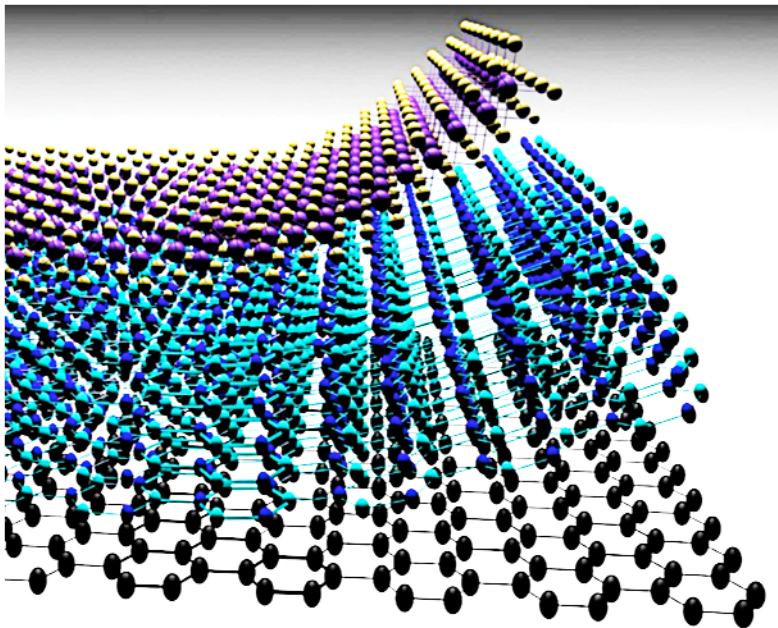
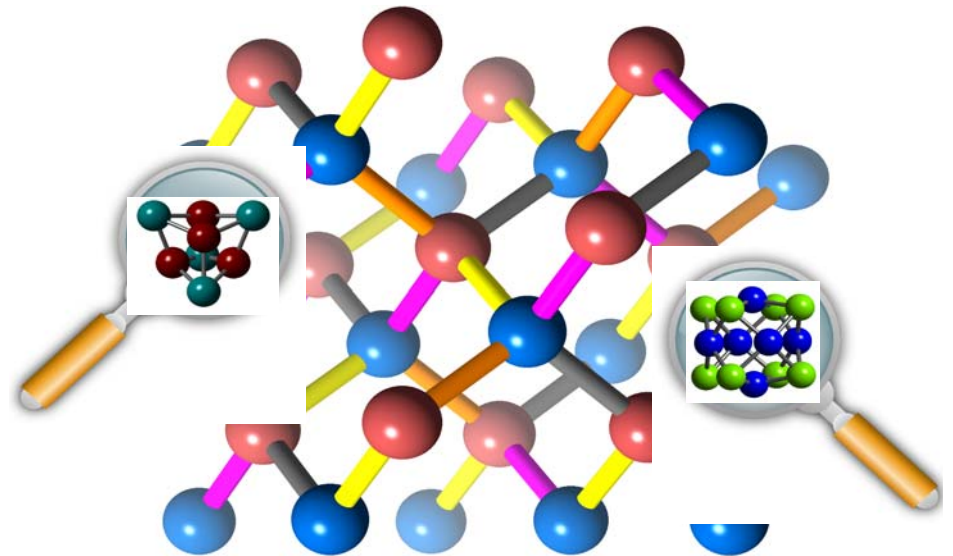


