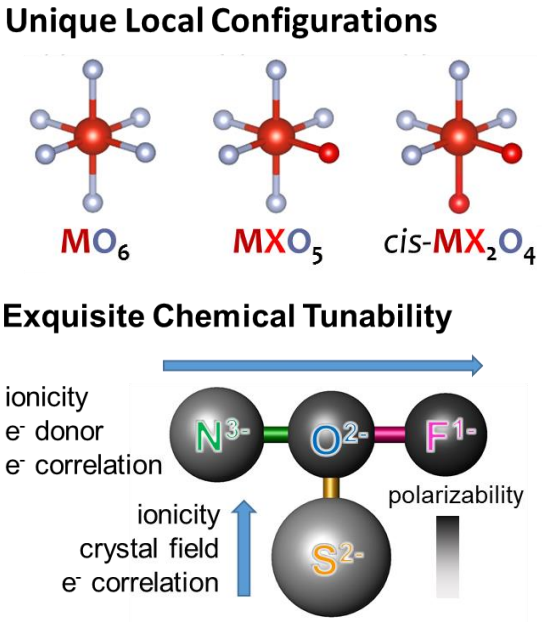
Computational Prediction


Rondinelli
MatSci
Applied Physics

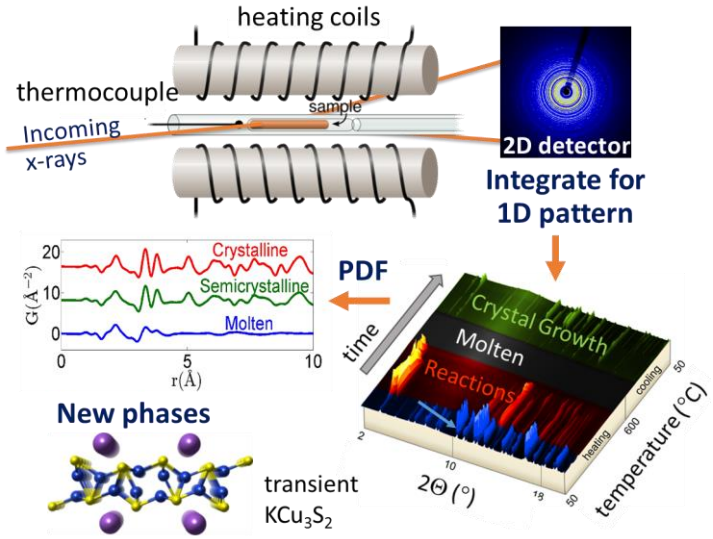

Wolverton
MatSci
Applied Physics

IRG-2 Grand Challenge and Research Thrusts

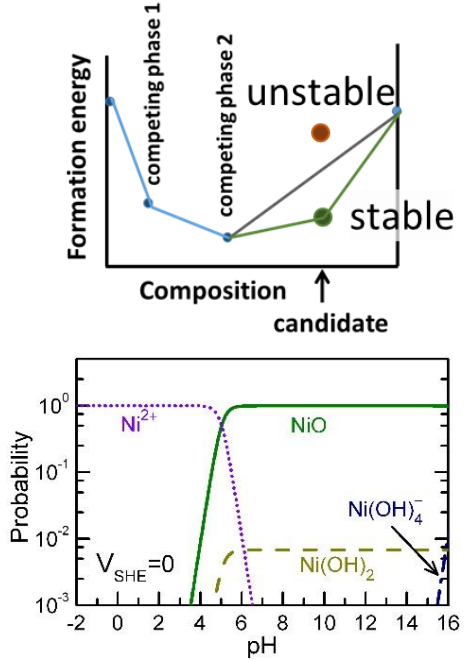
Creation of novel heteroanionic materials with unprecedented functions via the science of synthesis



