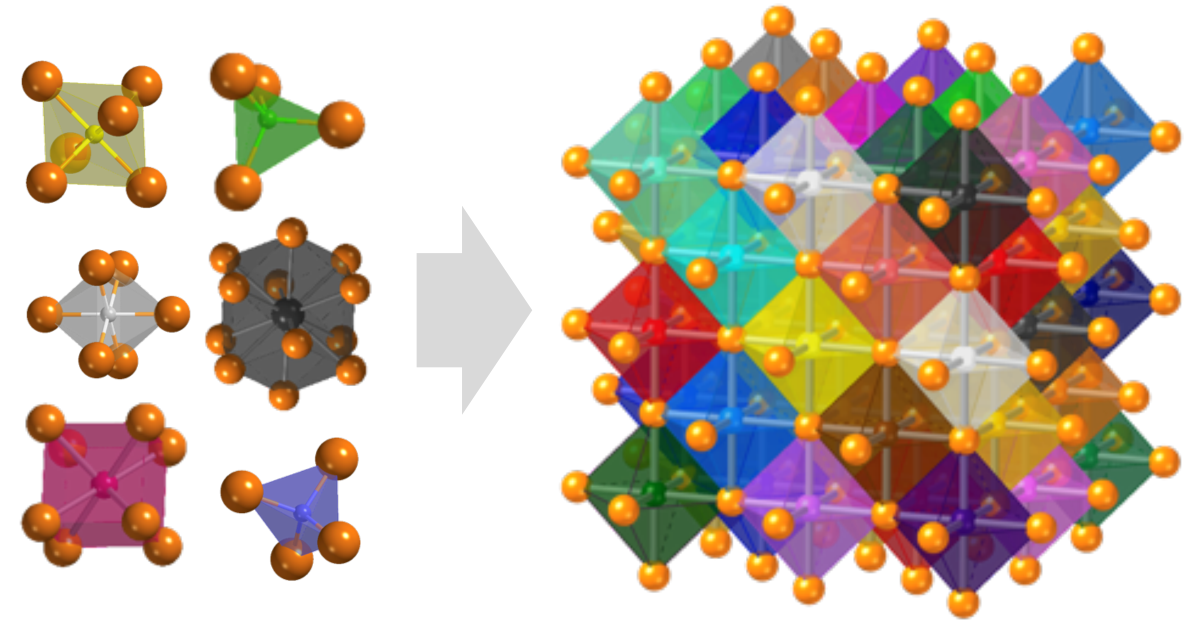
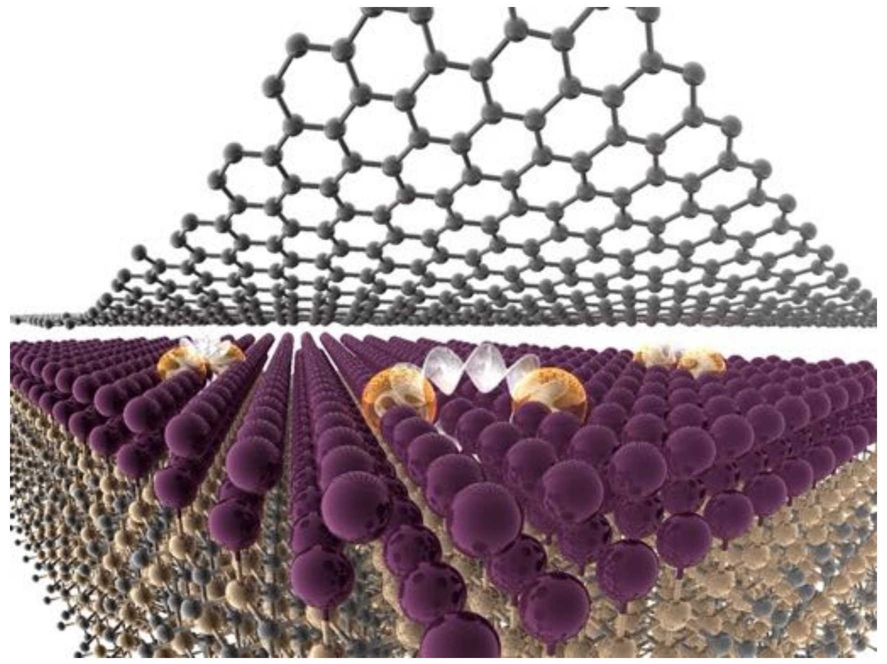
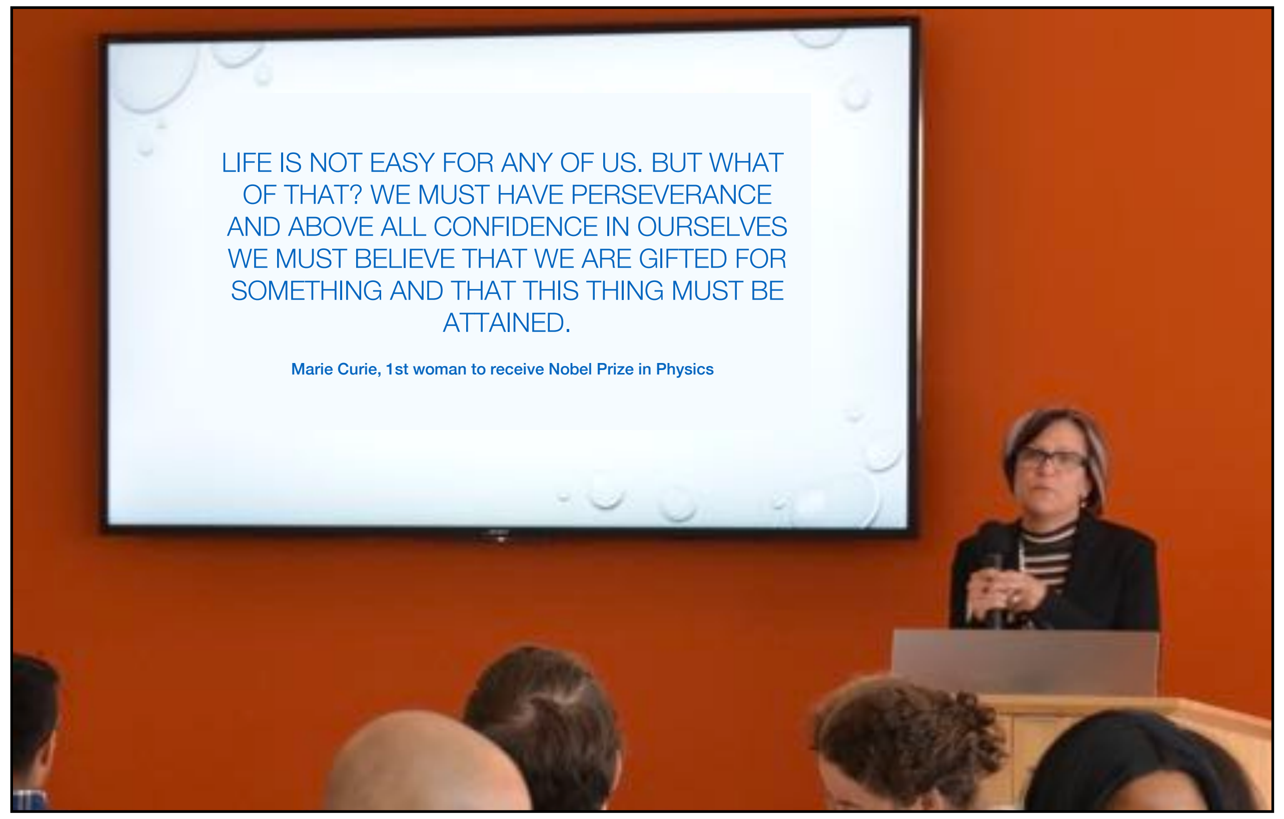




The Penn State Center for Nanoscale Science

New materials platforms created by close collaboration across disciplines



inclusion

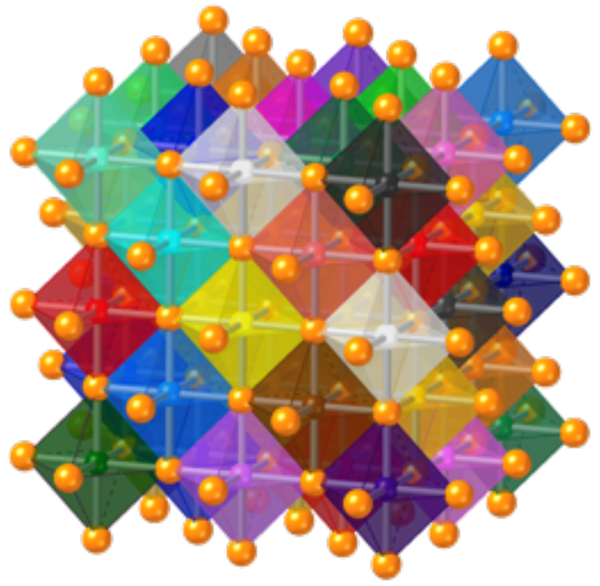
diversity

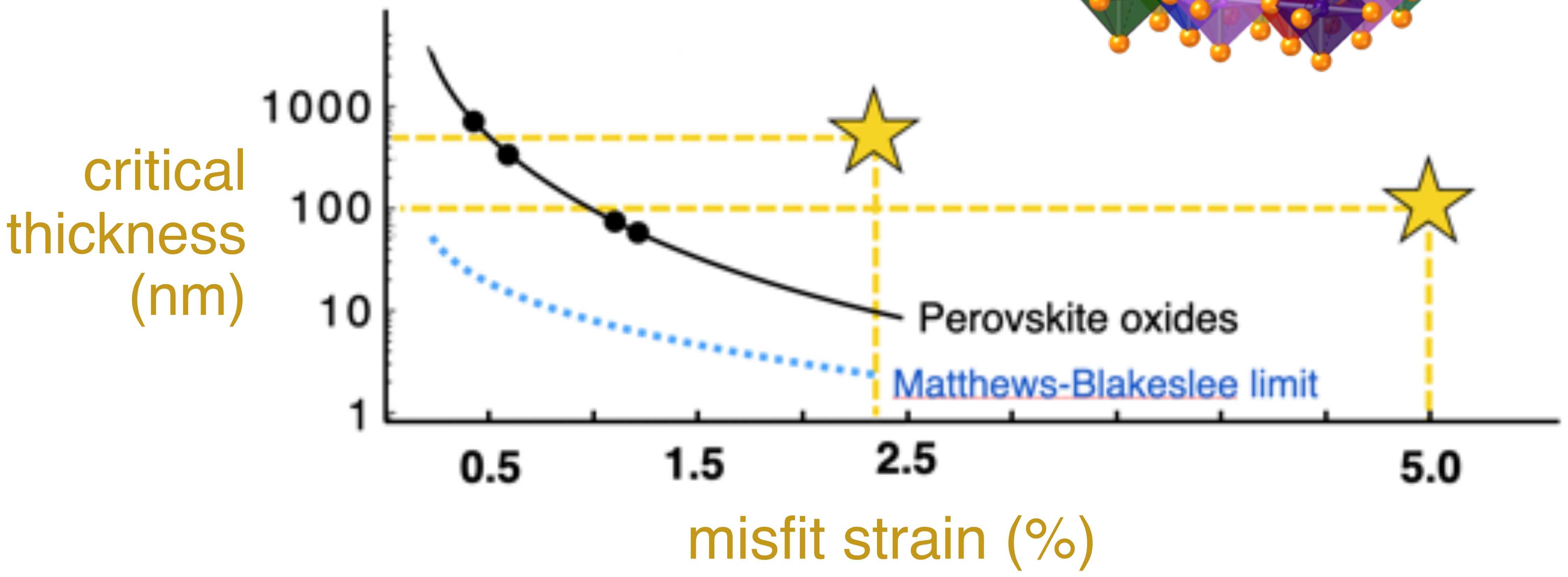
mentoring

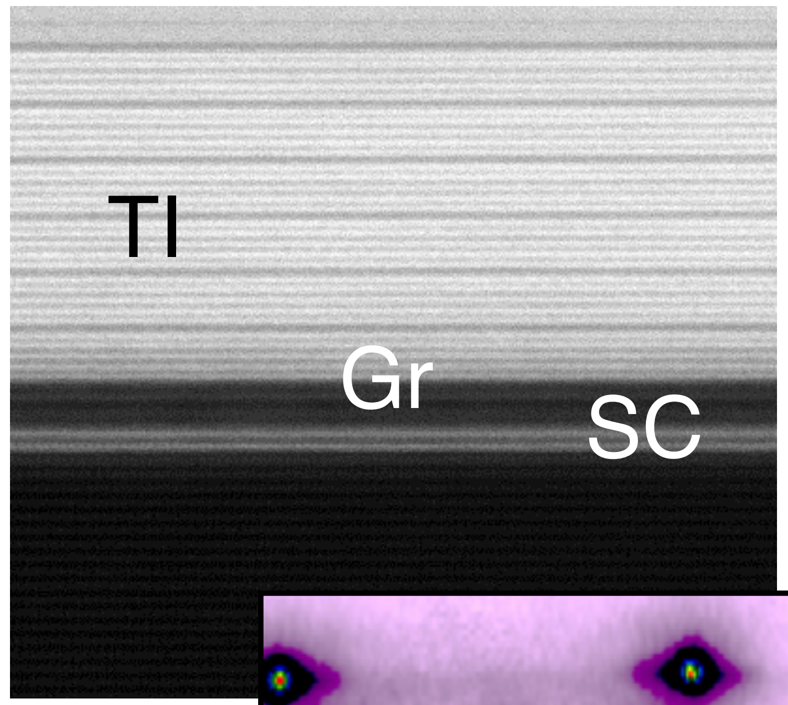
Center rationale & research mission

To combine special capabilities in nanoscale synthesis, fabrication, measurement and theory/design…

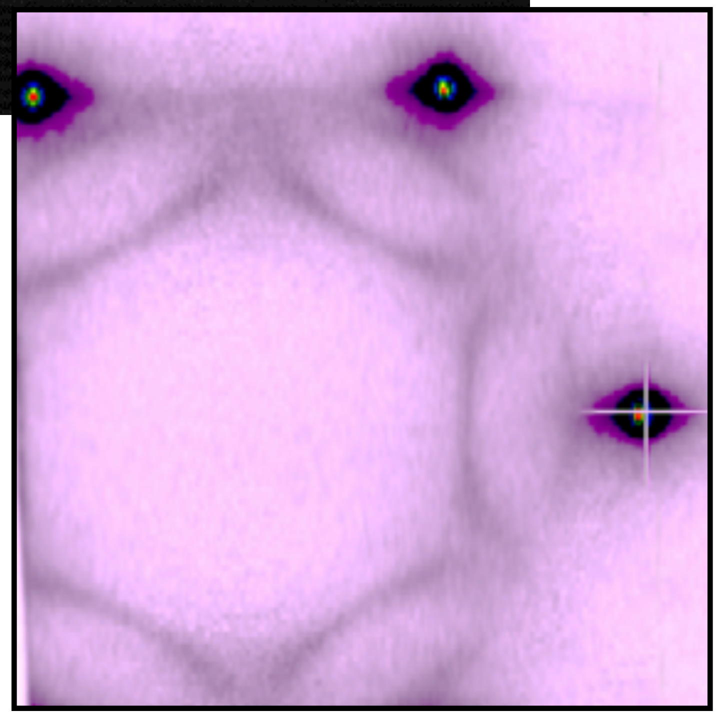
Films that deploy a **diversity of local configurations** in service of extraordinary epitaxy.







Topological insulators on super-conductors with **ideal interfaces**, with graphene interposed.



Strong spin-split Fermi surface of **air-stable** atomically thin 2D heavy metals.

…to establish new means of materials organization and behavior with unprecedented function at the nanoscale.

Management Philosophy: Continuous renewal to pursue **the most compelling emerging science**

2000: Established as a single-IRG MRSEC

2002: New award added **two new IRGs**

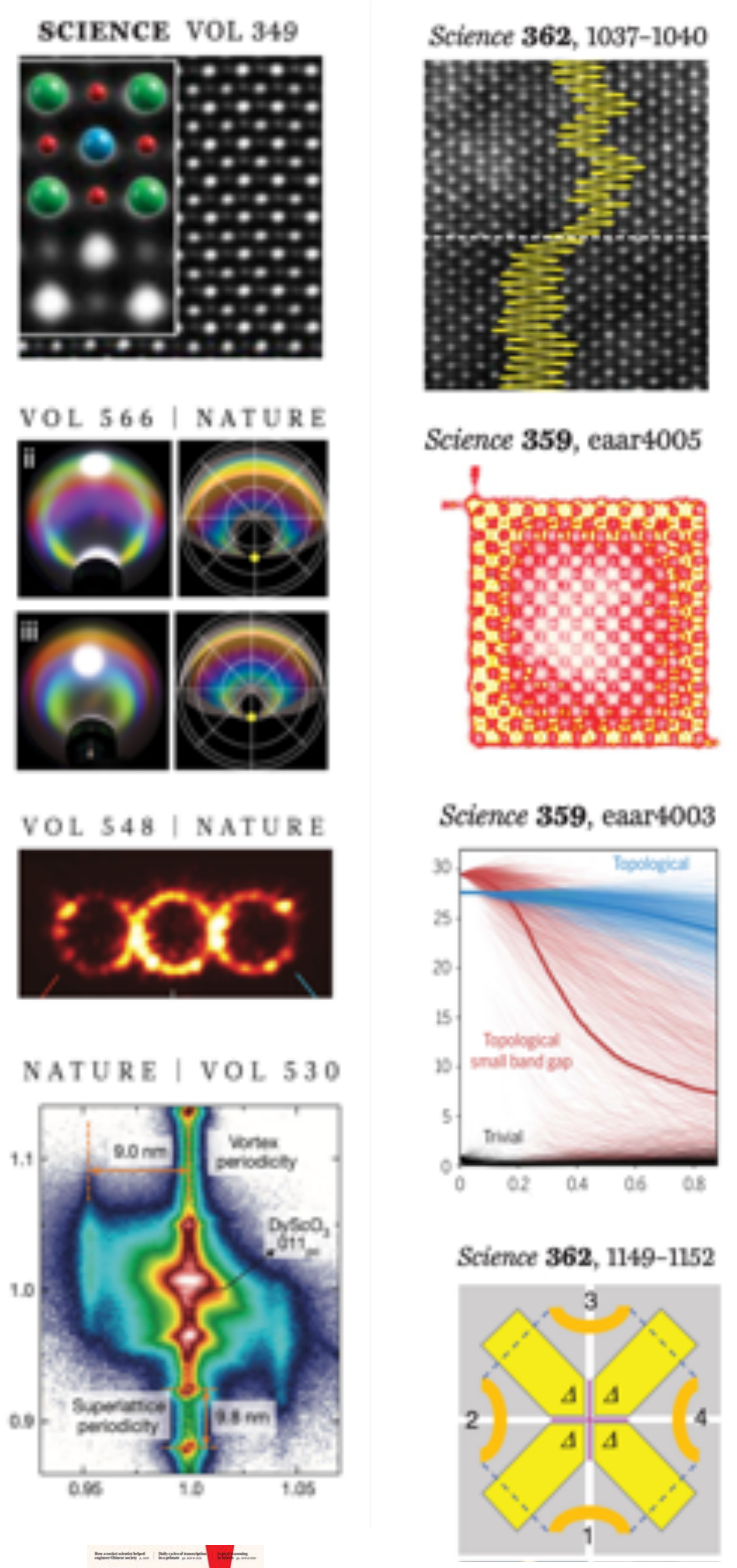
2004: Part of original MRSEC **phased out** at birth of new IRGs

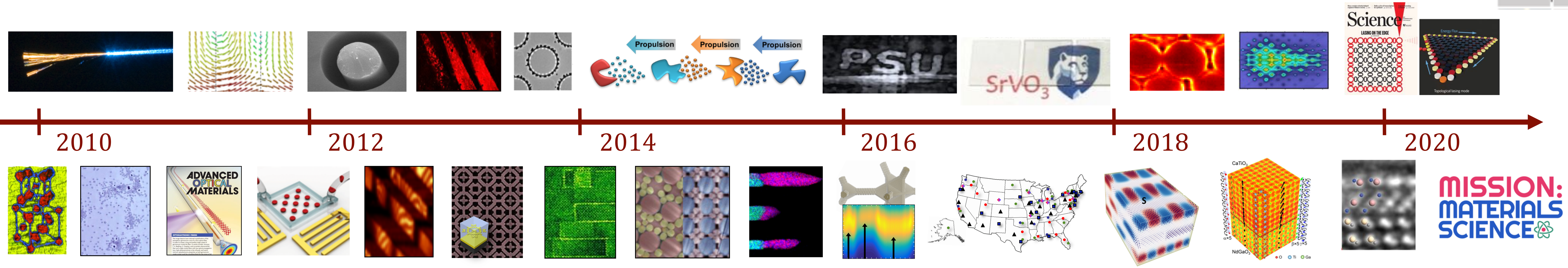
2008: Recompeted with **~25% overlap to prior IRGs**

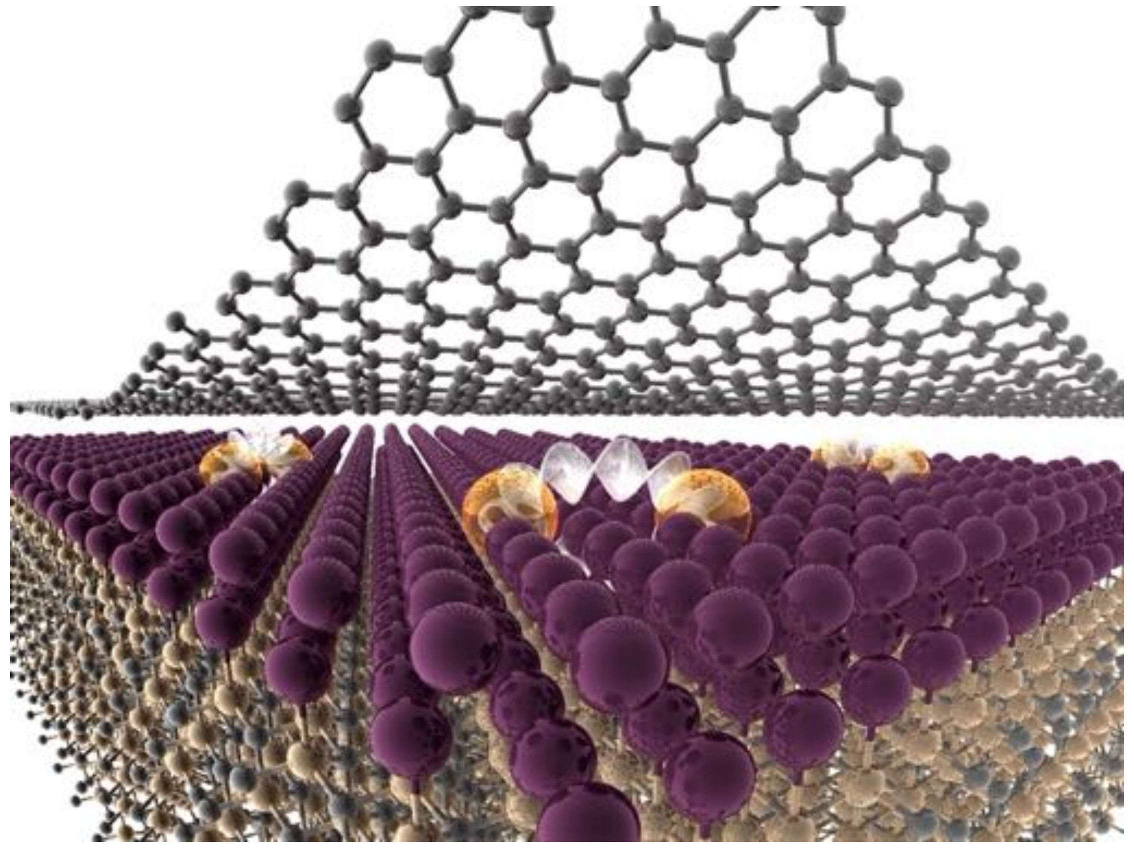
2012: Redirection substantially **refocused every IRG**

2013: Recompeted with **~40% overlap to prior IRGs** (down-selected from 9 internal white papers)

2019-20: 9 internal IRG white papers down-selected internally to three proposed and two funded IRGs with minimal overlap to prior IRGs. One began as Seed, other is de novo.



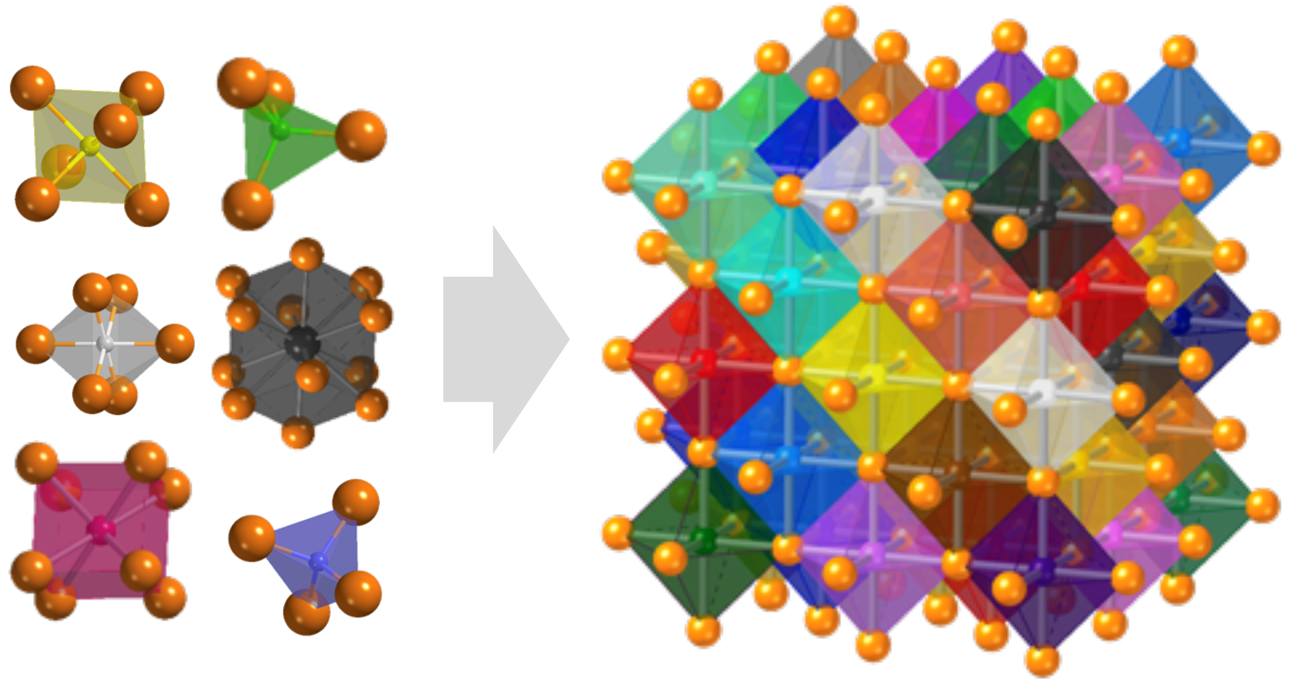




IRG1: 2D Polar Metals and Heterostructures

Air-stable, quantum-confined 2D metals with broken inversion symmetry for emergent electronic and optical phenomena.

Co-leads:
Joshua Robinson
Jun Zhu



IRG2: Crystalline Oxides with High Entropy

Establish the transformative guiding science of crystalline inorganic compounds with high configurational entropy.

Co-leads:
Jon-Paul Maria
Ismaila Dabo

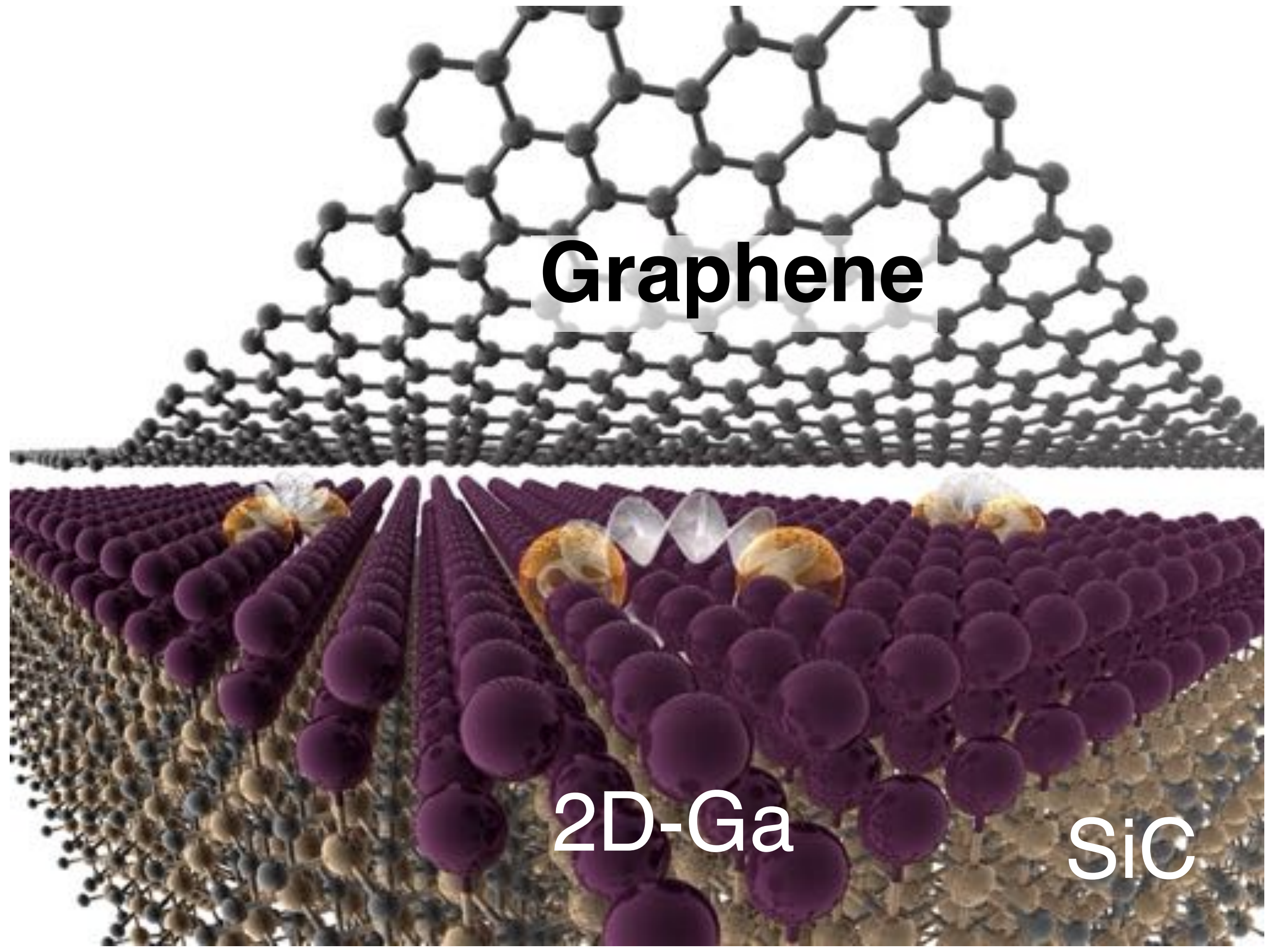
National Science Foundation MRSEC Materials Research Science and Engineering Centers

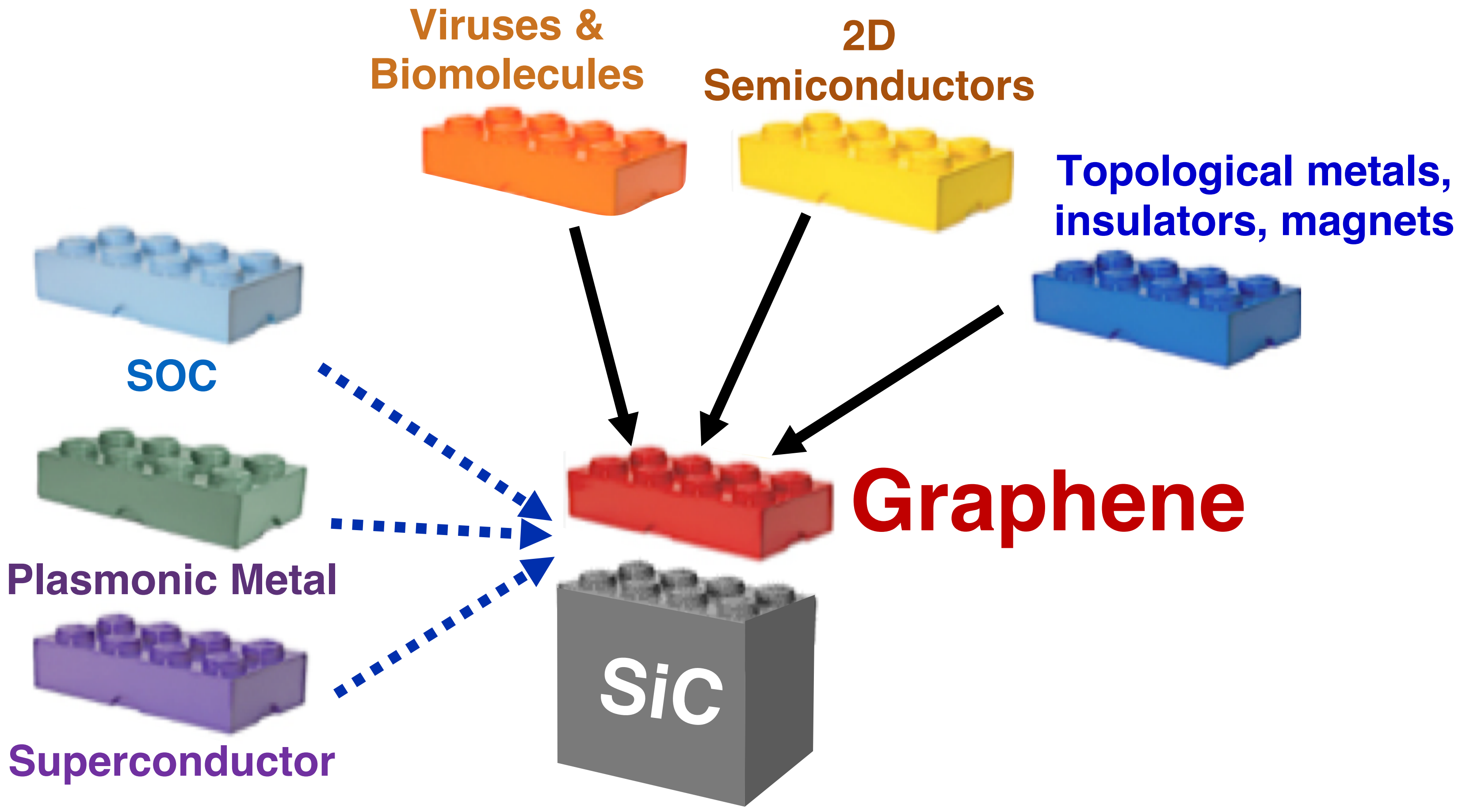
Center for Nanoscale Science

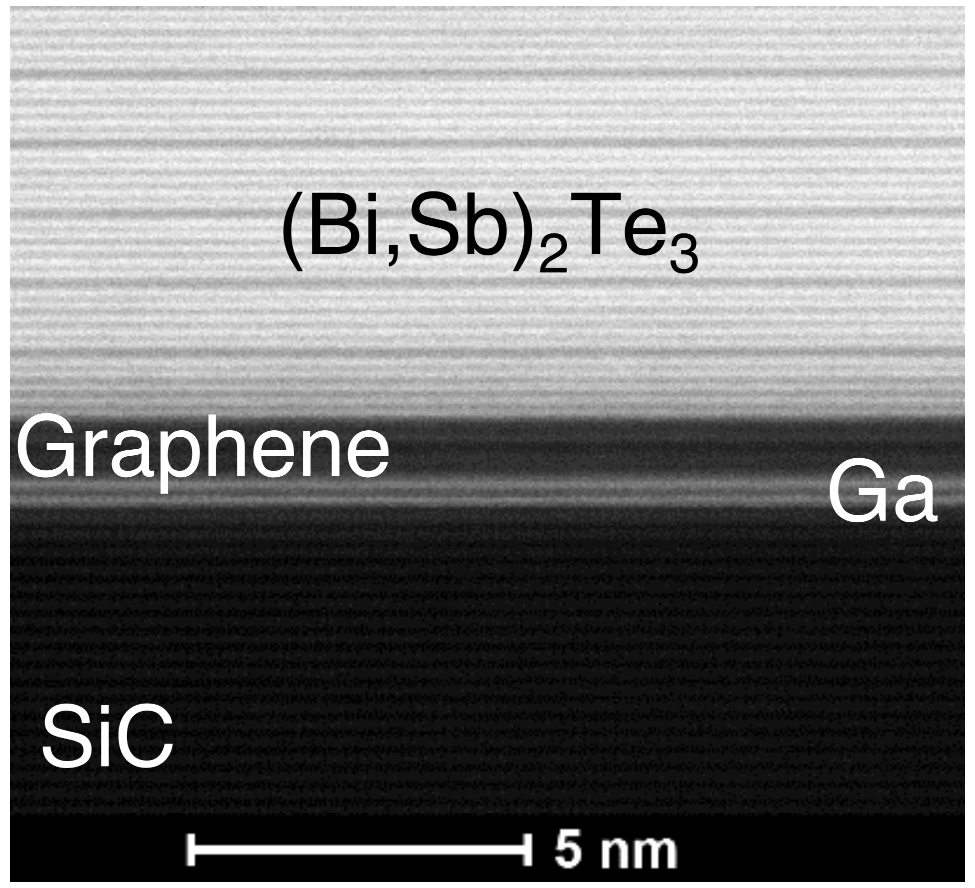
IRG 1

2D Polar Metals and Heterostructures

Co-leads: Joshua A. Robinson, Jun Zhu







Opportunity

Air stable, quantum-confined metals with broken inversion symmetry enable opportunities in emergent electronic and optical phenomena.

TOPOLOGICAL SUPERCONDUCTIVITY

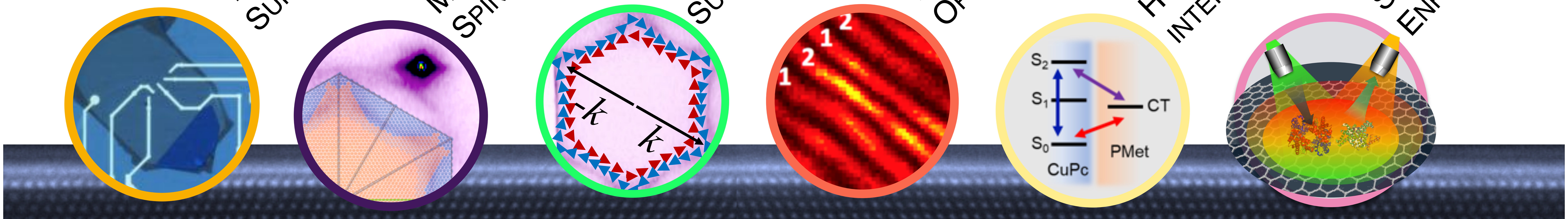
METAL-BASED SPINTRONICS

POLAR SUPERCONDUCTORS

NON-LINEAR OPTICS

HYBRID LIGHT-MATTER INTERACTIONS

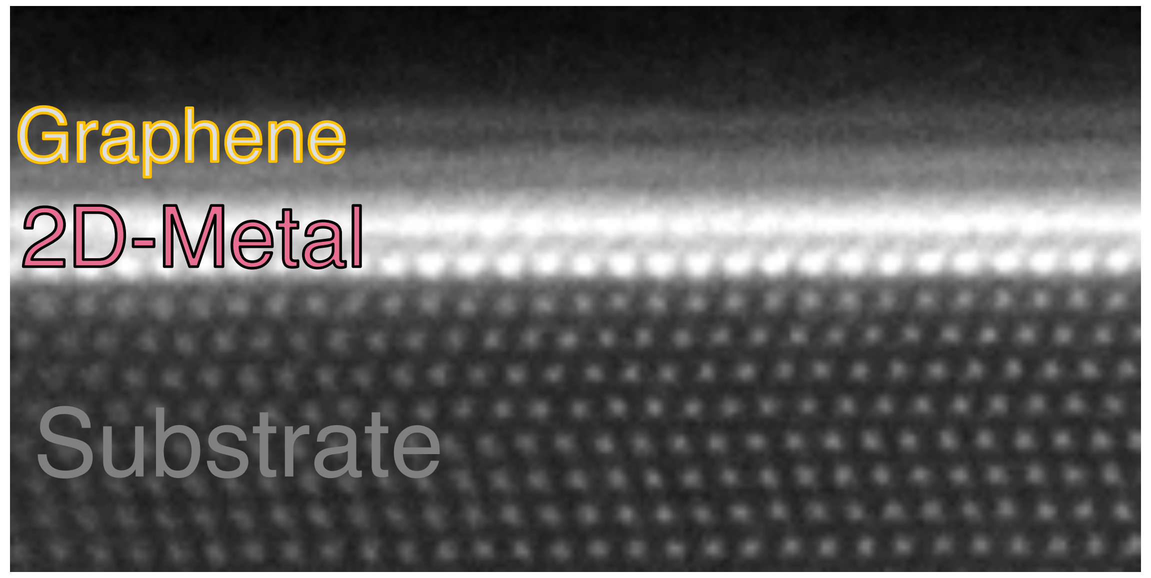
SURFACE-ENHANCED RAMAN



Challenge

Most metals are not stable when scaled down to a few atoms thick.

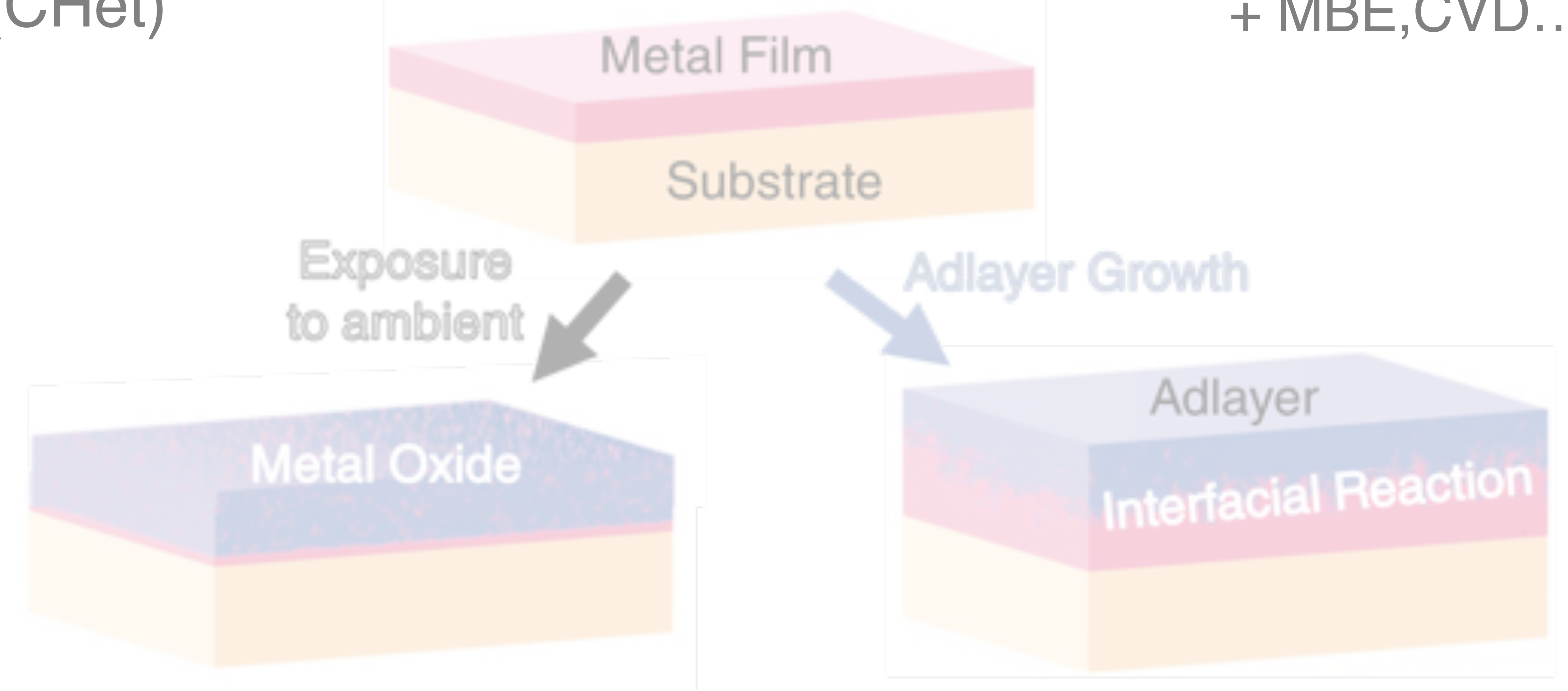
Air-stable, crystalline 2D metals



Confinement Heteroepitaxy

(CHet)