Functionality Beyond Homoanionic Materials



***In Situ* Identification of New Heteroanionic Compounds and Synthesis Pathways**

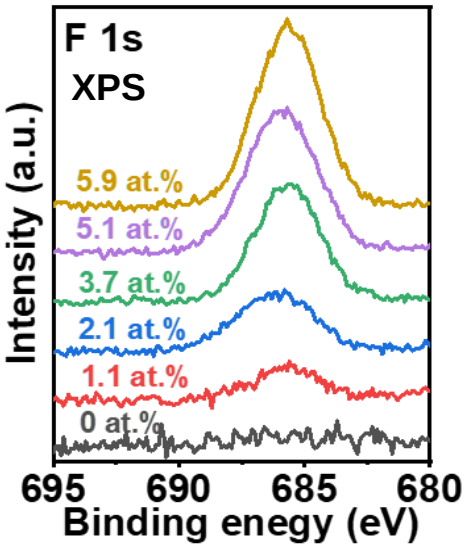


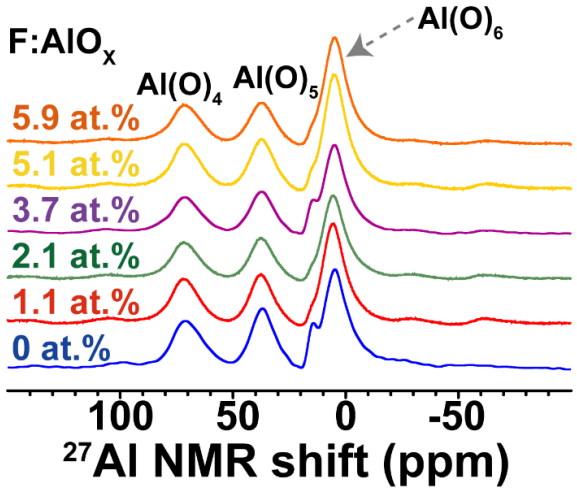
Computationally Guided Synthesis

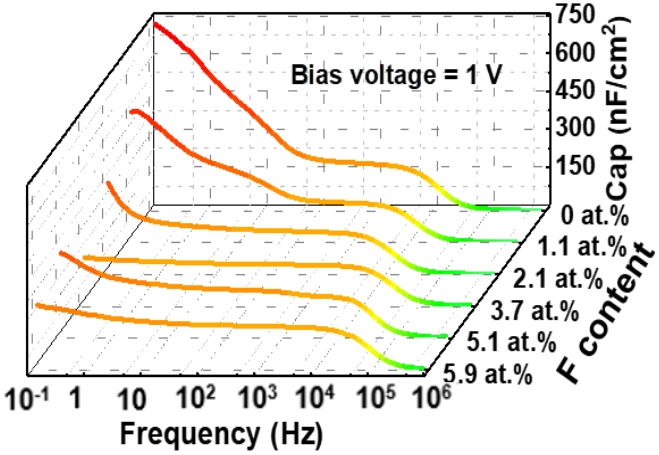
Heteroanion Derived Functionality

Marks, Dravid, Facchetti, Hu, Medvedeva

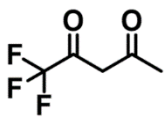
Fluorine doping of amorphous alumina enhances dielectric properties







Fluorine incorporated by combustion synthesis with novel precursor:

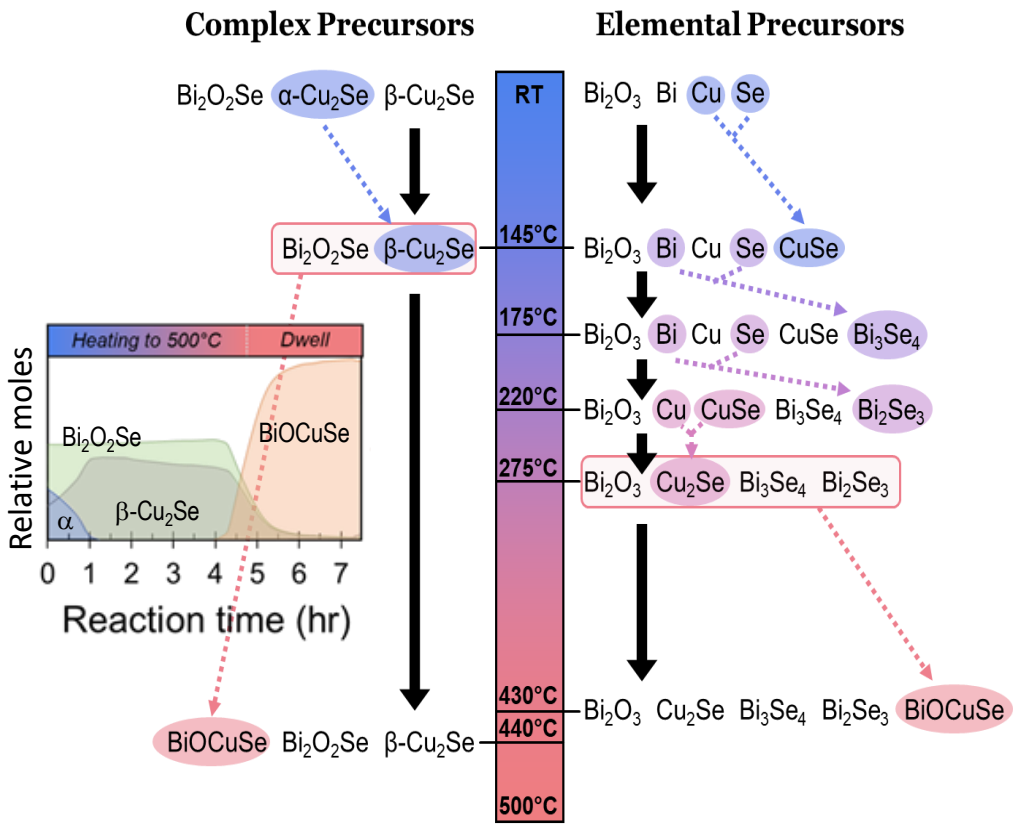


Solid-state NMR shows F incorporated as AlO-F with increasing Al octahedral coordination as F increases

Doping enhances frequency stability of capacitance; also lowers hysteresis, increases on/off ratio in amorphous oxide transistors

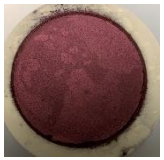
Probing Reaction Pathways

Kanatzidis, Dravid, Wolverton, Poppelmeier

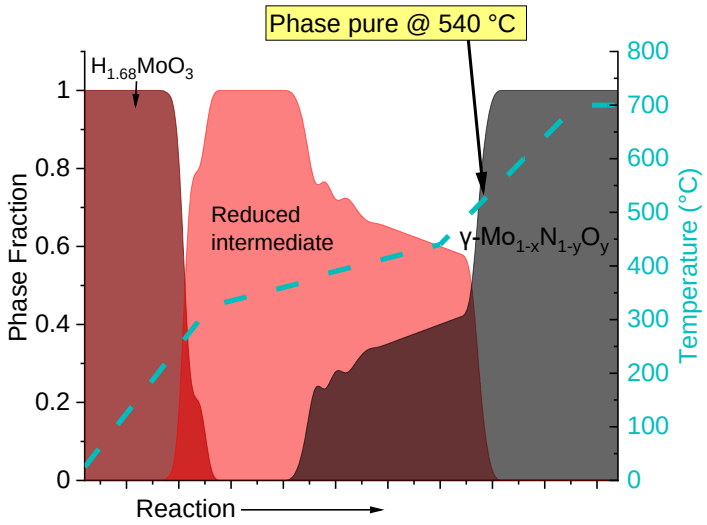


Probing reaction pathways *during* synthesis reveals that complex precursors lead to more direct and efficient oxyselenide formation

Haile, Bedzyk, Dravid, González Avilés, Wolverton



Monoclinic $H_{1.68}MoO_3$ + NH_3



Complex precursors also add value for oxynitride synthesis:
- reduced temp phase formation
- record surface area (206 m^2/g)