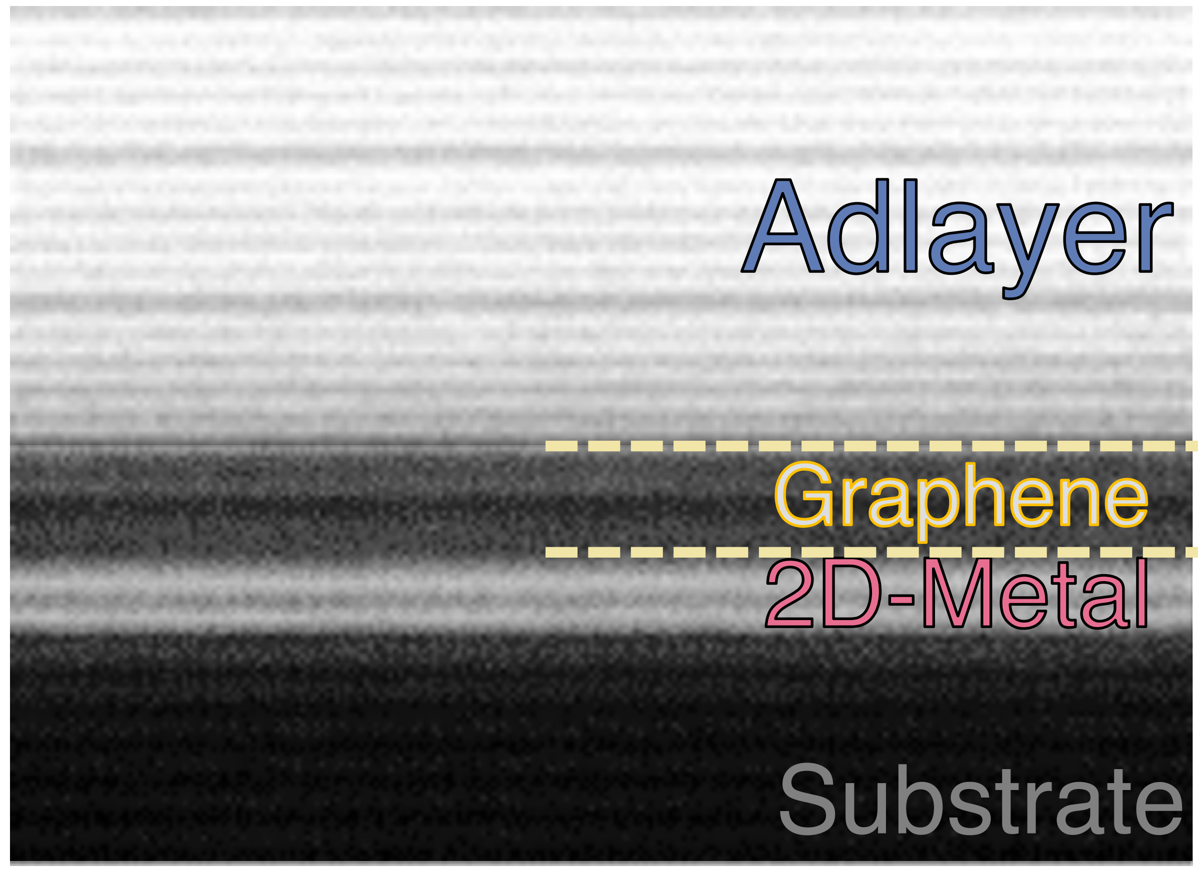
Traditional Routes



Confinement Heteroepitaxy

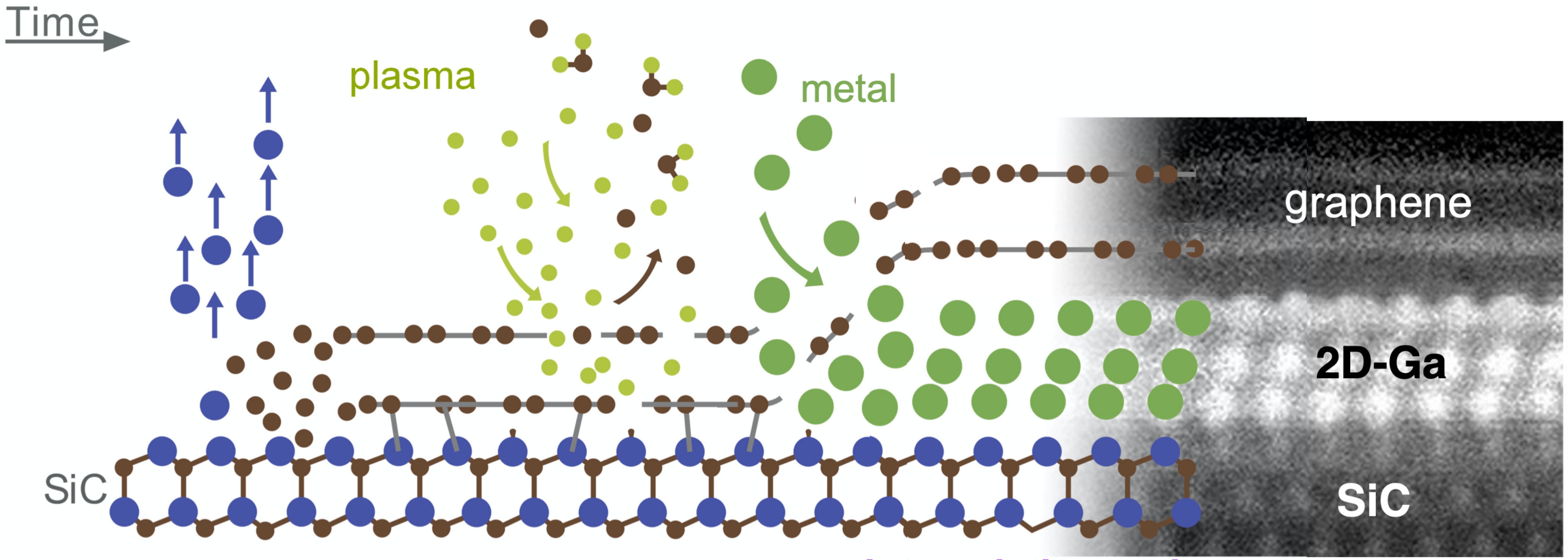
+ MBE,CVD…

2D-metal-based heterostructures with pristine interfaces



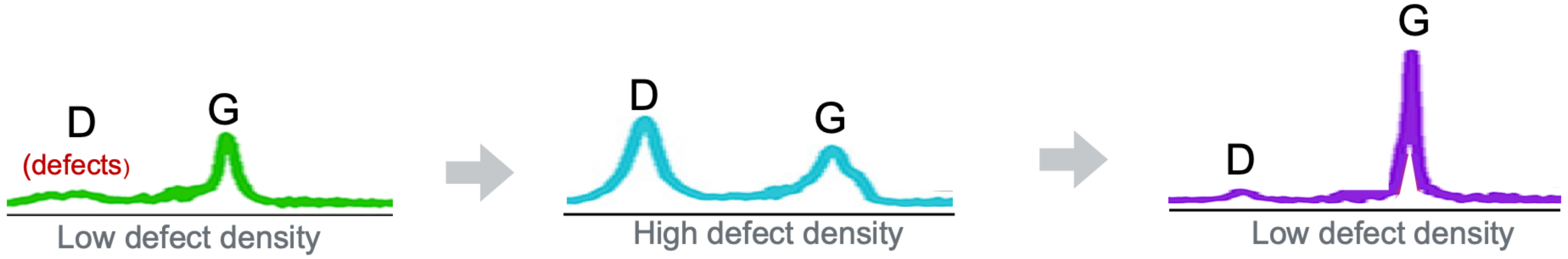
Confinement Heteroepitaxy

CHet produces **air-stable**, crystalline 2D polar metals (2D-PMets).



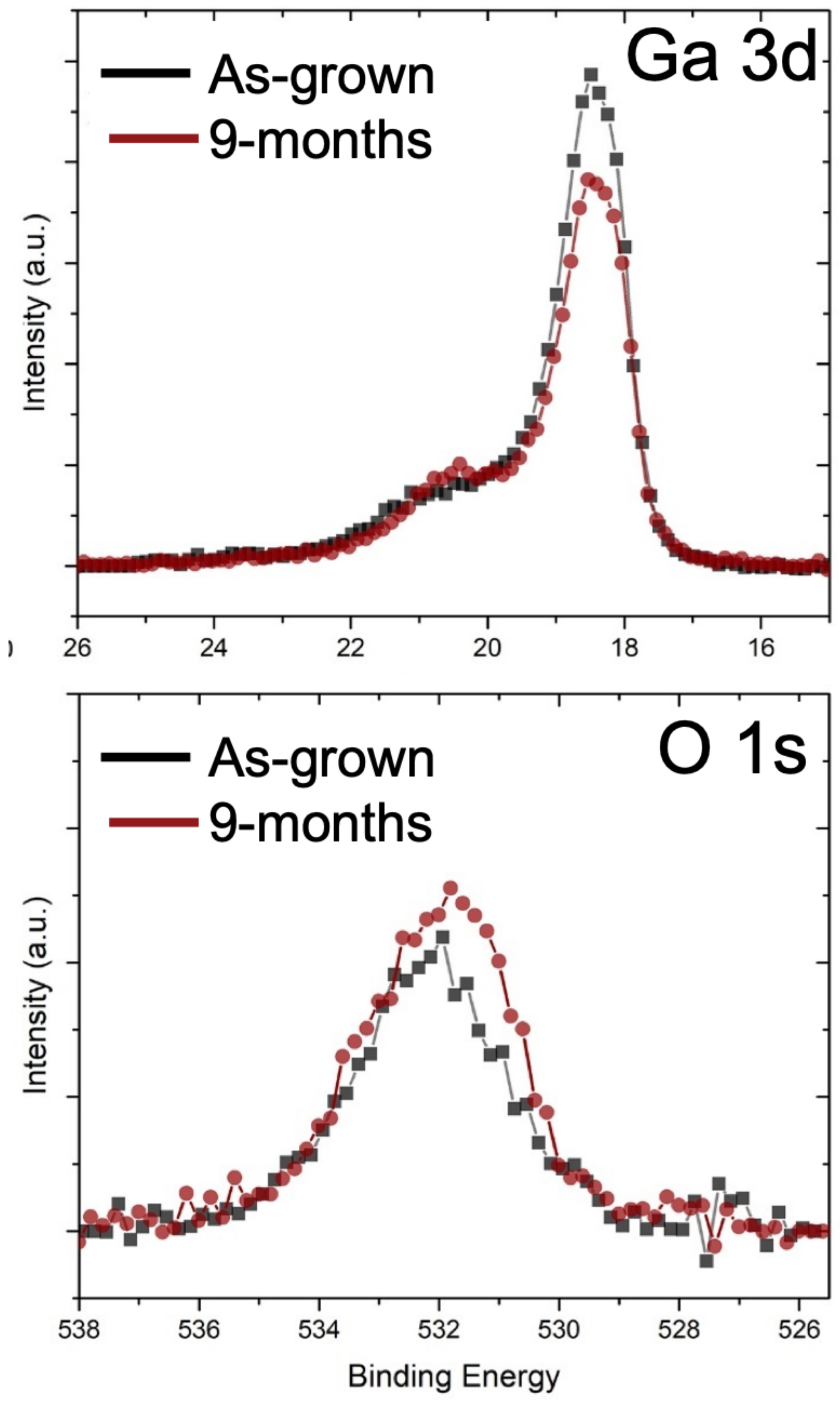
graphene forms by Si sublimation ➡ defects provide gallery access ➡ intercalation and graphene healing | **TEM Image**

Graphene Defect Evolution



Intercalation heals the graphene cap

2D-Metal stability in air



Briggs *et al.* Nanoscale 11 (33), 15440-15447
Briggs *et al.* Nature Materials; doi.org/10.1038/s41563-020-0631-x (2020)

2D Polar Metals and Heterostructures

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

Electronic

Topological/Unconventional 2D Superconduct.
Robinson, Zhu, Chang, Samarth, Crespi, Liu

Quantum Spintronics
Samarth, Knappenberger, Crespi, Liu

Ga Nb Nb_3Sn Sn Bi Pt … Pb

Synthesis

Controlled formation of 2D-PMets & Heterostructures
Robinson, Terrones, Chang, Samarth, Crespi

Sn Ag Zn Au In … Ga

effects of non-centrosymmetry

Seed efforts targeting new CHet substrates

2D Plasmonics & Non-linear Optics
Knappenberger, Giebink, Crespi, Fullerton-Shirey

Surface-enhanced Raman Sensing
Huang, Terrones, Jensen, Robinson

Photonic

Team

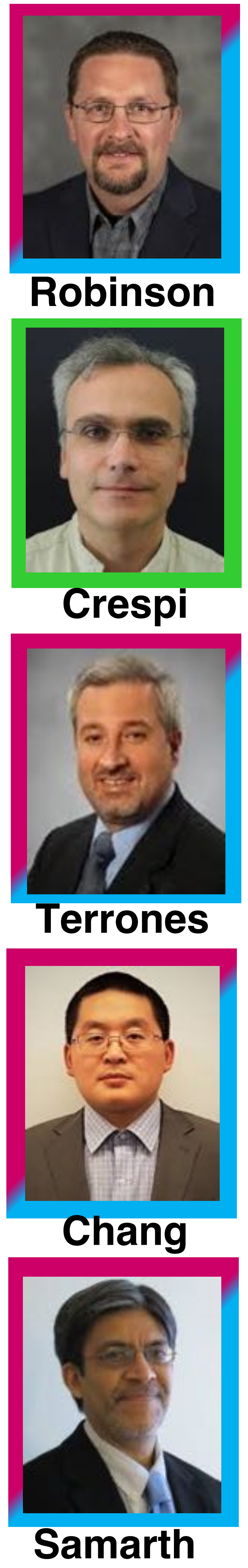
National Science Foundation
MRSEC
MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTERS

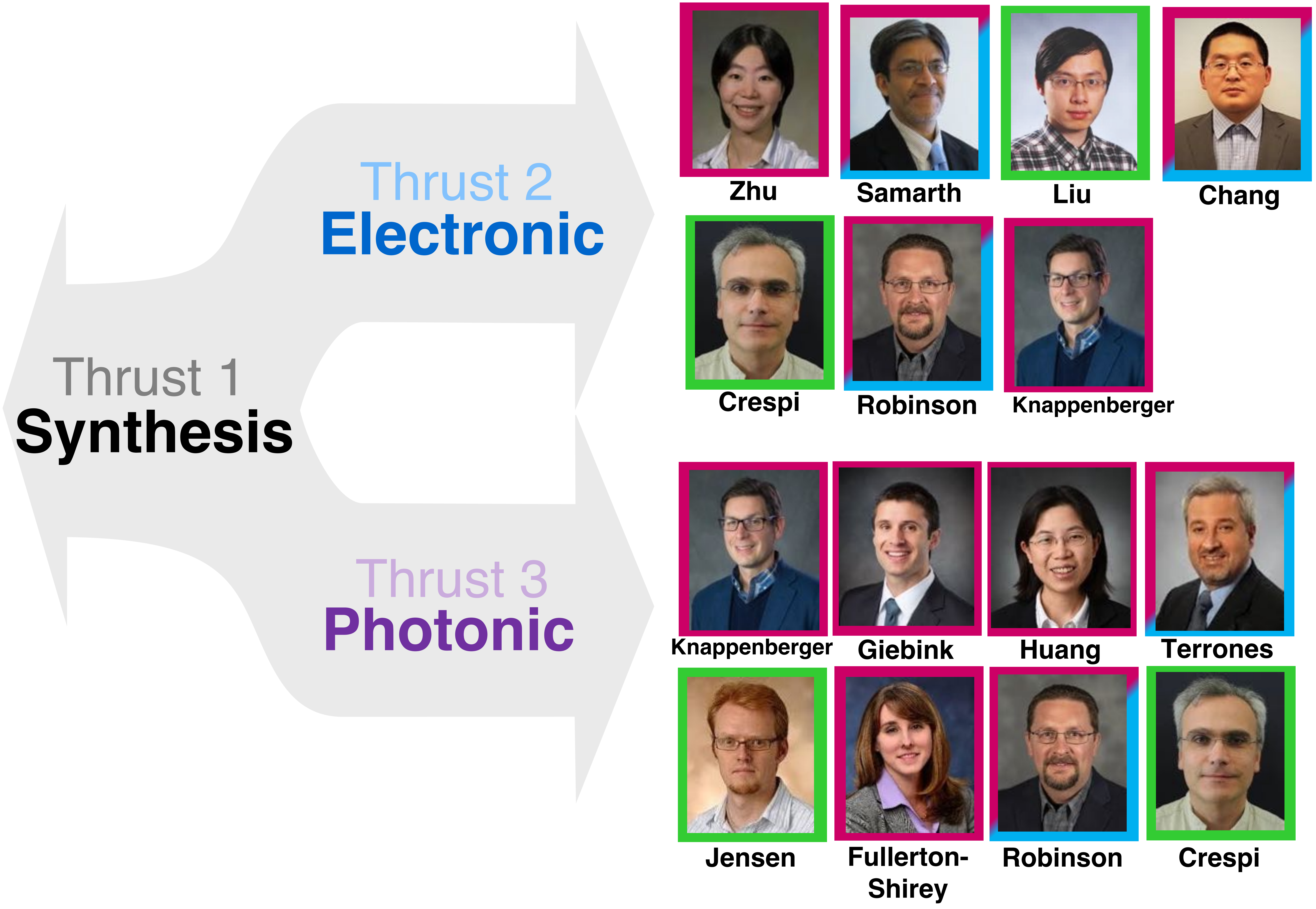
Theory/computation
First-principles methods
Reactive force fields
Analytical modeling

Characterization
Chemical/structural properties
Electronic properties
Non-linear optical properties
Magnetic properties
Raman spectroscopy
Electrolyte gating

Synthesis
Confinement heteroepitaxy
Molecular beam epitaxy
Chemical vapor deposition

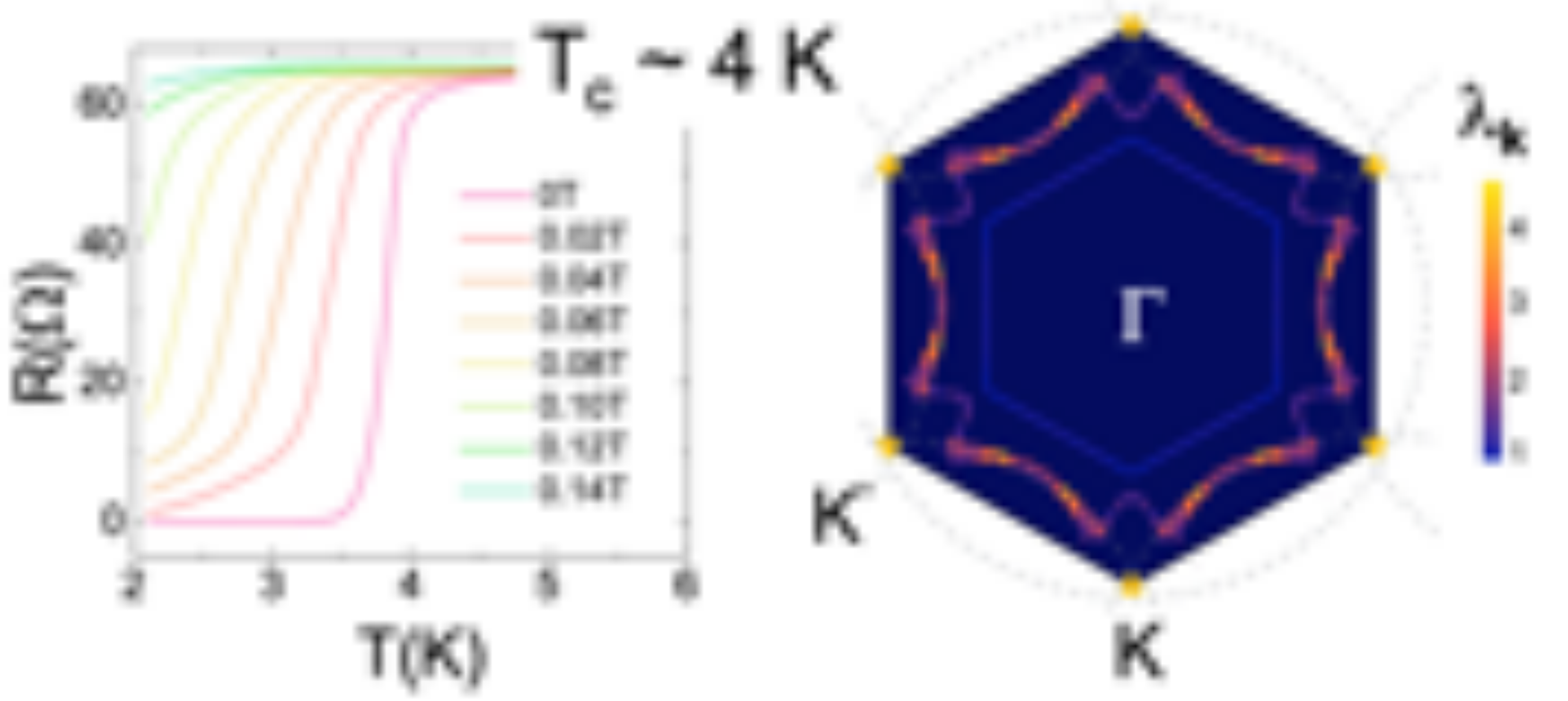
5 departments



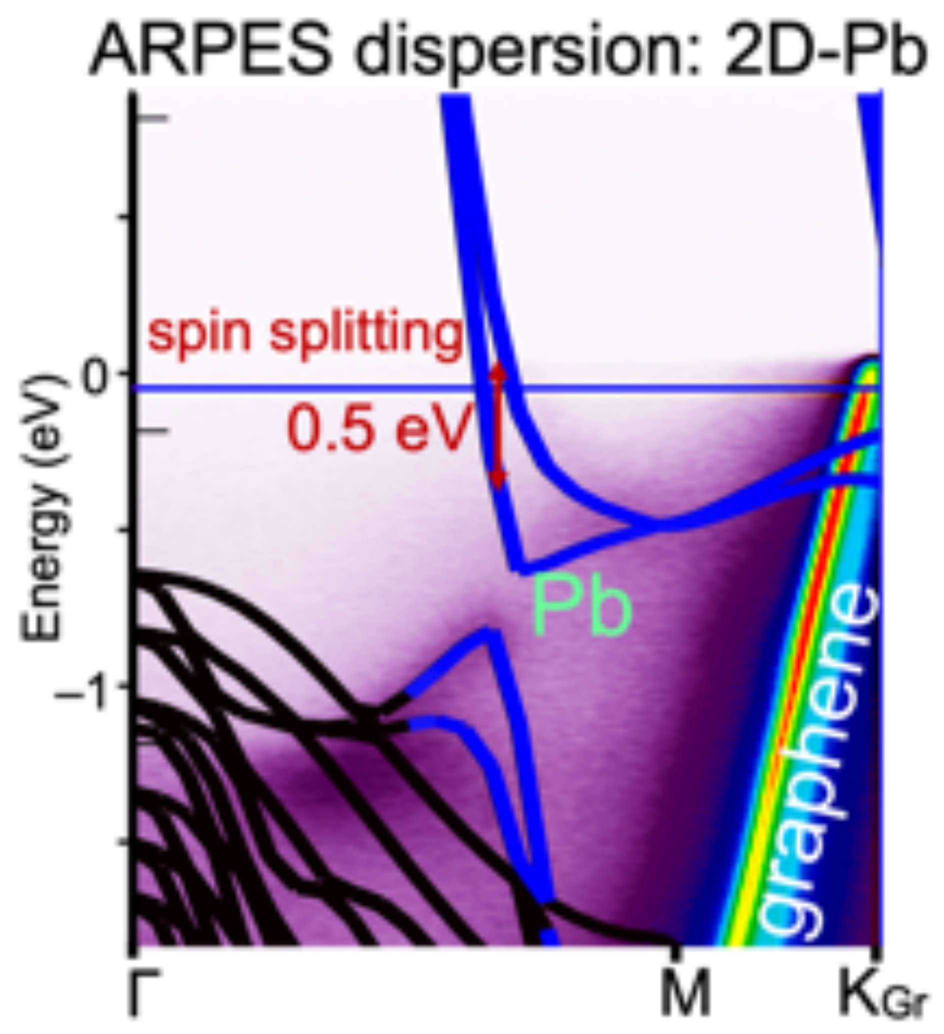


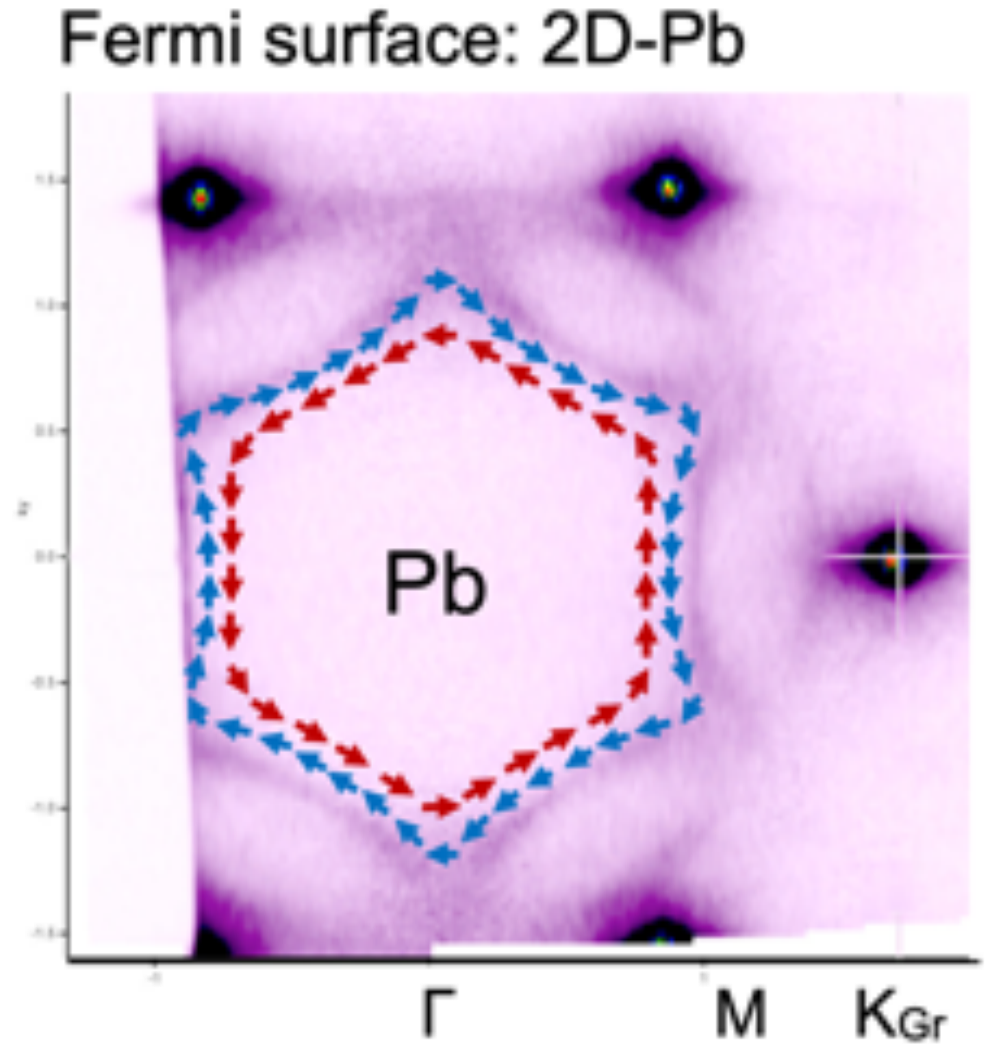
Unique electronic phenomena in 2D-Pmets

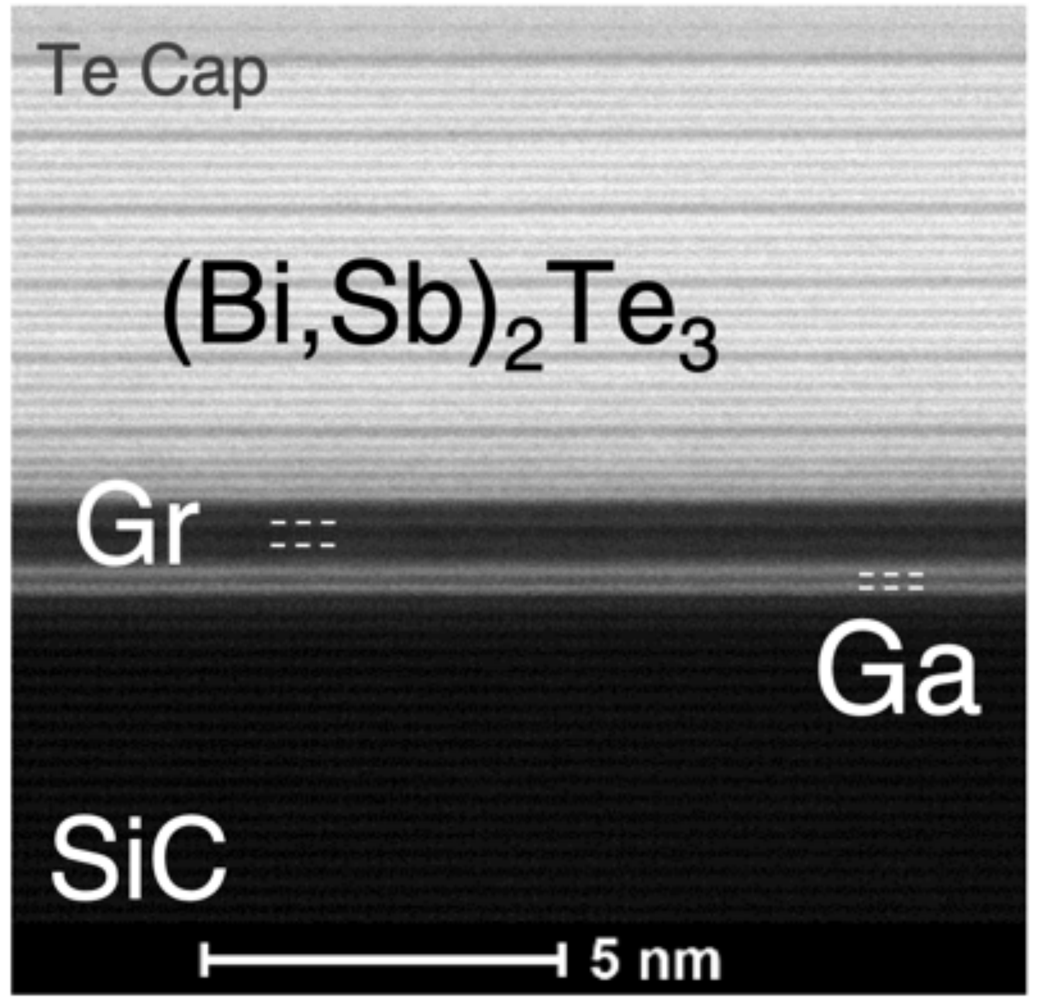
Superconductivity in few-layer Ga



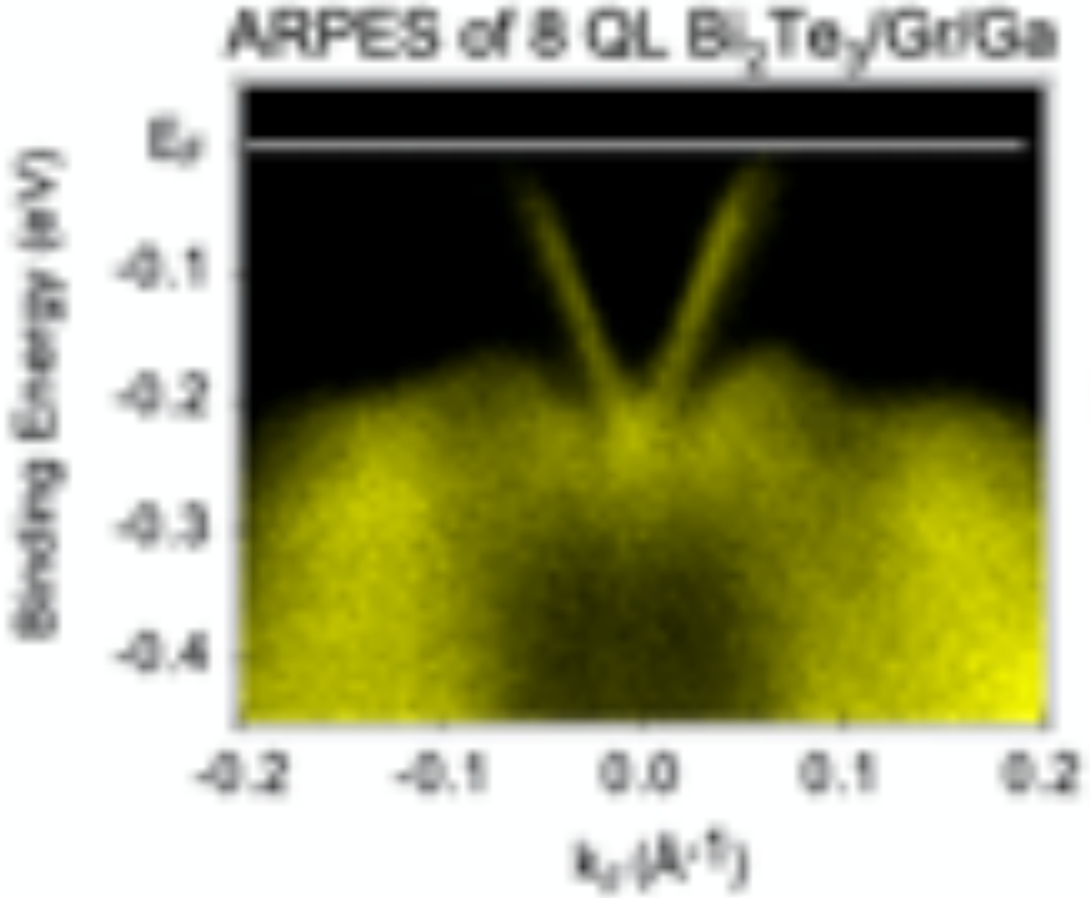
Briggs et al, Nat. Mat. doi.org/10.1038/s41563-020-0631-x (2020)

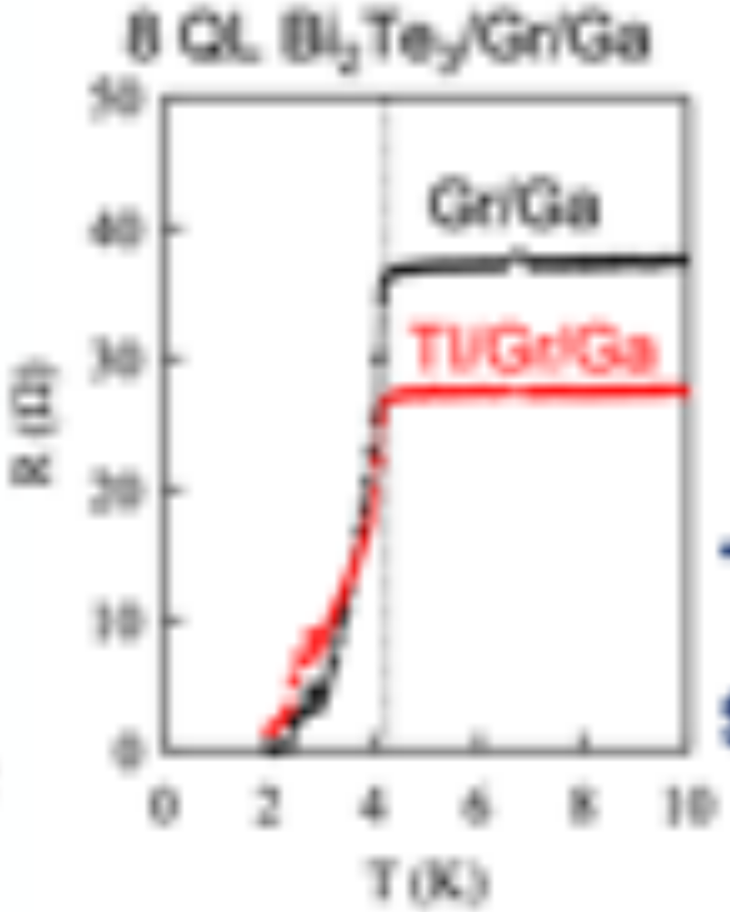






Tl/Gr/SC heterostructures



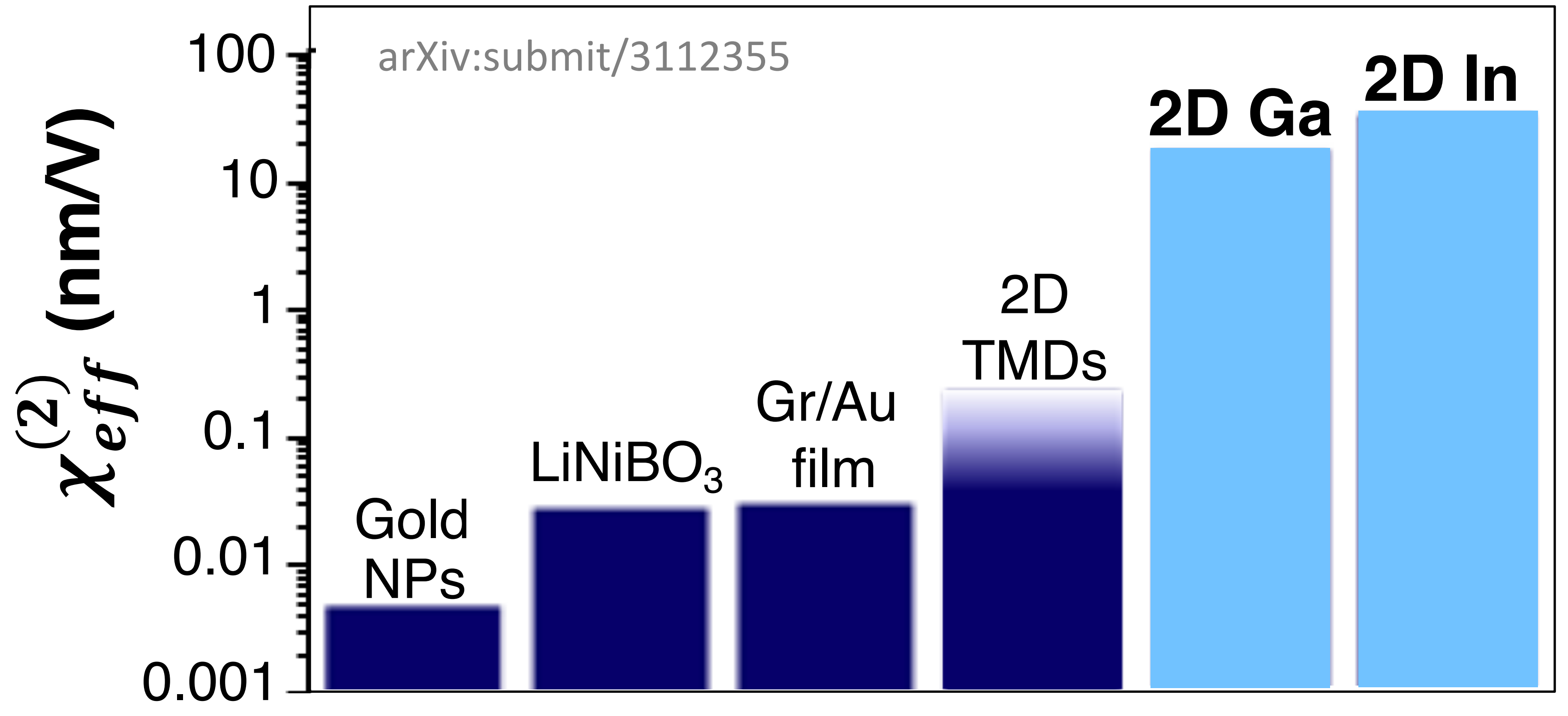


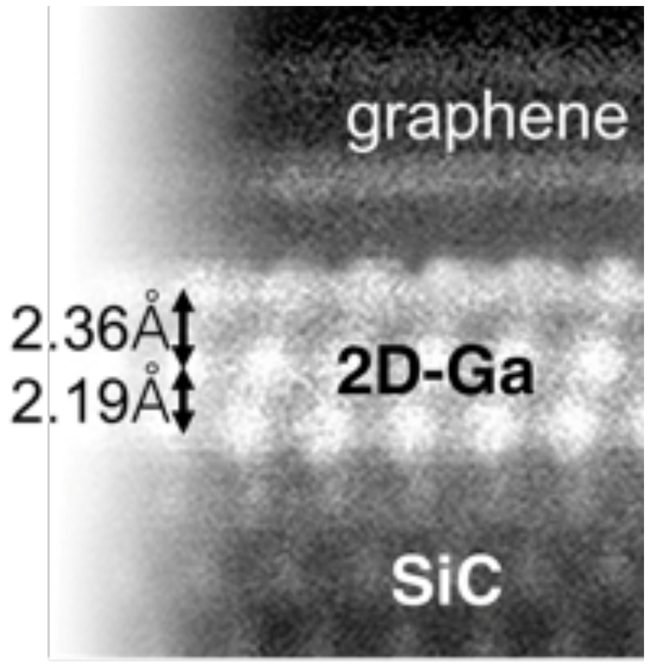
Tl growth preserves the superconductivity of Ga.

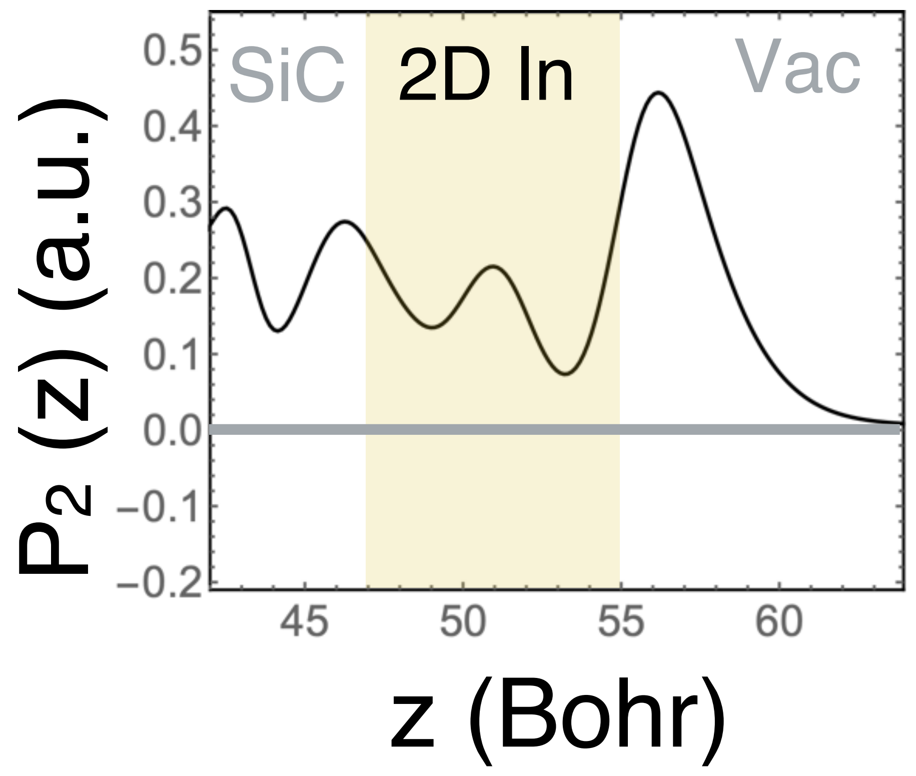
New Standards for Near-Infrared Nonlinear Optics

National Science Foundation MRSEC Materials Research Science and Engineering Centers

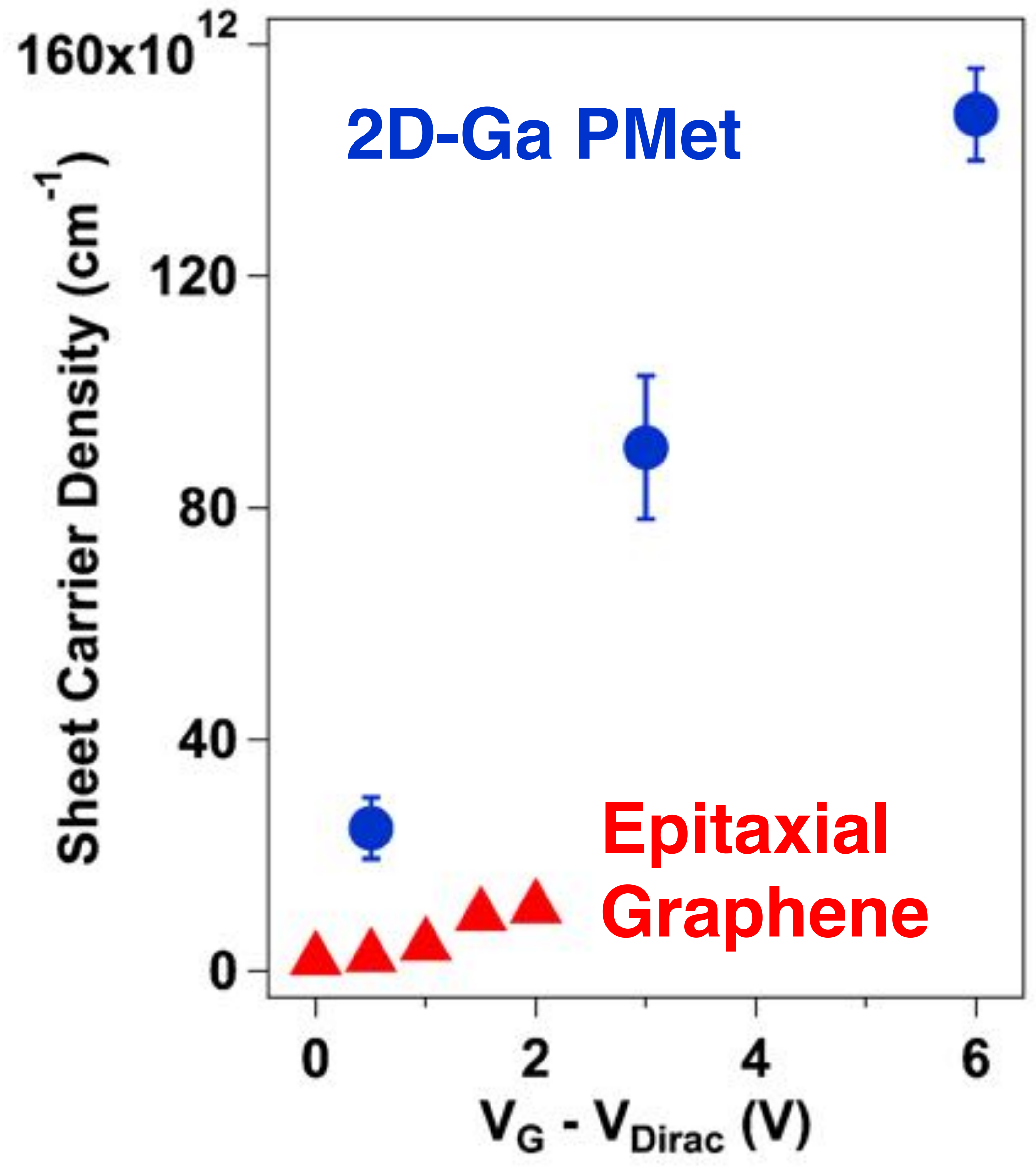
2D polar metals demonstrate the largest second-order nonlinear susceptibility ($\chi^{(2)}$) in the NIR

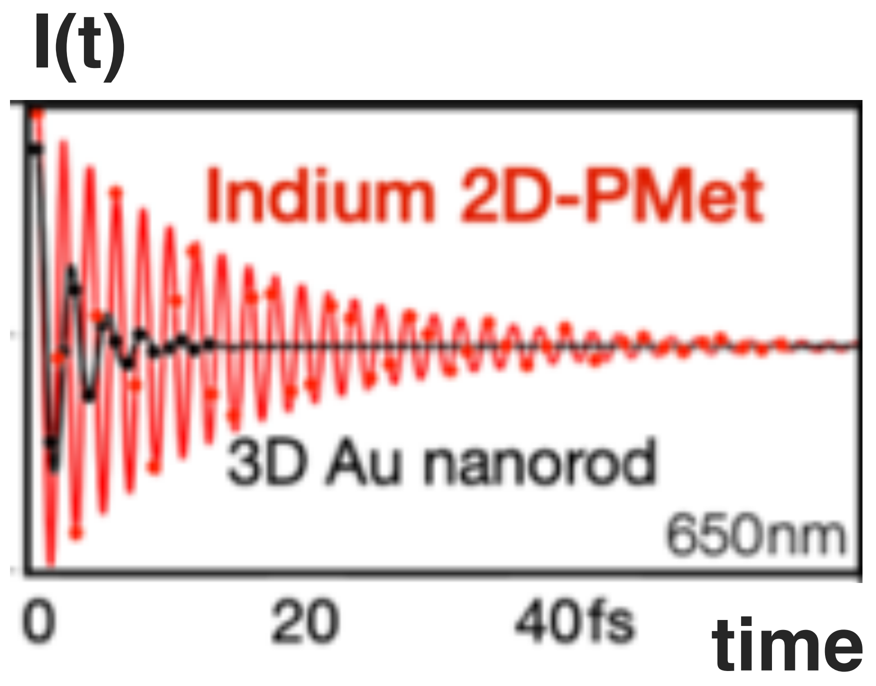


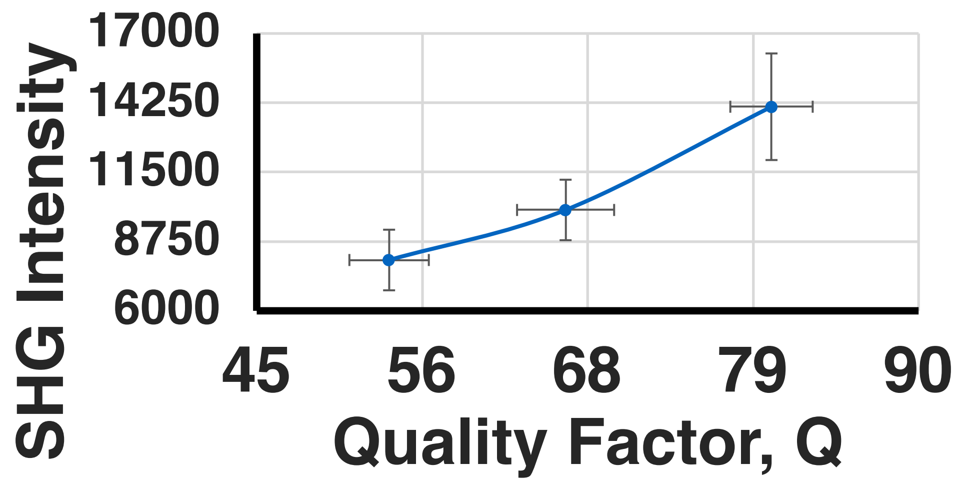




- out-of-plane symmetry breaking
- quantum confined electronic resonances in the Vis-NIR