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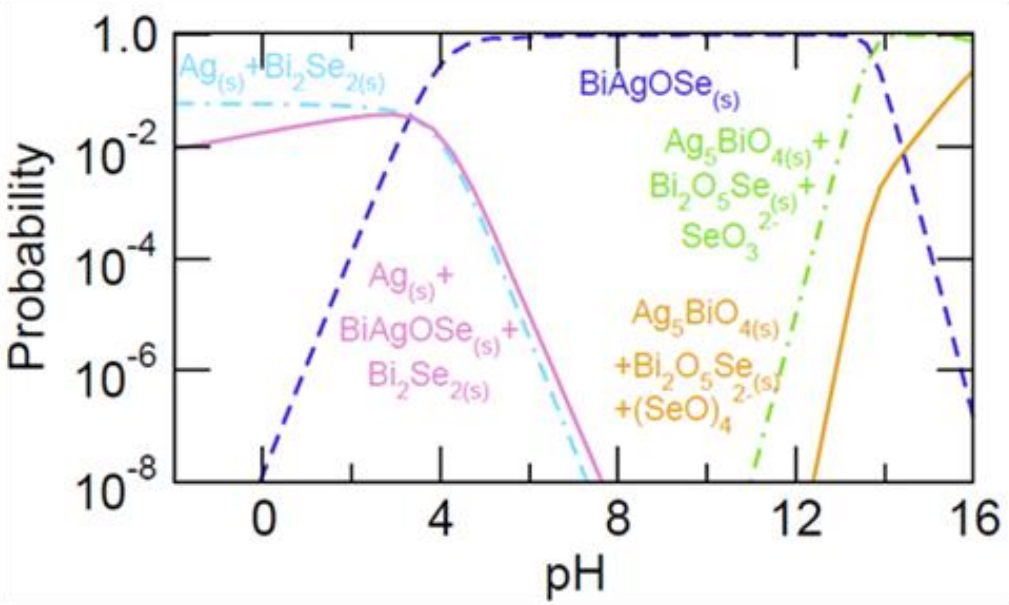
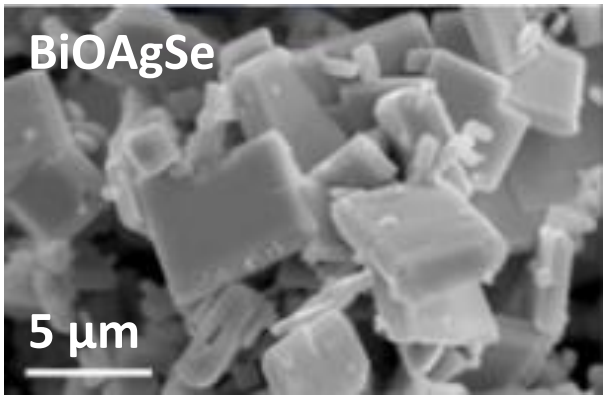
Computationally Guided Synthesis

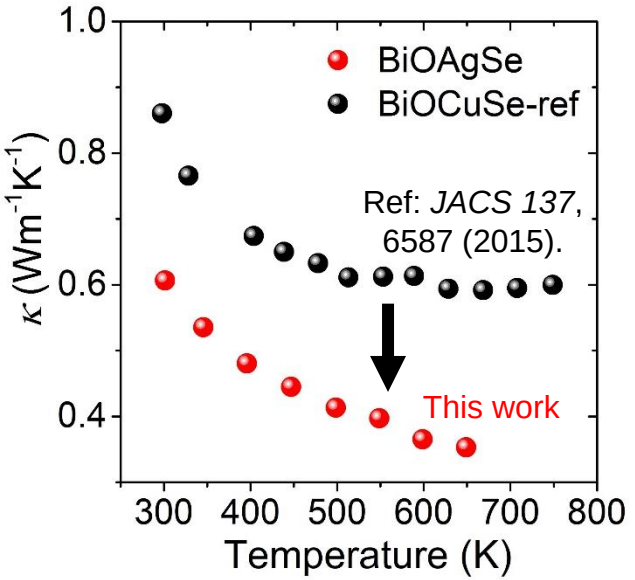
BiOAgSe is barely thermodynamically stable, presenting significant synthetic challenges



- Multi-step hydrothermal synthesis pathway developed using computational guidance
- Single phase BiOAgSe product has lower thermal conductivity than BiOCuSe, as computationally predicted