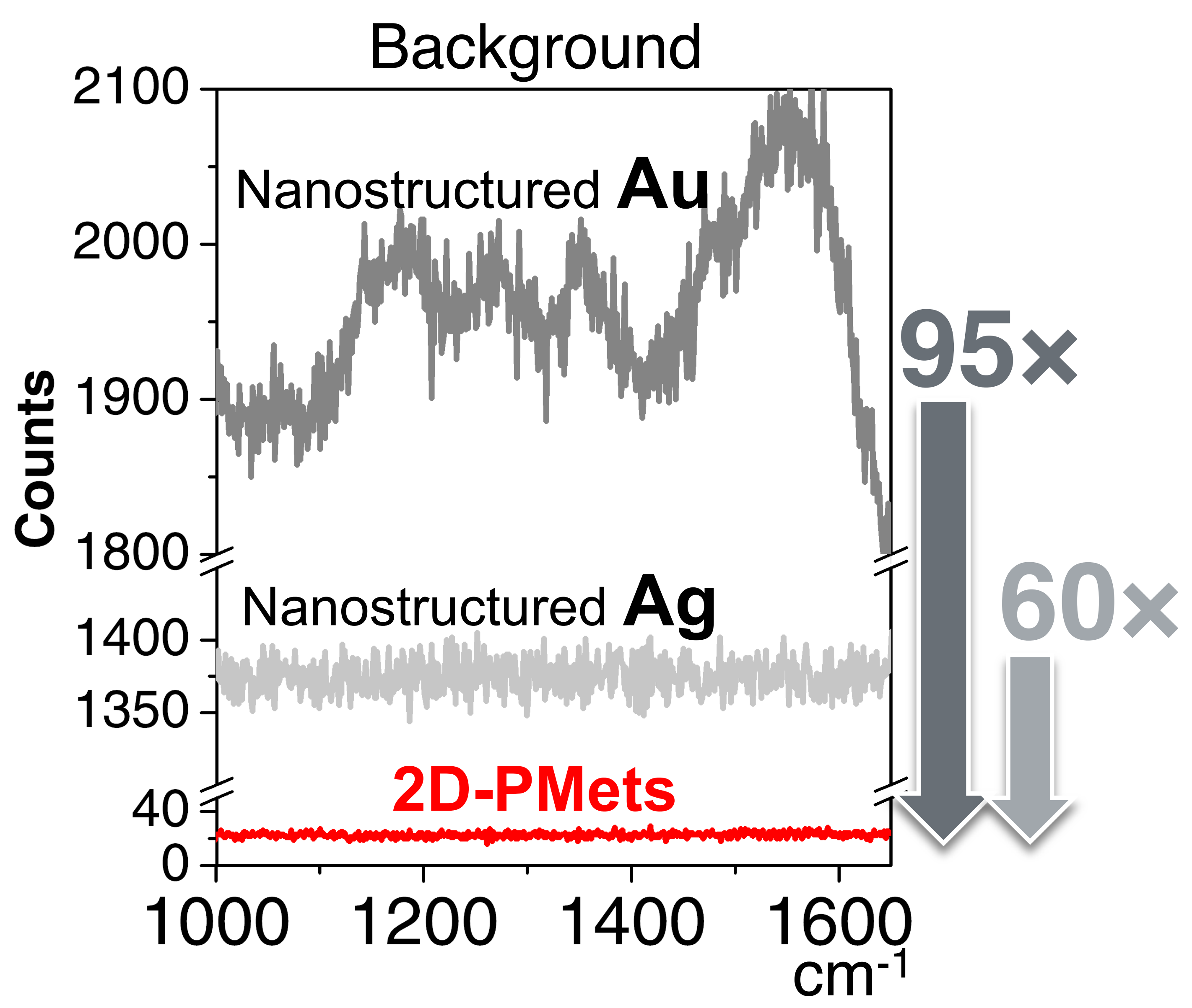


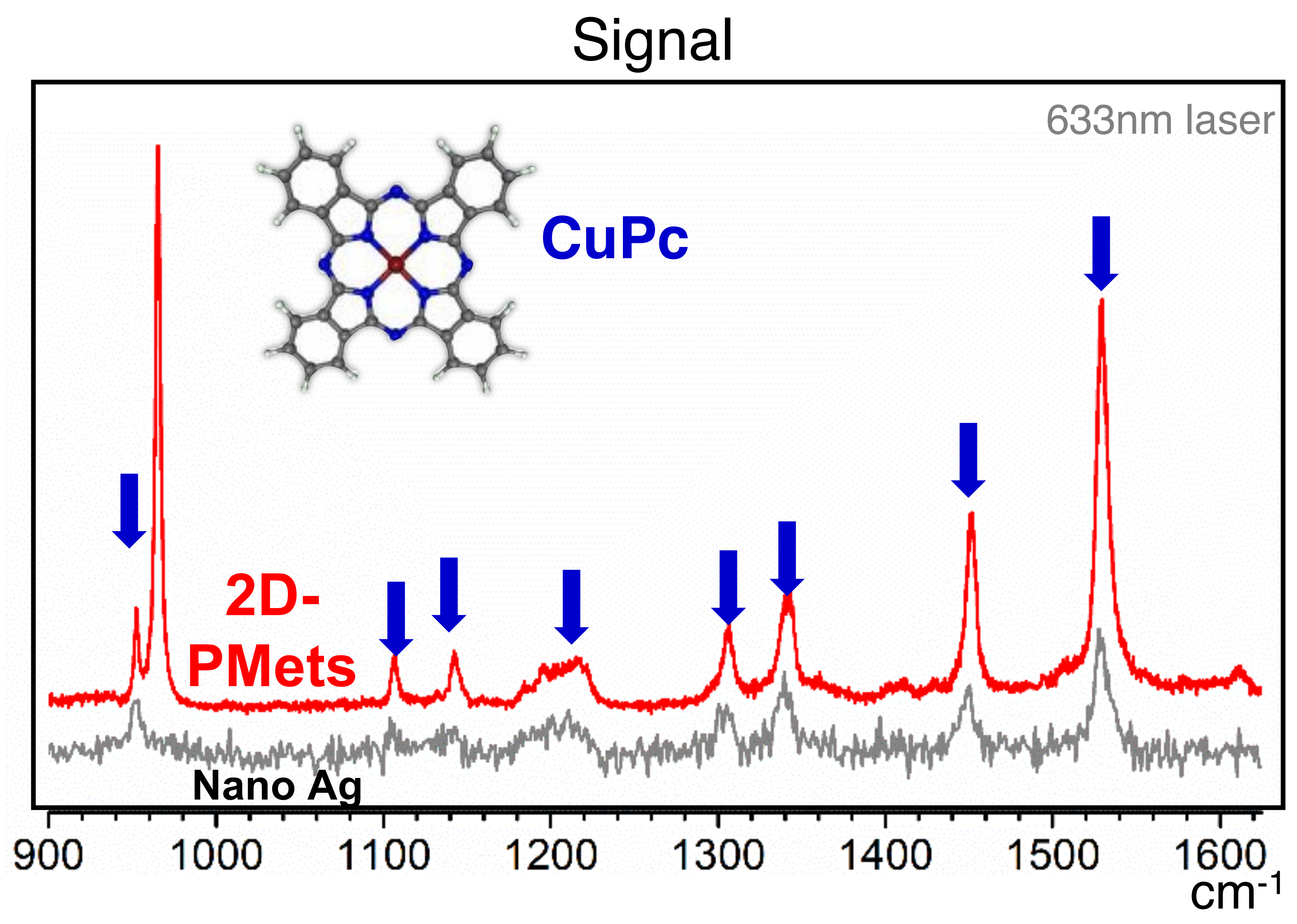
Control electronic resonances of 2D-PMets by electrolytic gating and chemical composition.

Knappenberger, Crespi, Robinson, Giebink, Fullerton-Shirey

2D-Polar Metal Enhanced Raman Spectroscopy

Traditional substrates produce large plasmon enhancement with large background, or low background with small chemical enhancement.





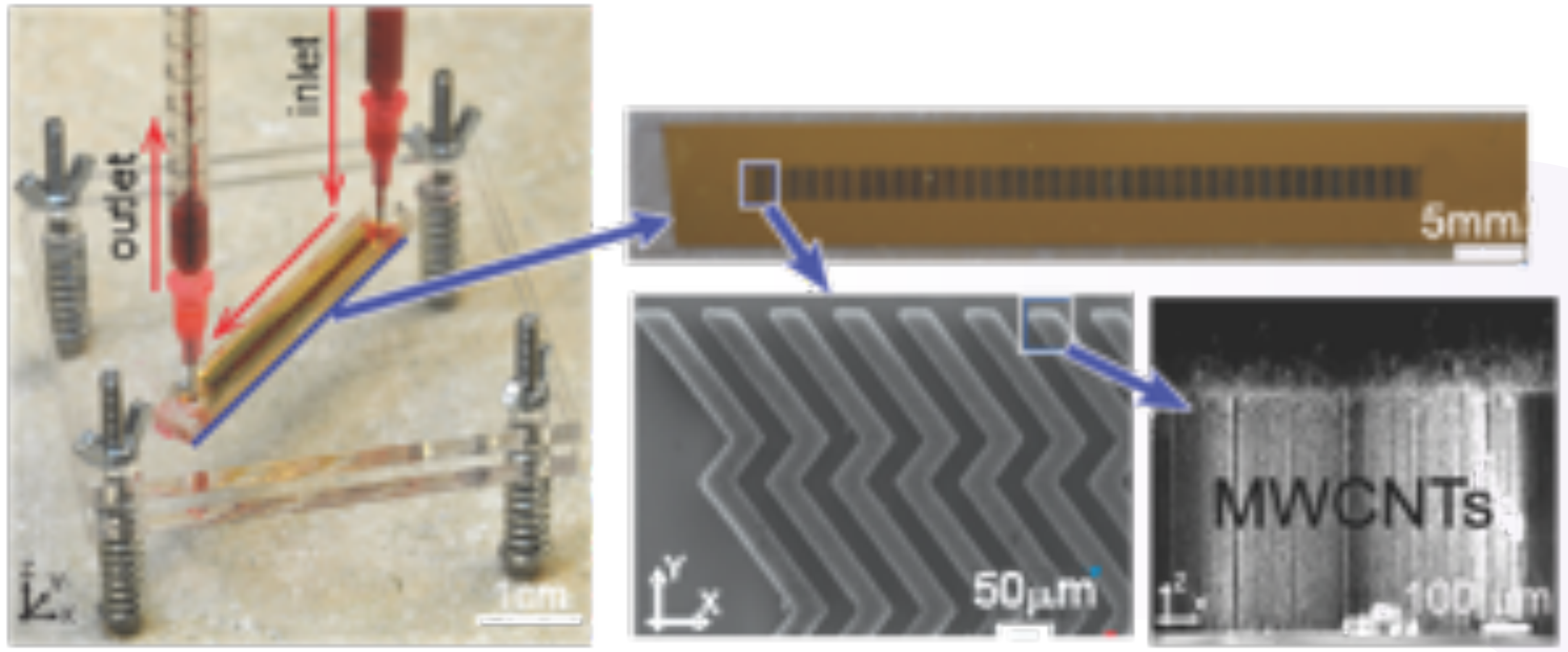
50-100× lower background
>2× stronger signal
>2× narrower peaks
>100× signal uniformity
>5× longer shelf lifetime

2D-PMets provide large Raman enhancement with low background, making them promising substrates for rapid detection of molecules with high specificity and sensitivity.

Terrones, Huang, Jensen, Robinson

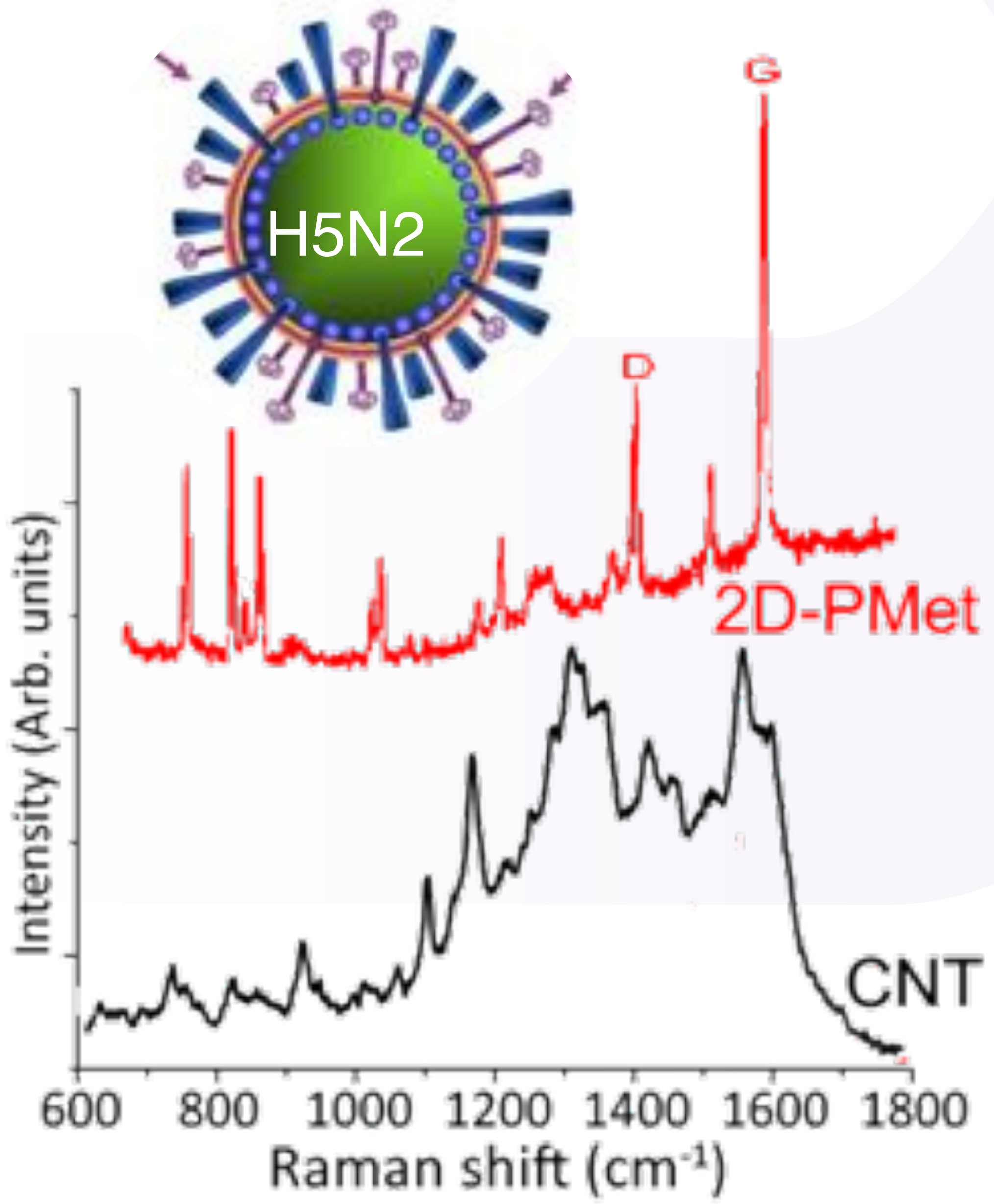
2D-Polar Metal Sensor Convergence

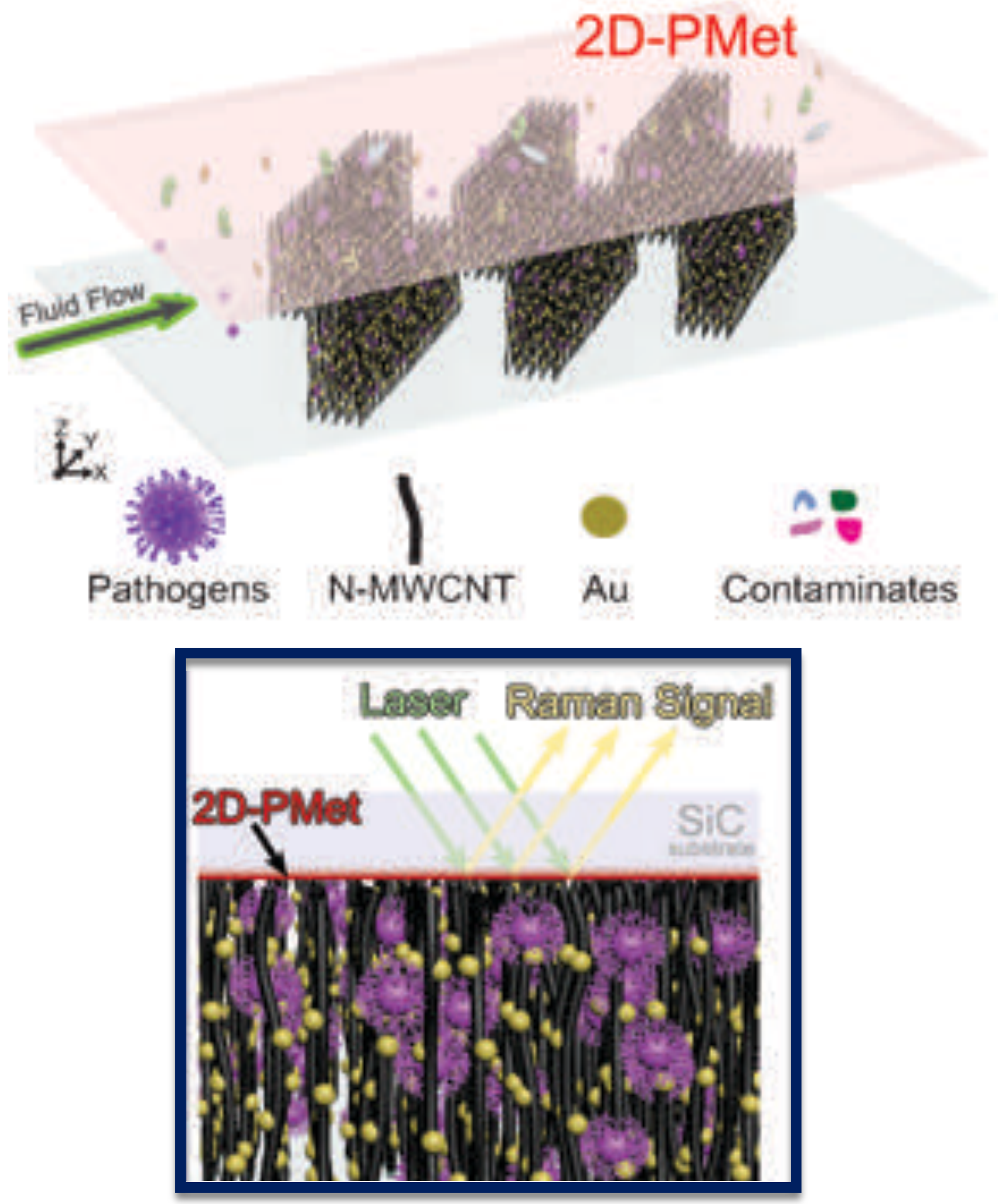
Terrones developed a **carbon nanotube-based virus concentrator**



(NSF-ECCS 1934977)

2D-PMets exhibit >10× sharper signal





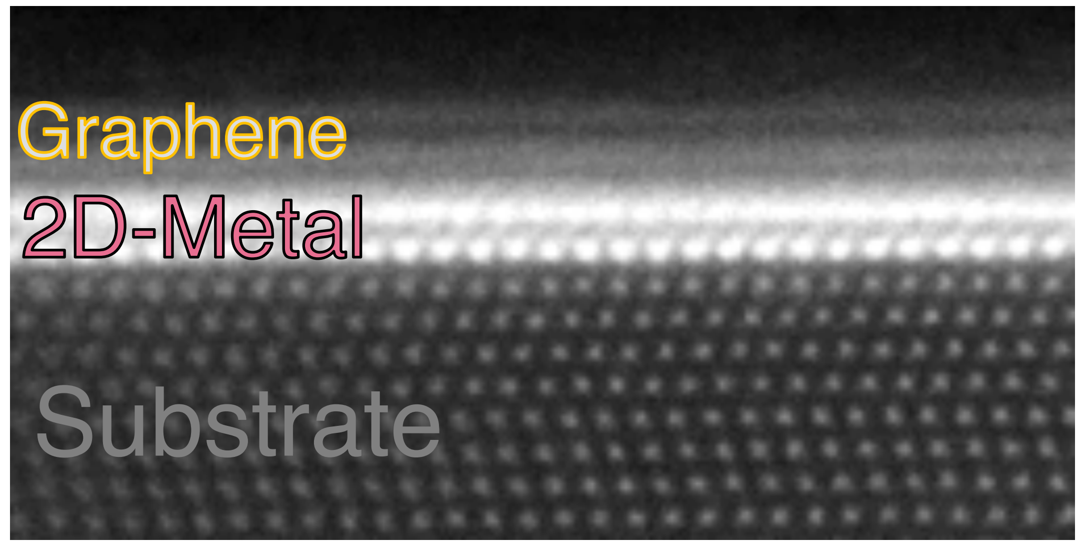
Real-time detection of viruses and molecules with high sensitivity and specificity.

Terrones, Robinson, Huang (with NSF-ECCS 1934977)

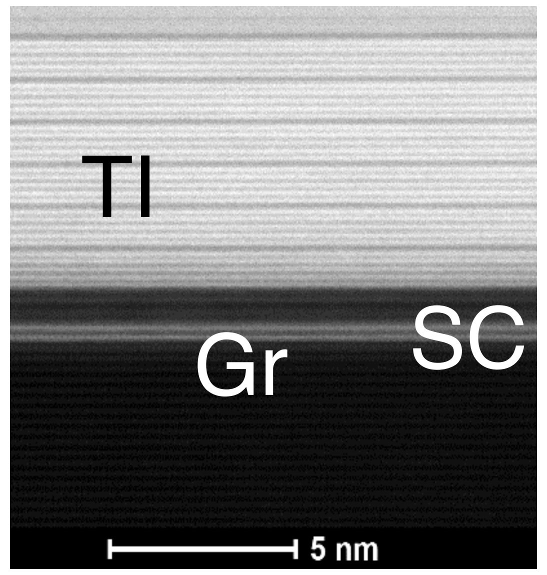
What is success?

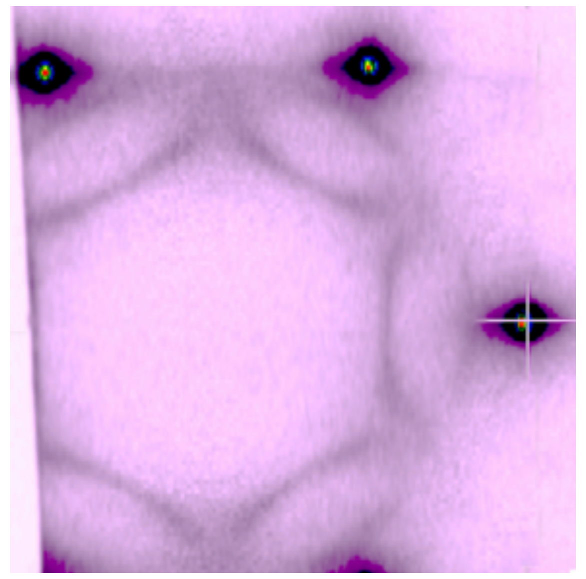
National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

Establish a large family of air-stable 2D polar metals, alloys and heterostructures at the wafer scale.

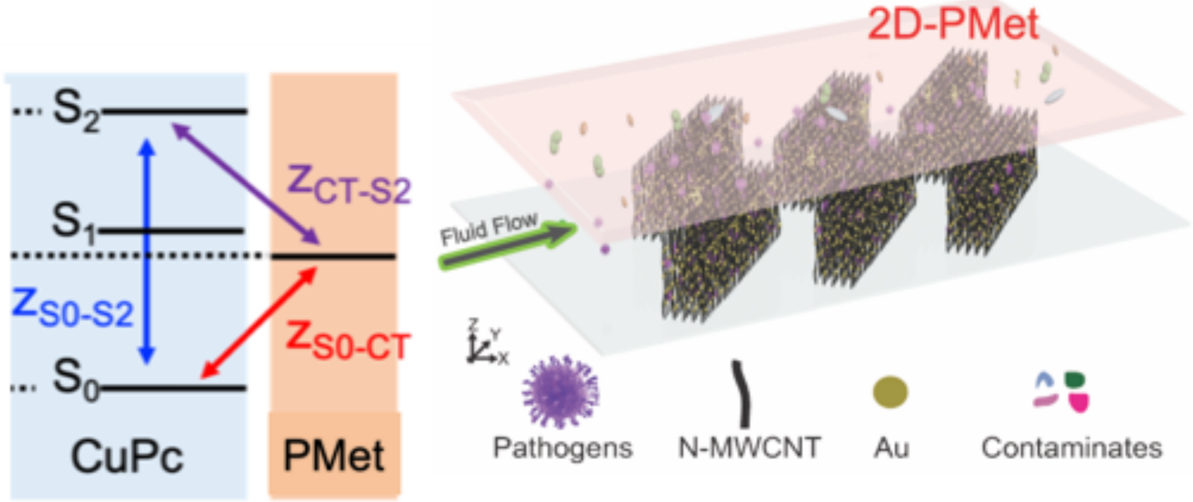


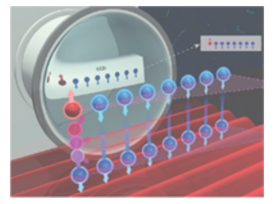
Discover new fundamental phenomena and achieve topological superconductivity in TI/Gr/SC heterostructures.





Achieve state-of-the-art nonlinear optical performance in the NIR and establish Raman sensing with high sensitivity and specificity.



 Quantum Leap

 Growing Convergence

 Rules of Life

 Harnessing Data

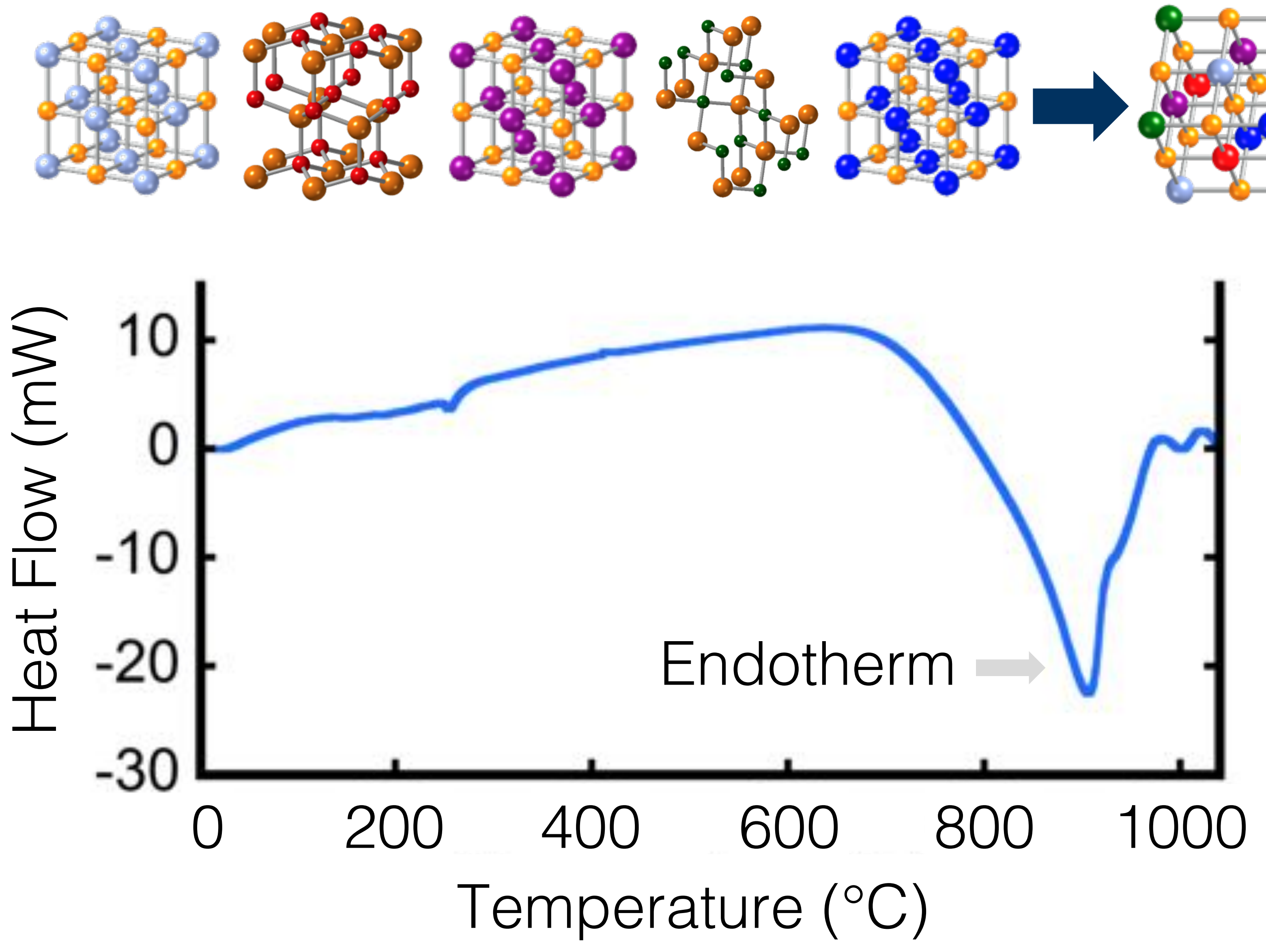
National Science Foundation MRSEC Materials Research Science and Engineering Centers

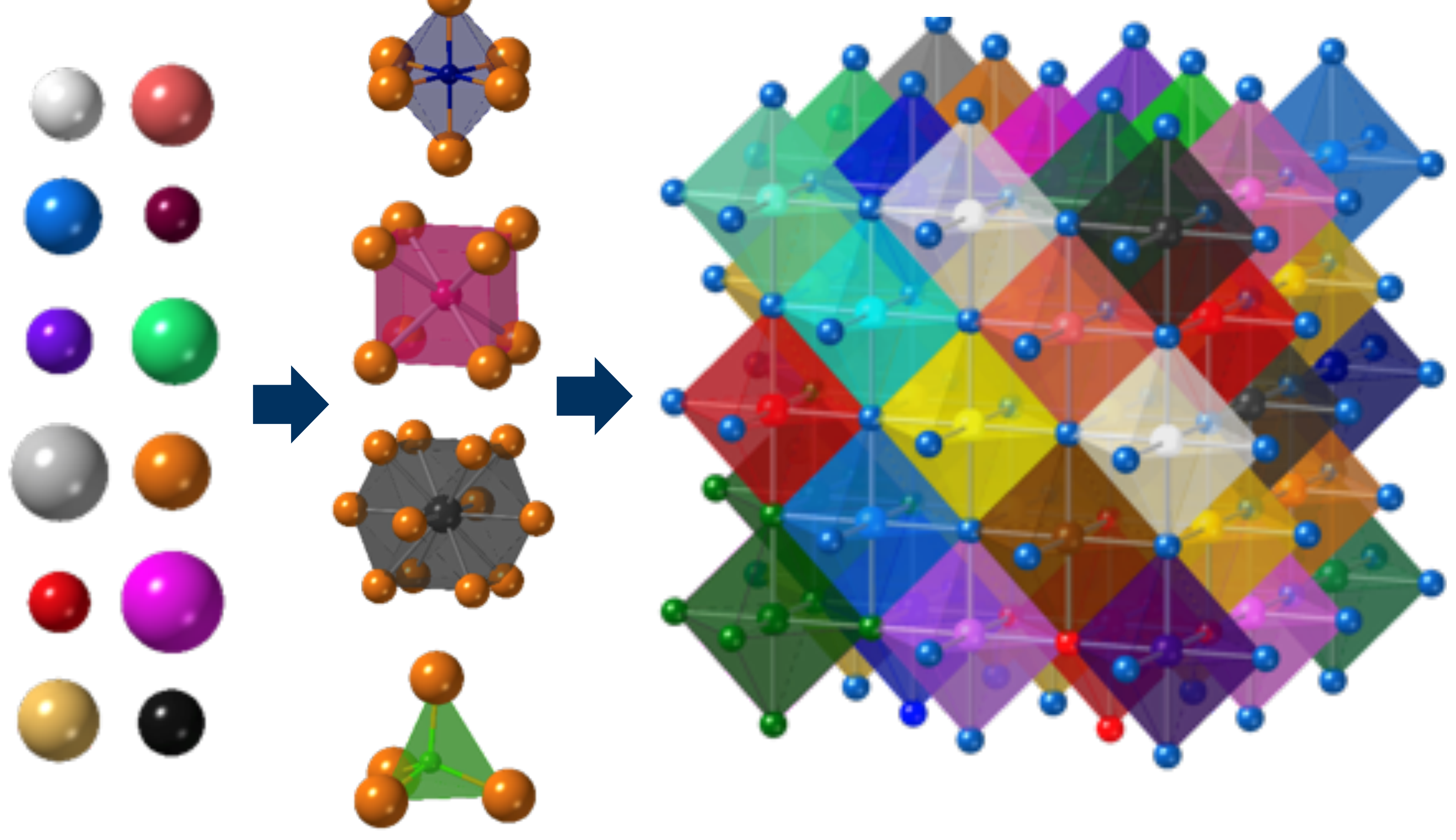
Center for Nanoscale Science

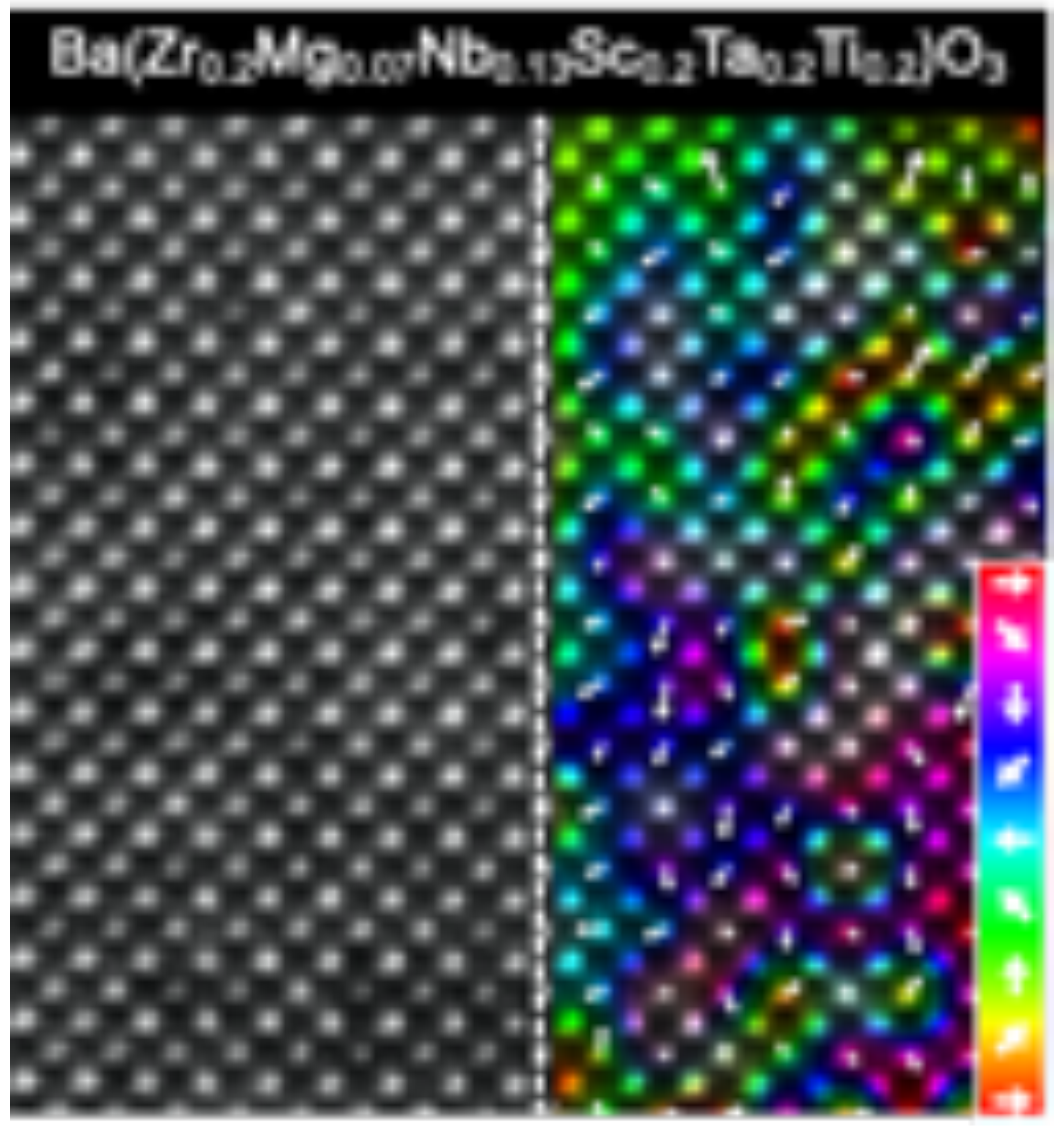
IRG 2

Crystalline Oxides with High Entropy

Co-leads: Jon-Paul Maria, Ismaila Dabo



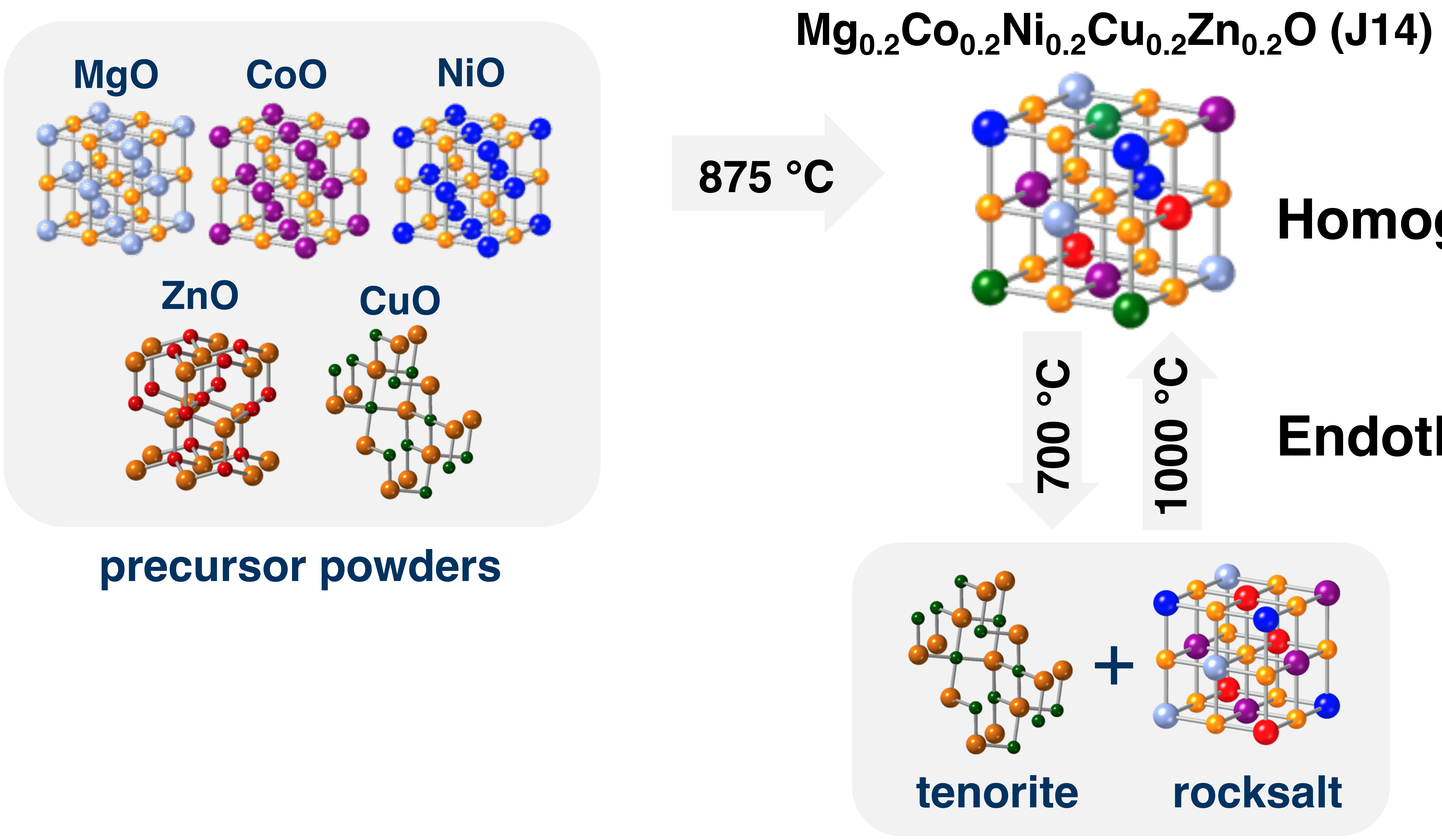




Proof for Entropic Stabilization

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

In 2015 **entropic stabilization** was demonstrated in complex oxides…



Homogeneous solid solution

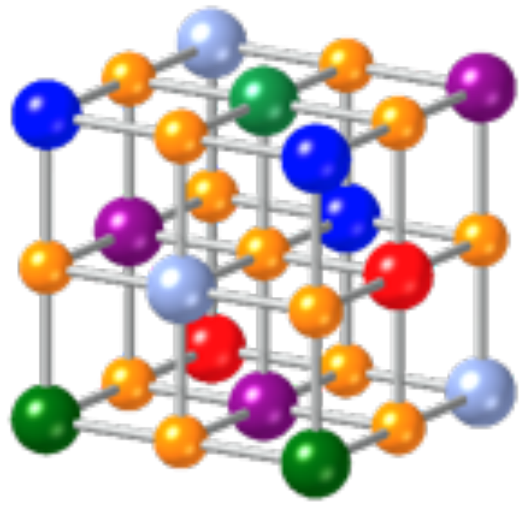
Endothermic & Reversible transition

Penn State researchers demonstrated new phases stabilized by entropy. This stimulated a vibrant and growing international body of work on oxides, nitrides, sulfides, silicides, and carbides.

Maria Group: Nat Comm., Sep 29 (2015)

Defect Chemistry in High Entropy Crystals is Complex, Unusual and Unexplored

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers



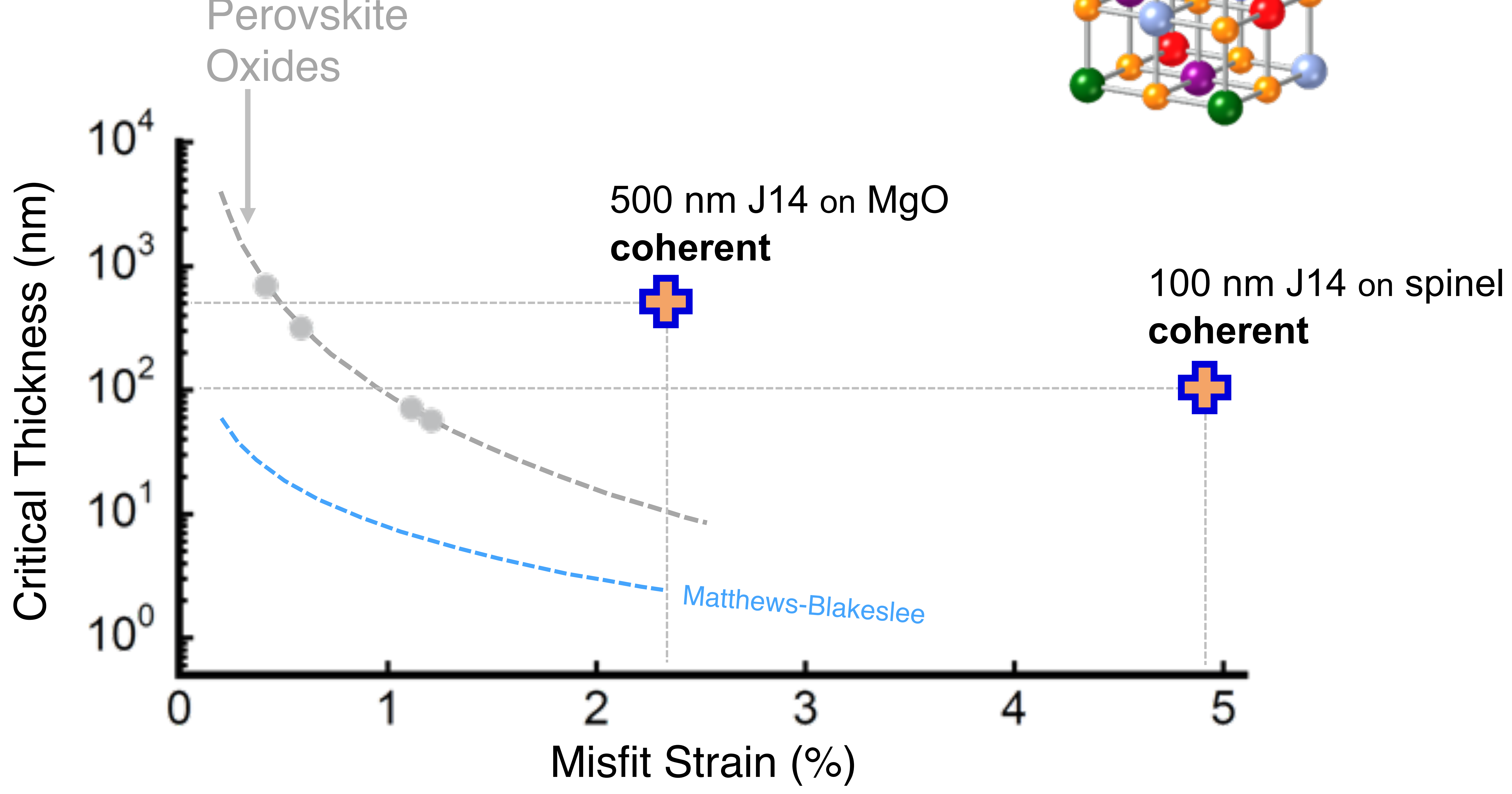
Large doping distortions

Modified oxidation

Huge relaxation thickness

Ease of synthesis

Each observation is related to the host crystal's entropy budget



The distortions, oxidation, crystalline fidelity, and relaxation resilience are without precedent. The science relating them to the "entropy-budget" will be exciting to uncover and understand.