Poeppelmeier, Dravid, Rondinelli, Wolverton





Super-Seed: Molecularly Precise Membranes for Efficient Chemical Separations

William Dichtel
COF Synthesis

Omar Farha
MOF Synthesis

Nathan Gianneschi
Microscopy, Defect Analysis

Benito Mariñas
Membrane Characterization

Monica Olvera de la Cruz
Computation

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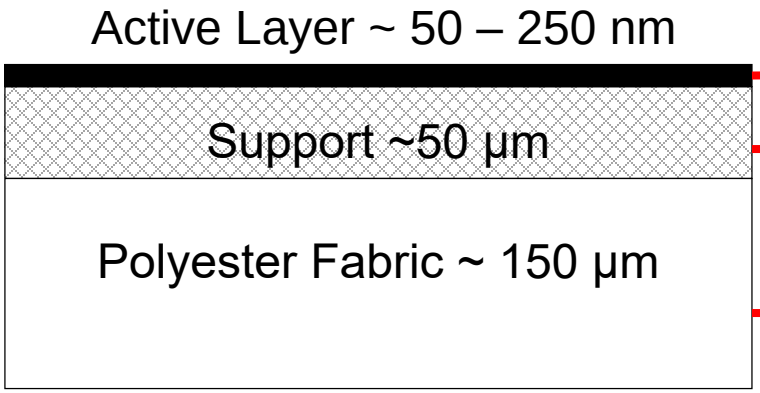
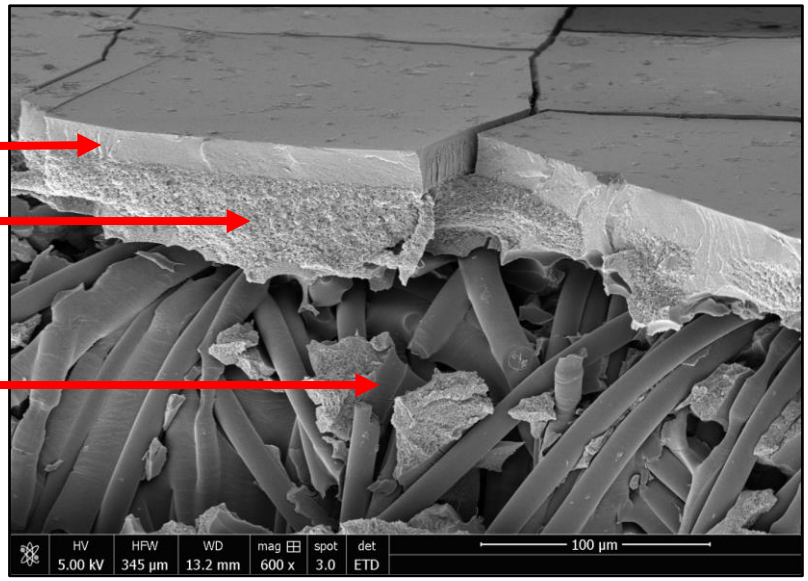
12

Super-Seed Goal: Integrate Precise Porous Materials into Nanofiltration Membranes

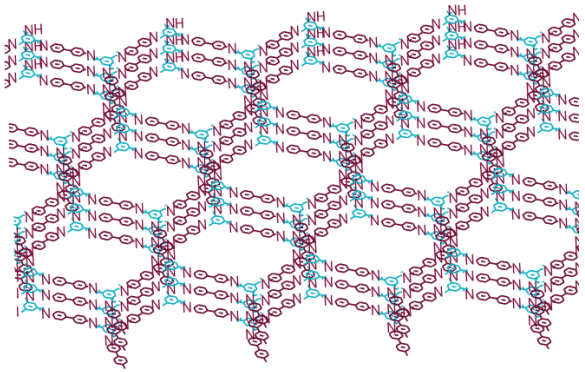
Commercial membranes use a thin-film composite structure:





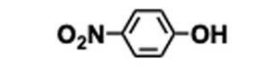
Current active layers: poorly defined crosslinked polyamides

Project goal: Replace polyamides with molecularly well-defined porous framework materials (MOFs/COFs)

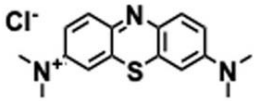


Incumbent COF Membranes Actually Separate Based on Adsorption Affinity (not size)

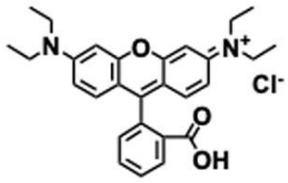
Separation of a three-dye mixture in flow based on adsorption affinity (not size)



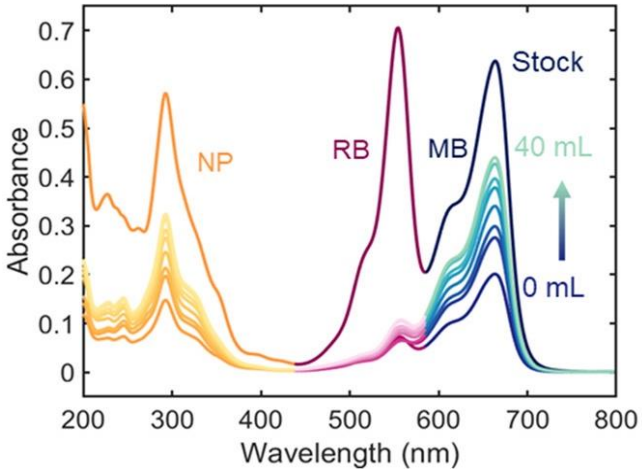
4-nitrophenol
(**NP**)