Chen *et al.*, APL 91, 252906 2007

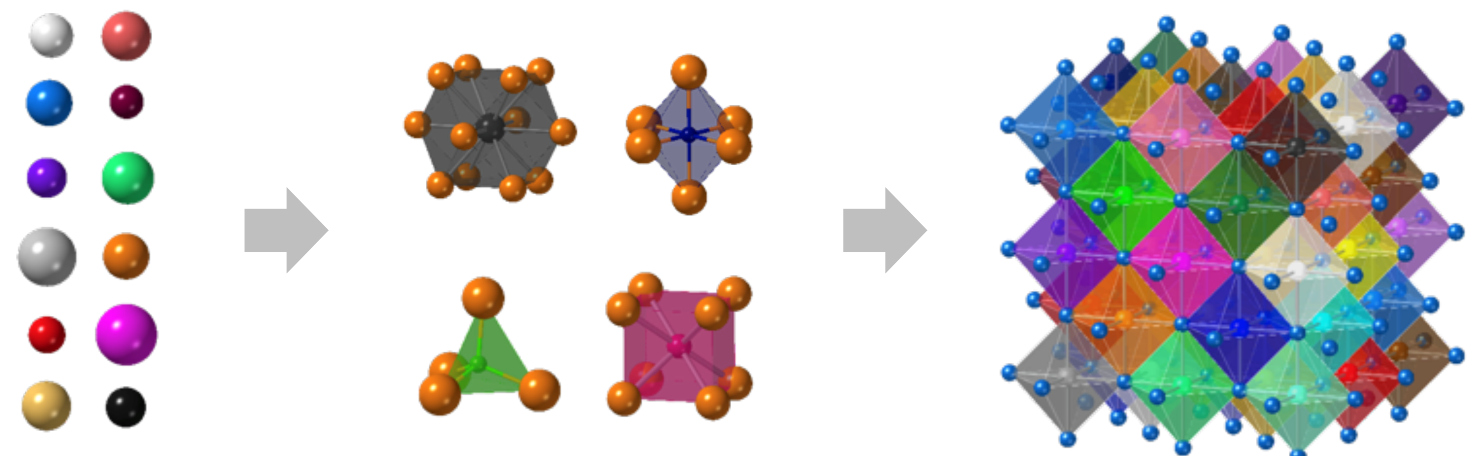
Meisenheimer *et al.*, Scientific Reports volume 7, Article number: 13344 (2017)
Meisenheimer *et al.*, Phys. Rev. Materials **3**, 104420, 28 October 2019

Trolier-McKinstry, Alem, Chen, Engel-Herbert, Gopalan, Rost

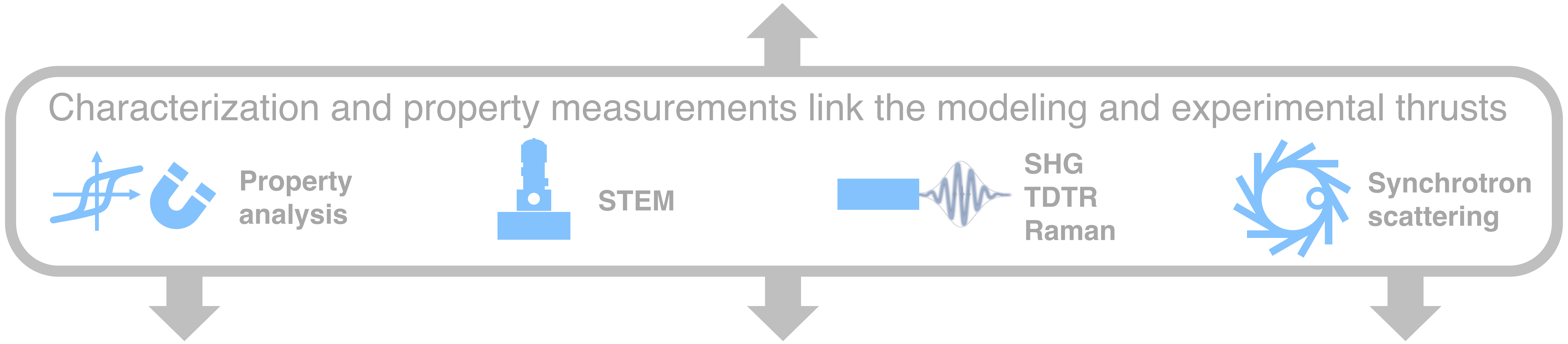
IRG 2: Team and Expertise

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

T1: Multiscale models that capture combinatorial complexity



I. Dabo
L-Q. Chen
V.H. Crespi
S.B. Sinnott
S. T-McKinstry



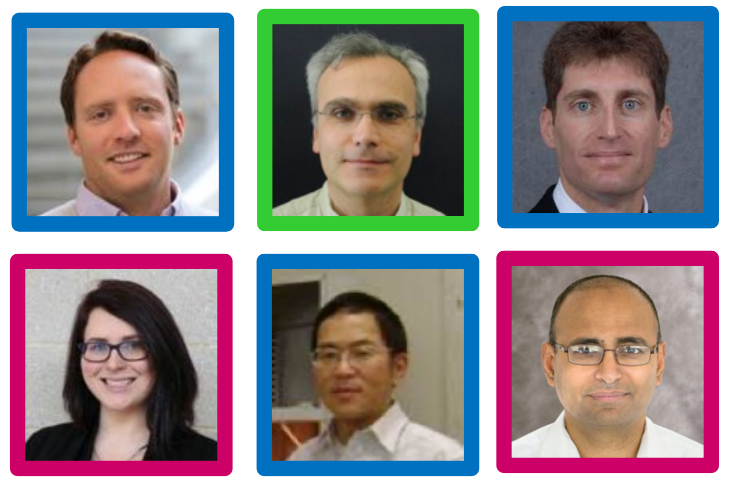
T2: Transport properties in high entropy crystals

R. E-Herbert, N. Alem, L-Q. Chen, I. Dabo, J-P. Maria, S. Sinnott

T3: Entropy engineered distortions and symmetry

S. T-McKinstry, N. Alem, L-Q. Chen, V. Gopalan, R. E-Herbert, C.M. Rost

T4: Entropy, solubility, e⁻ correlation and magnetism



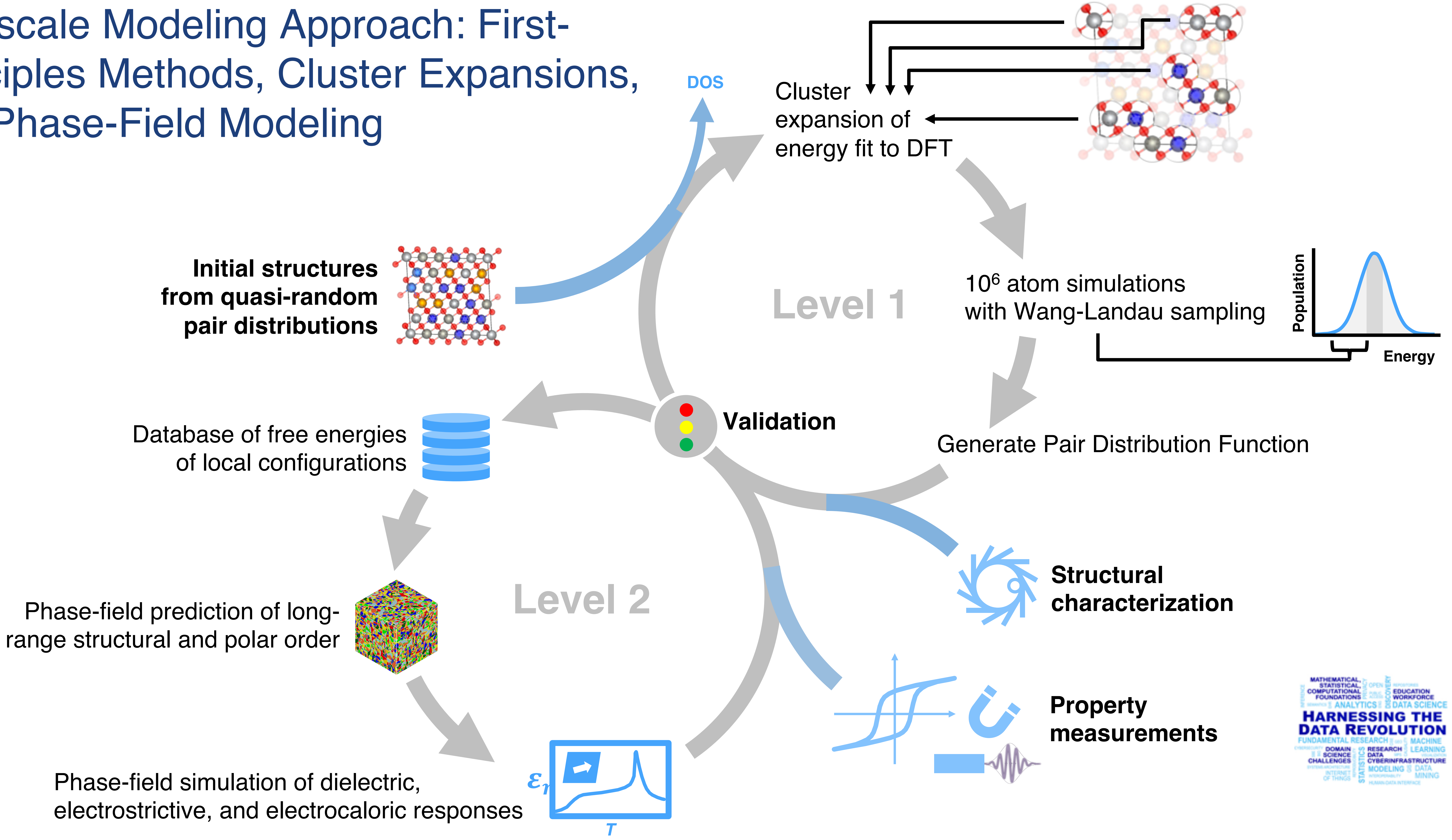
J.T. Heron, V.H. Crespi, J-P. Maria, Z. Mao, V. Gopalan, C.M. Rost

Theory/computation
First-principles methods
Cluster expansions
Phase-field modeling
Monte Carlo sampling

Characterization
STEM & Synchrotron scattering
Non-linear optics
Electromechanical properties
Magnetic properties

Synthesis
Sputtering
Laser ablation
Molecular beam epitaxy
Single crystal growth
Bulk ceramics

Multiscale Modeling Approach: First-Principles Methods, Cluster Expansions, and Phase-Field Modeling



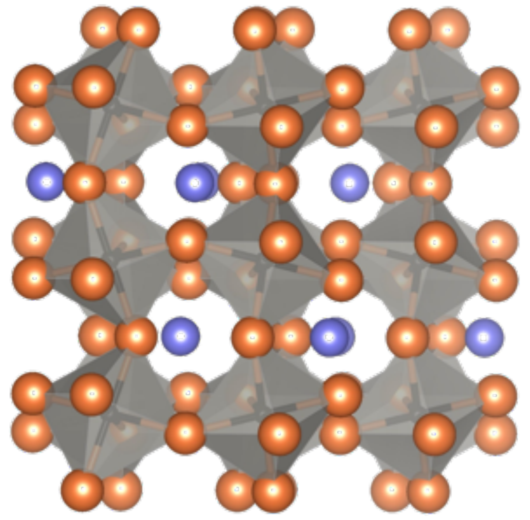
Dabo, Alem, Chen, Crespi, Maria, Rost, Sinnott, Trolier-McKinstry

Overcoming Limits of UV-Transparent Conductors

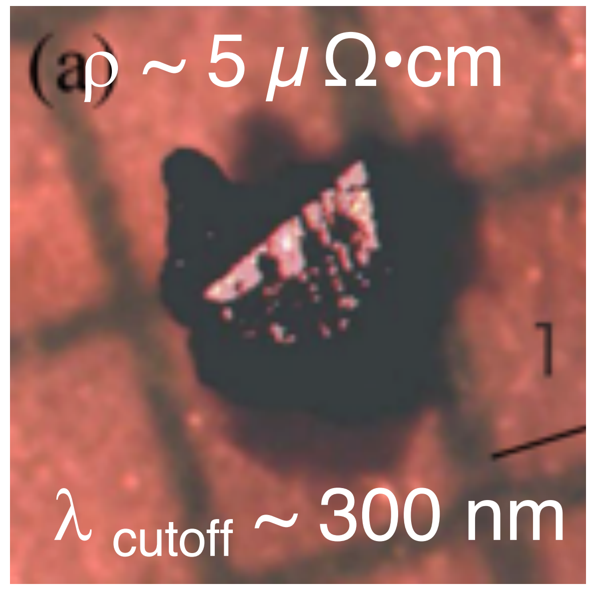
National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

Opportunity: Realize metallic molybdate and tungstate perovskites using configurational entropy; these are necessary and enabling materials for **ultra-violet optoelectronic** systems.

$Sr_{1-\delta}MoO_3$ & $Sr_{1-\delta}WO_3$
unstable as ABO_3



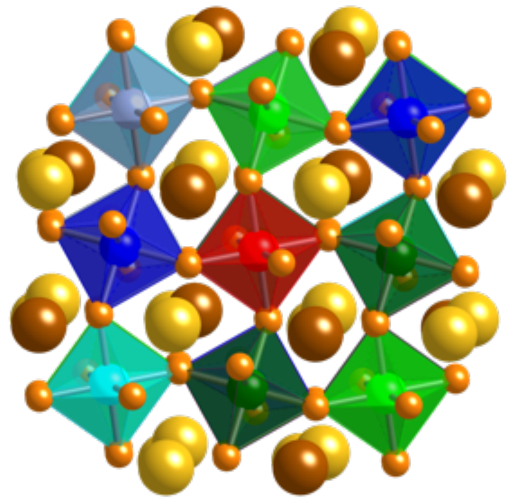
Heroic efforts to stabilize



Metastable ABO_3
2000 K + 10^{-25} pO_2

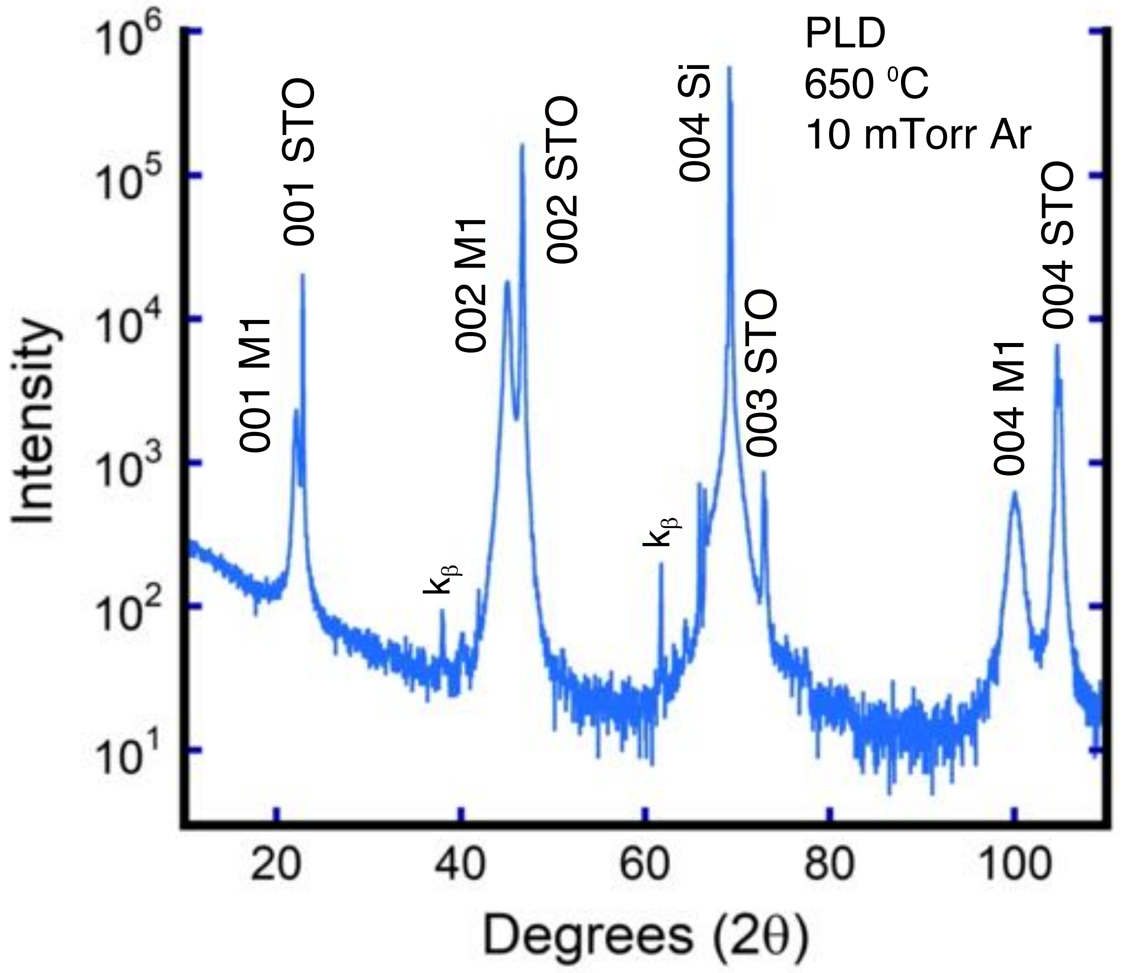
Propose high entropy solution:
$(Sr,Ca,Ba,La)_{1-\delta}(W,Mo,Ta,Nb,Ti,V)O_3$

High *TS*



B-site for maximum valence e^-
A-site to compensate ΔH^{mixing}
Theory informed composition

$Sr(V_{0.2}Nb_{0.2}Mo_{0.2}W_{0.2})O_3$



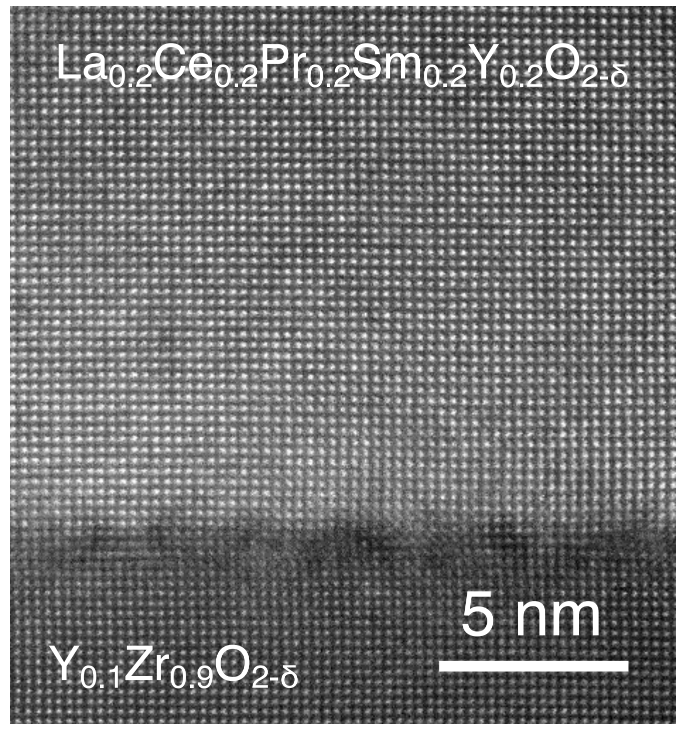
ρ < 150 μ Ω · cm

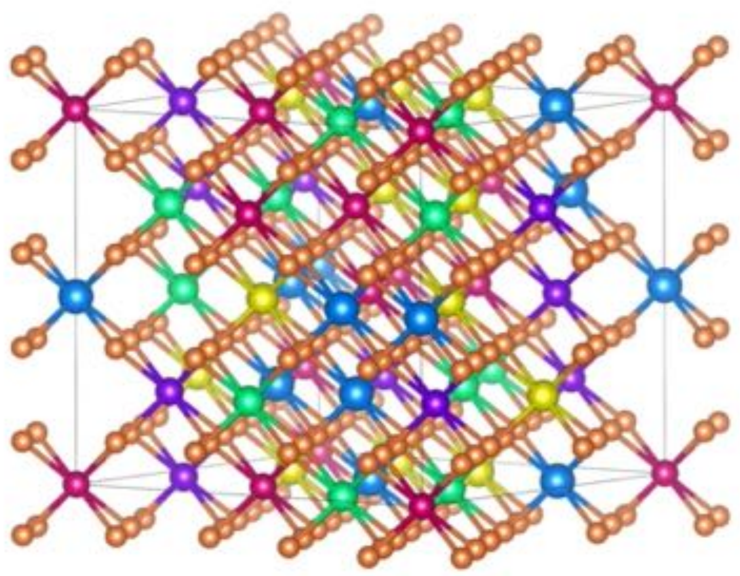
With minimal investment, preliminary experiments support the structure hypothesis, 150 $\mu\Omega\cdot$cm is a **very low** resistivity for perovskite oxide conductors. As with other high entropy systems, growth is straightforward.

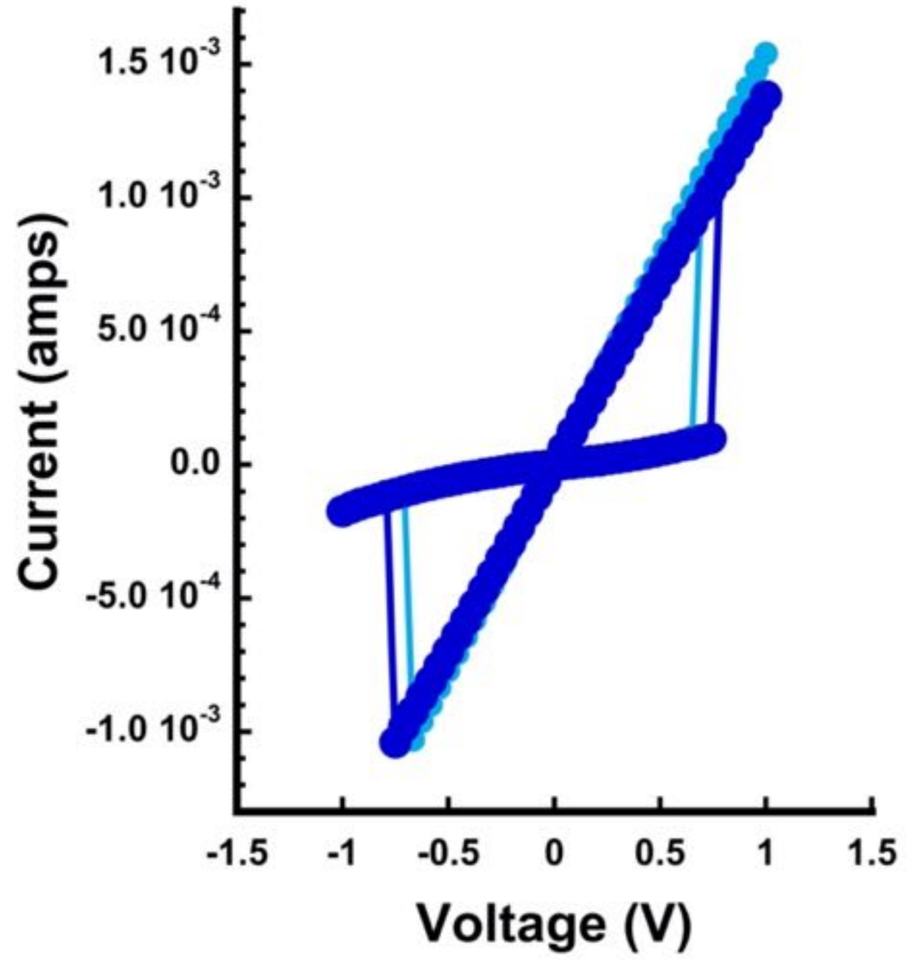
Engel-Herbert: Nat. Mat., v 15, Feb 2016
Radetinac, Journal of Applied Physics **119**, 055302 (2016)

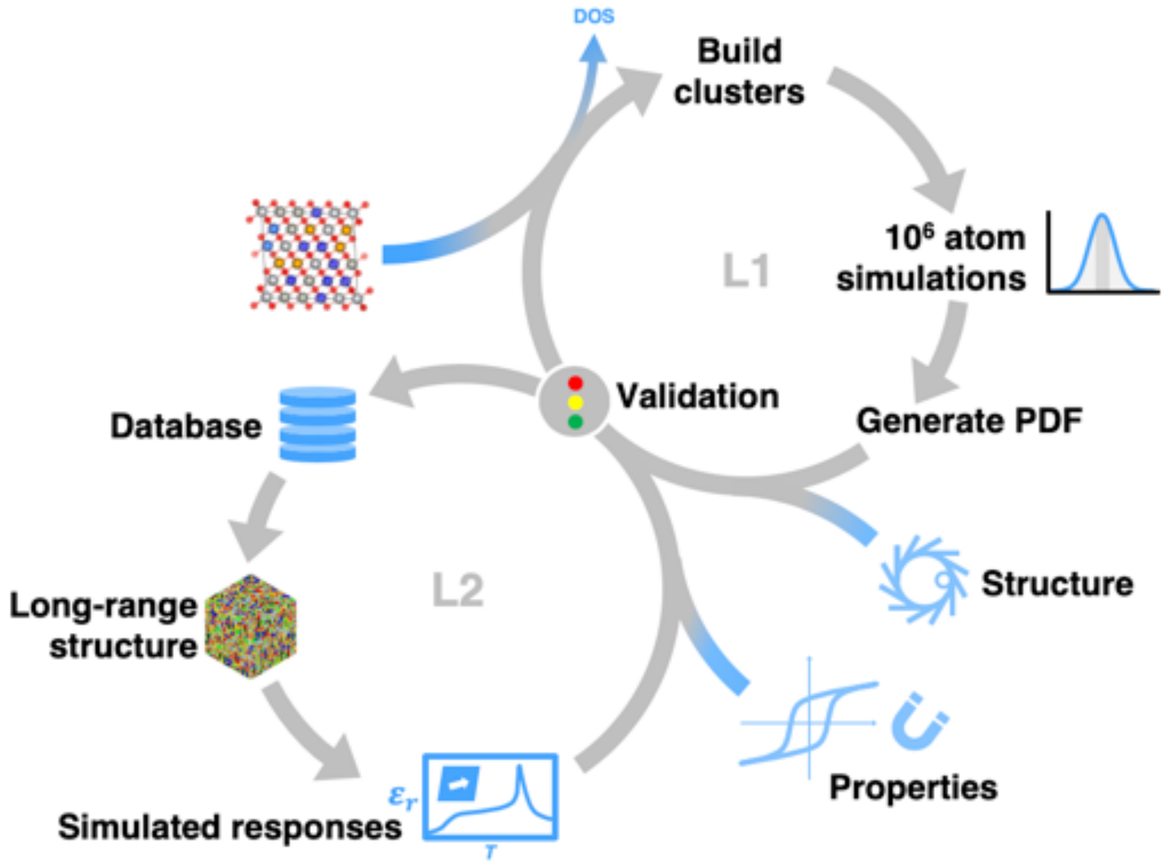
Engel-Herbert, Alem, Chen, Dabo, Maria, Sinnott