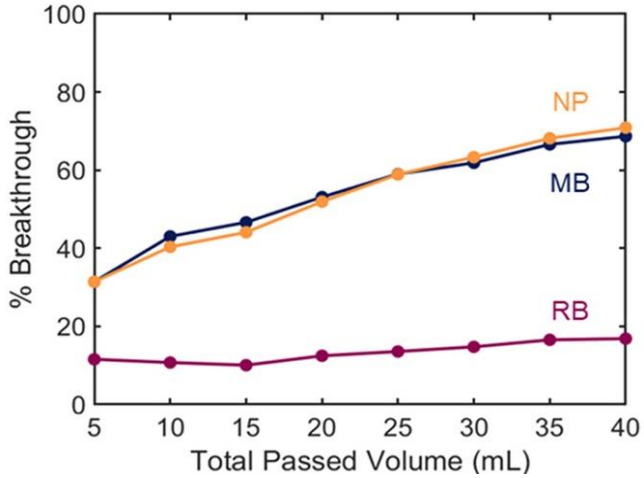


Methylene Blue
(**MB**)

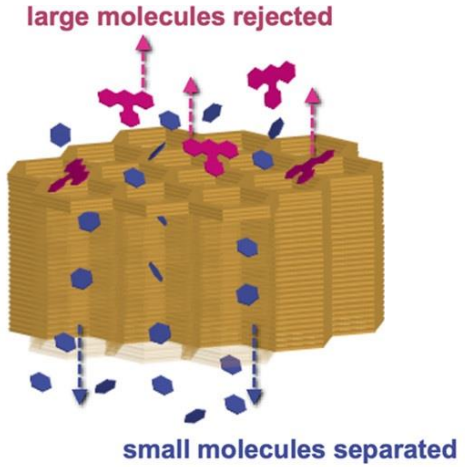


Rhodamine B
(**RB**)

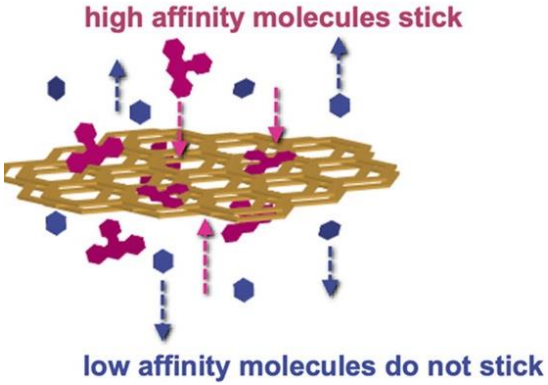




Expectation:



Reality:

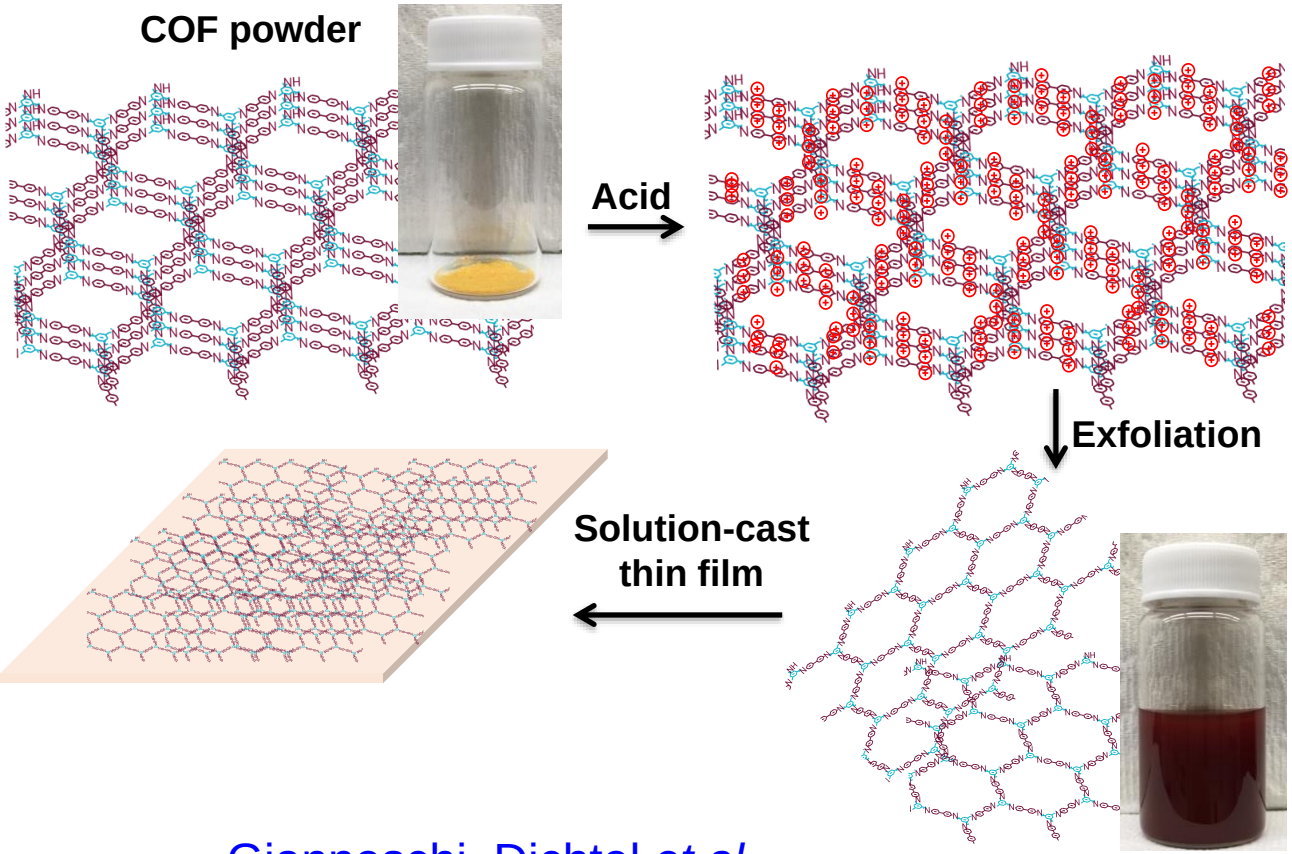


Olvera de la Cruz, Dichtel *et al.*
J. Am. Chem. Soc. **143**, 1466 (2021).

Towards Size-Selective COF Membranes

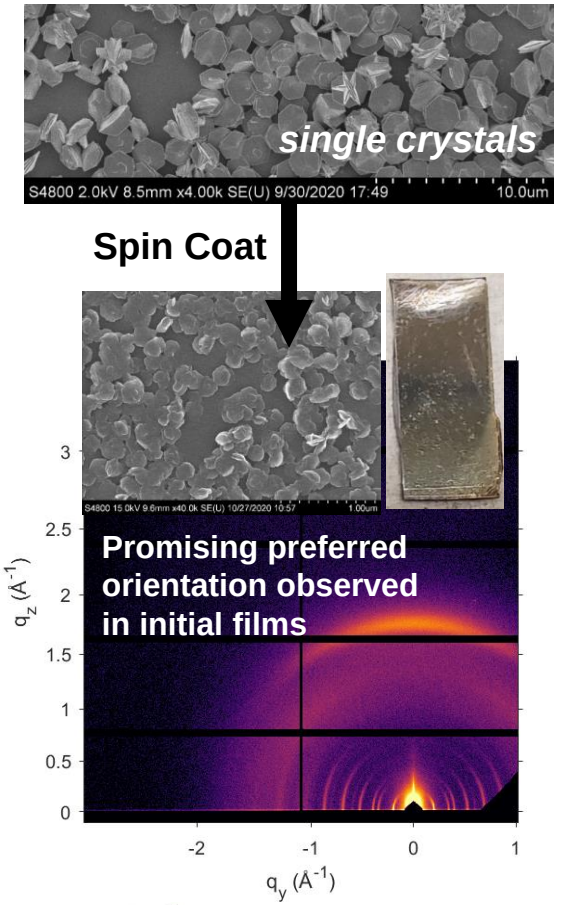
Exfoliation of 2D COF powders and solution-processed thin films

COF powder



Gianneschi, Dichtel *et al.*
Angew. Chem. Int. Ed. **59**, 5165 (2020).