Closed-Loop Materials Discovery of Fast Ion Conductors





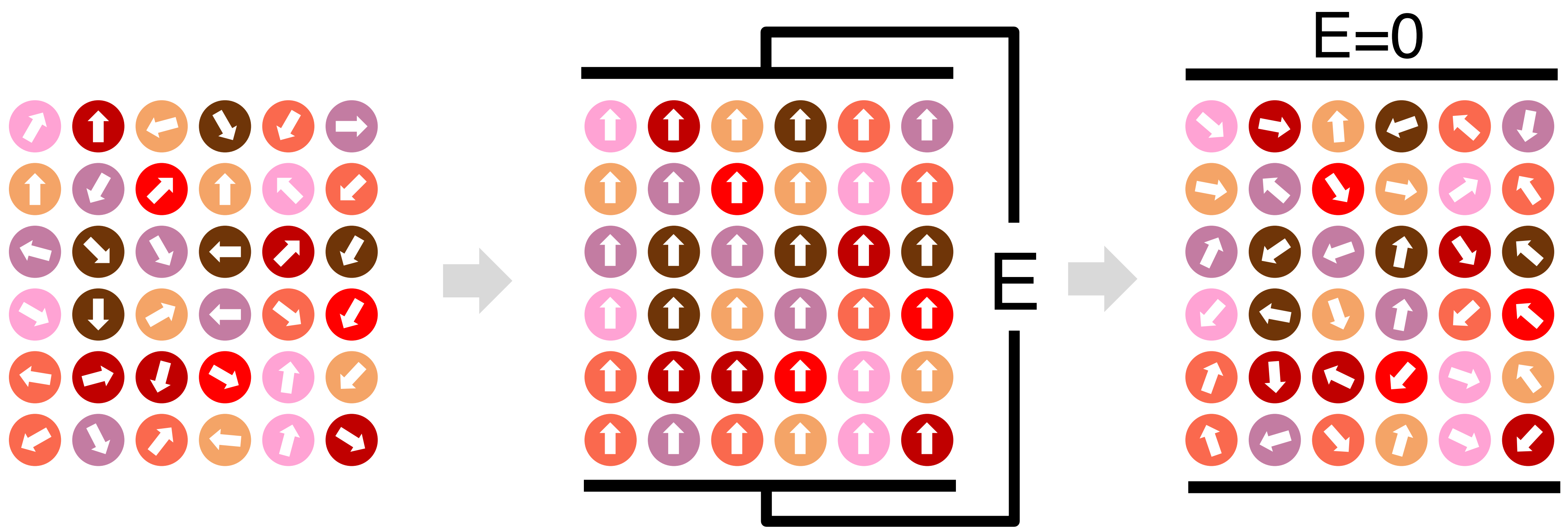




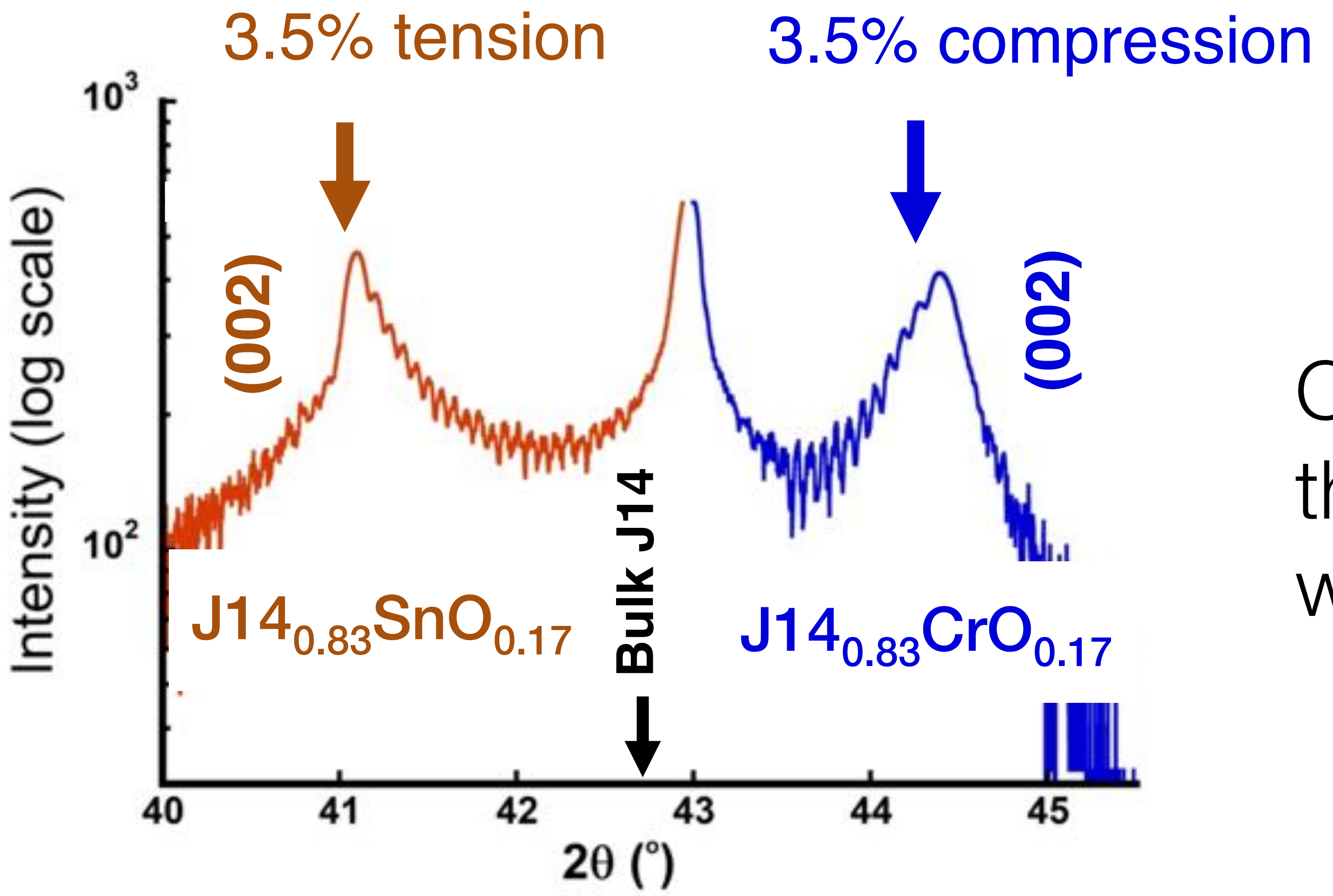
Entropy Control of Dipole Coupling for Electrocaloric Effects

(Ba,Sr,Pb,Bi)(Sn,Nb,Hf,Ti)O_3

Enormous atomic polarizability, weak dipolar coupling



Metal-Insulator Transitions Enabled by Entropy



Can chemically strain the J14 lattice by **7%** with substitution

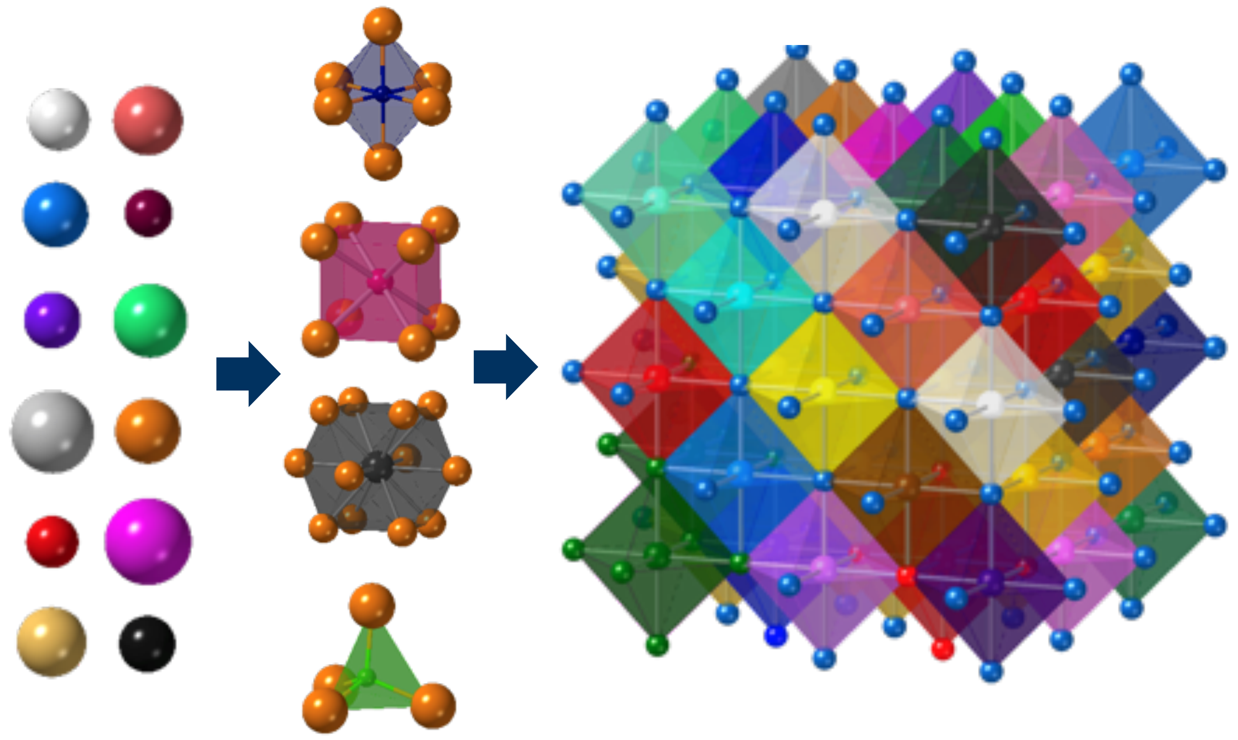
What is Success?

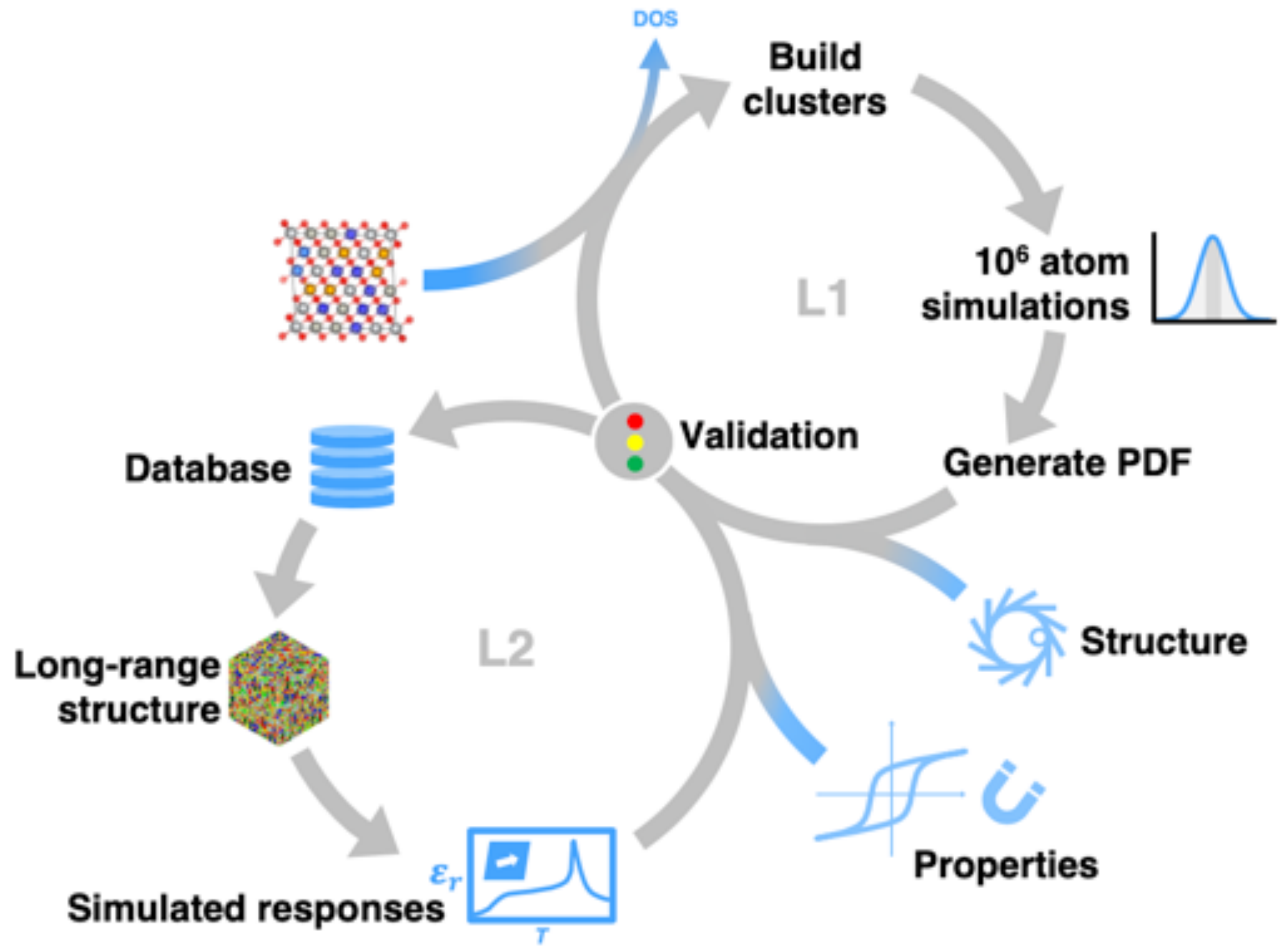
Understand composition-structure-property relationships for high entropy oxides.

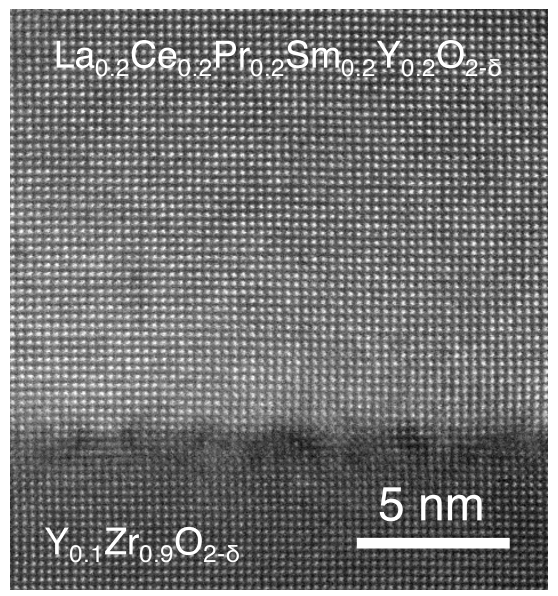
Create a multiscale theory engine for combinatorially complex systems that link atomistic, intermediate, and long-range phenomena.

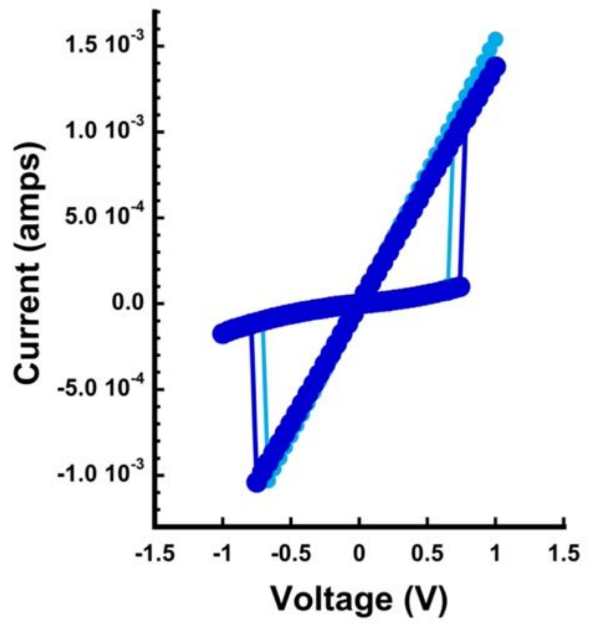
Discover new materials that exhibit transformative dielectric, magnetic, and transport properties.

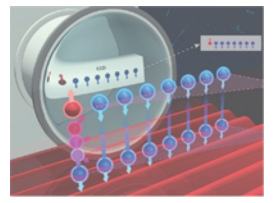
Establish design principles for high-entropy materials that can be extended beyond oxides.









 Quantum Leap

 Harnessing Data

Education, Outreach & Diversity

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

Partnerships for Research & Education in Materials

North Carolina Central Univ.

Cal State Univ. Los Angeles

Sustainability

Teams and Leadership Development

DIY Digital Platform

Cal State LA partnership

15 Collaborating Faculty
& Research Staff

multi-year/on-going collaboration

facility staff

Faculty/ staff visits	**PSU→CSULA**	**CSULA→PSU**
2016	3	1
2017	4	3
2018	8	3
2019	4	8
	19	15

10 Collaborating Faculty

student advisors

facility users

Summer student researchers:

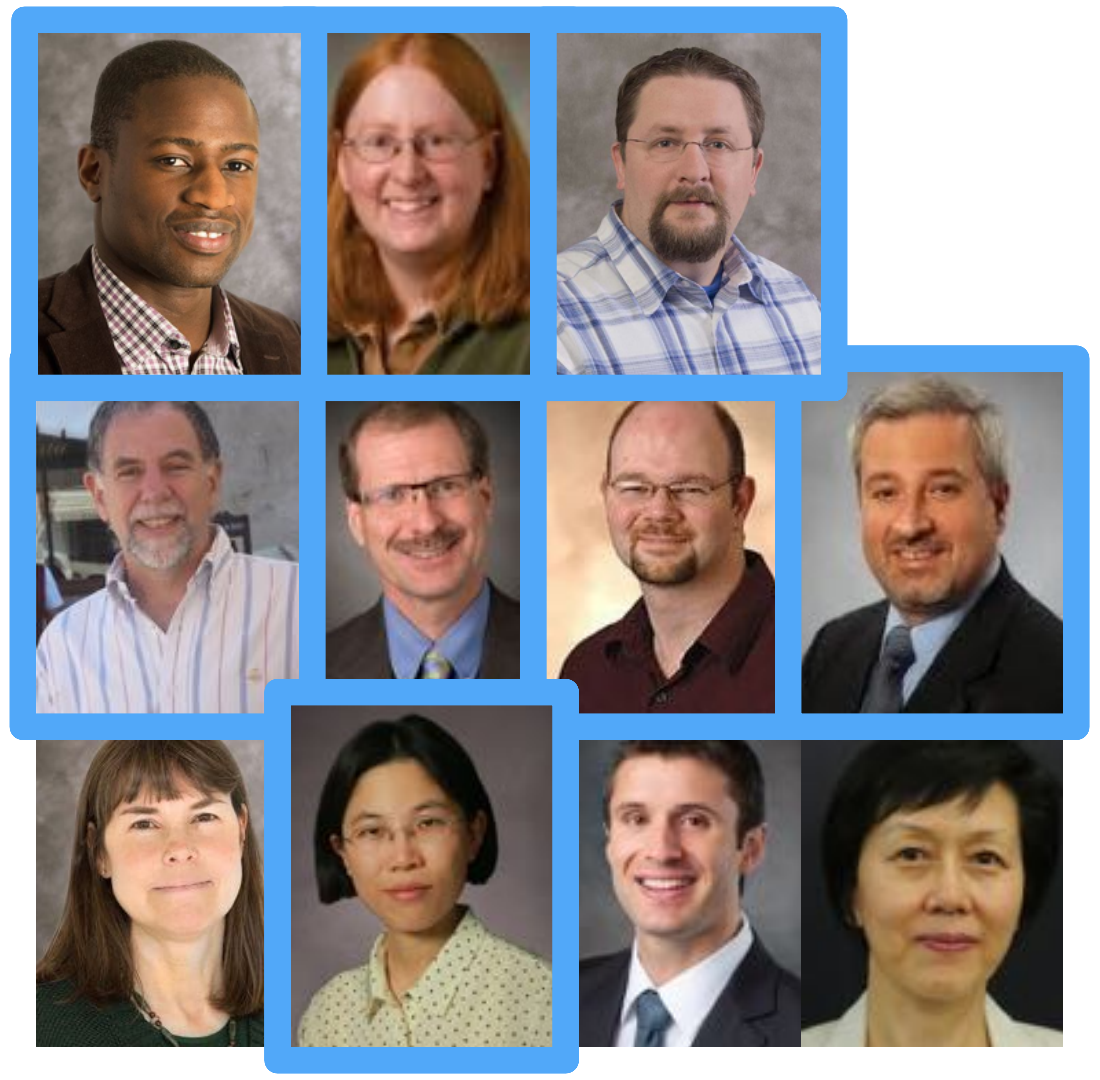
14 Undergrad and **6** Masters
12 URM and **7** female

60% enter STEM grad school, 1 @ PSU

North Carolina Central

National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

11 Collaborating Faculty



multi-year/on-going collaboration

Faculty/staf f visits	PSU→NCCU	NCCU→PSU
2015	3	1
2016	4	2
2017	2	3
2018	3	1
2019	1	3
	13	10

5 Collaborating Faculty

student advisors

Summer student researchers:

13 Undergrad and **5** Masters
14 URM and **9** female
(1 NCCU student is spending summer @ CSULA)

60% enter STEM grad school, 2 @ PSU, compared to 7% of non-PREM students

"Penn Pal" peer mentoring

Insights from experience…

Create a **distinct PREM identity** to the summer experience.

MRSEC staff build institutional memory, support students, and facilitate collaboration.

Faculty and students at MSI institutions face **unique challenges** and bring **unique strengths**.

Strong facility use: SEM, FIB, XRD, TEM, AFM, XPS, Raman, dielectric testing…

…inform future plans

Involve PREM partners in **Mission: Materials Science**.

Personal and workshop-based **grad admissions mentoring** (→REU).

Year-round professional development for all PREM students (and Undergrad ≠ Masters).

Support current & spark new collaborations with **multiple contact points throughout year**.

Measure the **specific impacts of the R1 experience** on PREM students and faculty at **both** sites.

Sustainable Research Practice and Outcomes

Both immediate research **practice** and long-term research **outcomes** have sustainability implications. By developing this mindset and skillset, we equip future leaders in industry and academia for career-long impacts.

Year 1, Groundwork: Awareness-raising, cross-IRG brainstorming, case studies, education in tools, resources, policy.

Years 2 & 3, IRG Action Plan: Identify goals, leaders, tasks, metrics and assessment.

Years 4+: Assess, adjust and expand across university and beyond.

sustainability INSTITUTE

FOCUS ON Sustainability

Partner with local (PSU) and national (MRS) programs to access tools and expertise.

my green lab certification.

SCIENCE U

MISSION: MATERIALS SCIENCE

Pursue my green lab certification and embed content in programs Center-wide (camps, at-home activities, teacher training, public events, industry speakers, etc.).

Follows a successful Center track record of spearheading institutional change, such as science camps, URM graduate recruiting events, and blind/low-vision camps.

Leadership/Professional Development

Outreach Teams develop leadership skills and benefit "both sides of the table"

Education & Outreach Team:

K-12 & public audiences, activity development, science communication training

Sustainability Team:

Researcher and public audiences, develop and implement education and awareness programs with PSU partners, support Green Lab Certification

Team Leaders receive regular mentoring and are recognized with a travel award.

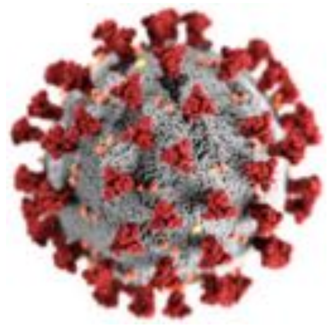
Science outreach at Arts Fest Kids Day with REU and Upward Bound

Student tour of research facilities from experienced grad guides

Grad/Postdoc Advisory Committee provides feedback on Center priorities and plans through quarterly meetings with the Executive Committee.

Outcomes include student-invited speakers, student-run activities at Materials Day, and altered MRSEC seminar timing.

Hands-on, At-home Science



National Science Foundation
MRSEC
Materials Research Science and Engineering Centers

An extensible web app platform for at-home DIY science coupled to interviews of MRSEC scientists on how research impacts daily life.

MISSION: MATERIALS SCIENCE

Build capacity at local grassroots science museum

Discovery Space
Where Science Takes Shape

Extend to rural communities through STEM Ecosystem

ENGINE OF CENTRAL PA

THE FRANKLIN INSTITUTE

Built in collaboration with our long-term museum partners, the Franklin Institute.

In-depth evaluation at summer camps

U SCIENCE

PREM partners & universities hosting other MRSECs are now extending and deepening the web app content.

Public outreach events provide wider visibility

USA SCIENCE & ENGINEERING FESTIVAL