<u>New</u>: Large single crystal colloids of 2D COFs enable higher quality films



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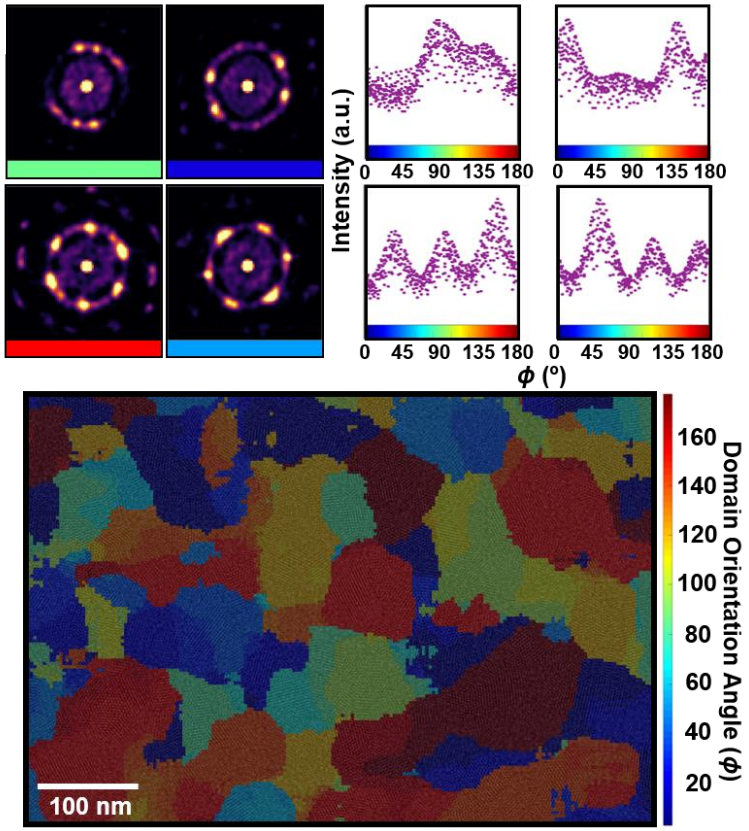
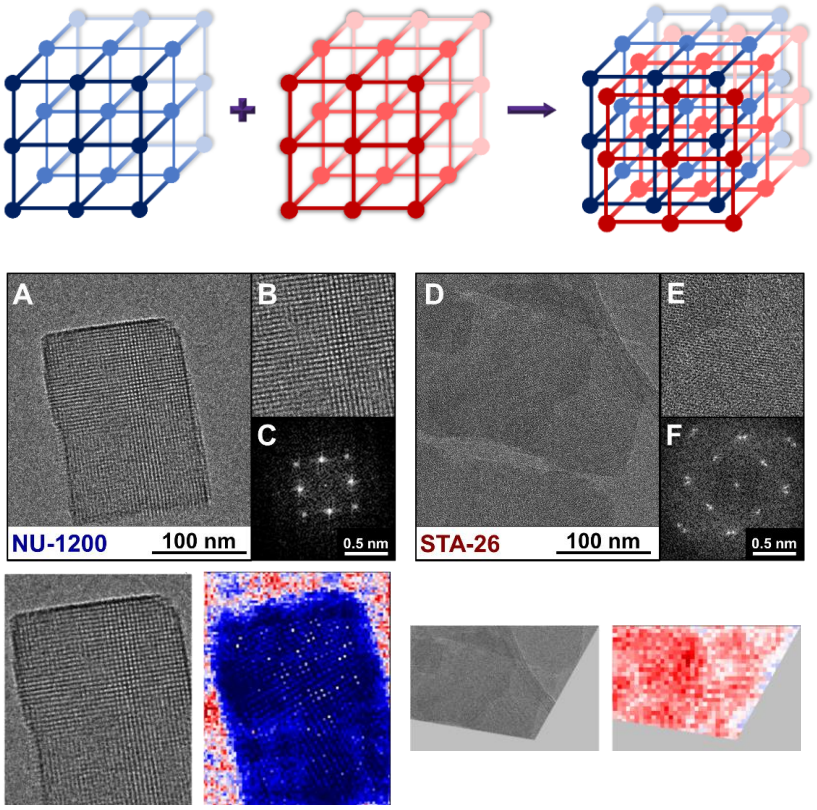
Transmission Electron Microscopy Imaging and Automated Mapping of MOFs and COFs

Assessing COF film quality via automated mapping of crystalline domains in TEM images



Dichtel, Gianneschi, *et al.*
Chem. Mater. **in press** (2021).

Differentiating between MOF structures using TEM images and automated mapping



Dichtel, Gianneschi, Farha *et al.*
J. Am Chem. Soc. **143**, 1503 (2021).

Acknowledgments

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

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NU-MRSEC

Faculty
Postdocs
Students
Staff