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COLUMBIA-CCNY

# Center for Precision Assembly of Superstratic and Superatomic Solids (PAS<sup>3</sup>)



Superstratic



Superatomic

# PAS The MRSEC Team

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COLUMBIA-CCNY



Hone



Nuckolls



Krusin-Elbaum



Zhu



Archibald



Barmak



Brus



Crowther



Cacciuto



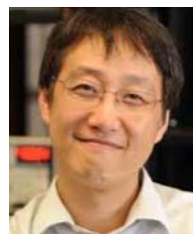
Dean



Herman



Heinz



Kim



Kymissi



Marianetti



McDermott



Millis



Campos



O'Brien



Oganessian



Pasupathy



Reichman



Roy



Steigerwald



Tamargo



Venkataraman

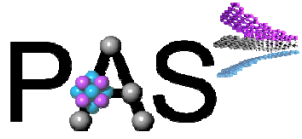


Ford

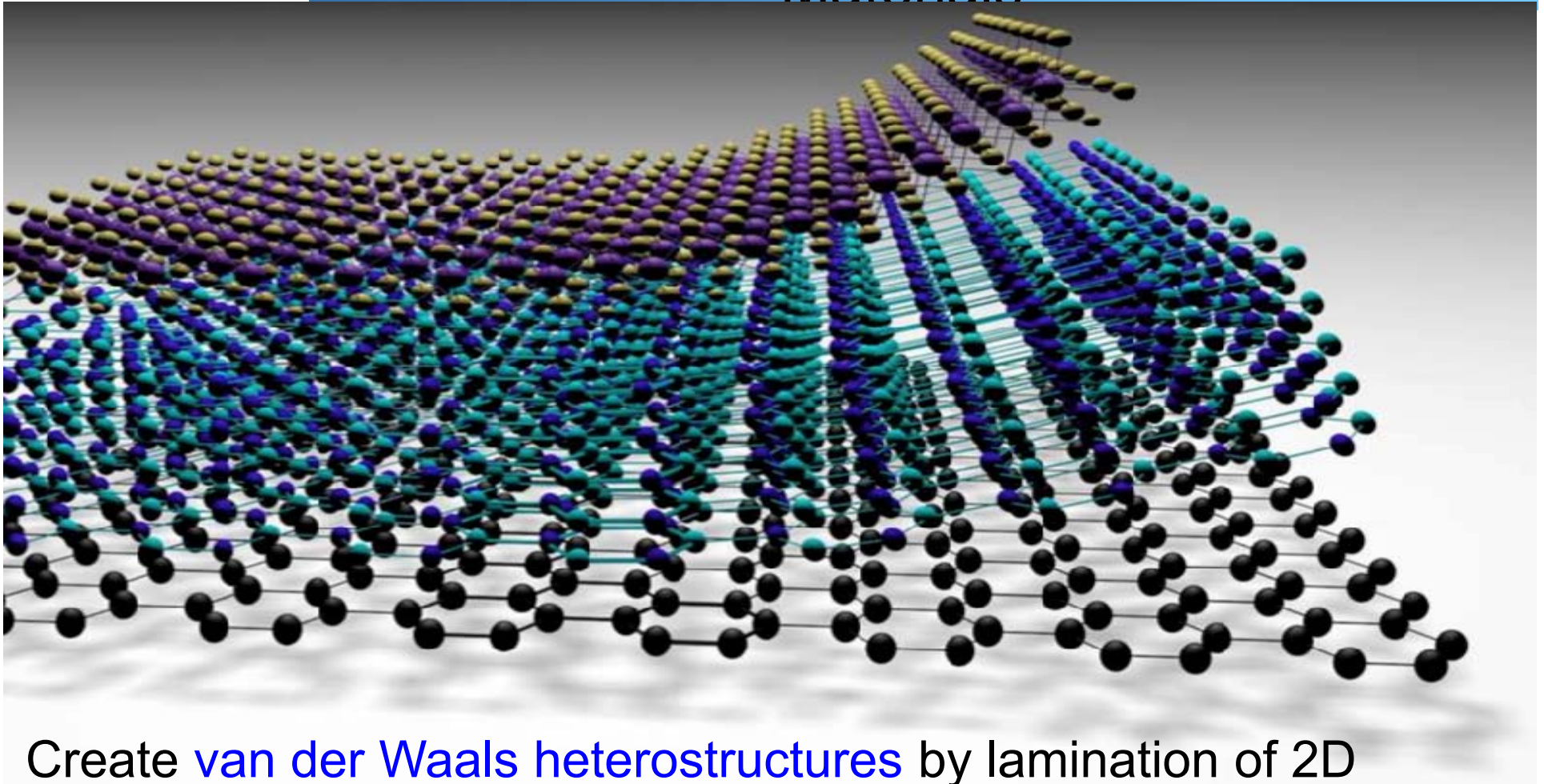
MRSEC fellows: Rebeca Ribeiro, Lukas Zhao (IRG 1),  
Alexandra Velian, Haiming Zhu (IRG 2)



Lowes

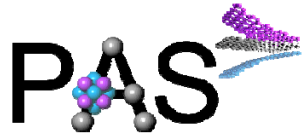


# IRG 1: Heterostructures of van der Waals Materials



Create [van der Waals heterostructures](#) by lamination of 2D materials

- Materials Properties
- Interactions and Emergent Behavior



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# IRG 1 Team

James Hone, Columbia Mechanical  
Engineering, Lia Krusin-Elbaum, CCNY  
Physics



Wayne Archibald  
UVI



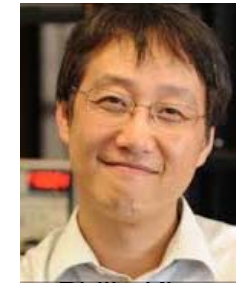
Cory Dean  
Columbia



Tony Heinz  
Columbia/Stanford



Irving Herman  
Columbia



Philip Kim  
Harvard



Chris Marianetti  
Columbia



Stephen O'Brien  
CCNY



Vadim Oganesyan  
CUNY



Abhay Pasupathy  
Columbia



Maria Tamargo  
CCNY

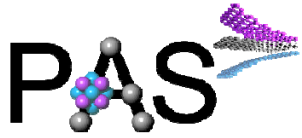


Latha Venkataraman  
Columbia



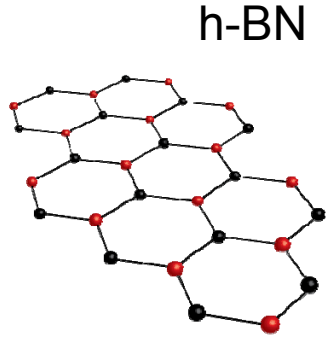
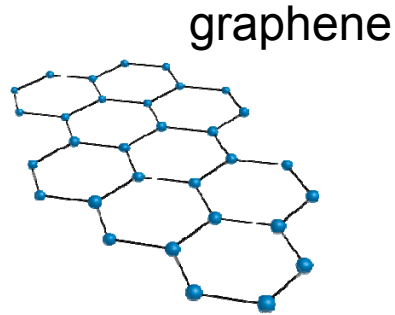
Theanne  
Schiros  
FIT

Key collaborators: Sfeir, Stach, Sutter (BNL); Adam, Castro-Neto (NUS); Low (IBM); Taniguchi, Watanabe (NIMS)

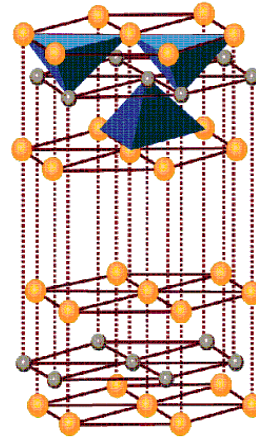


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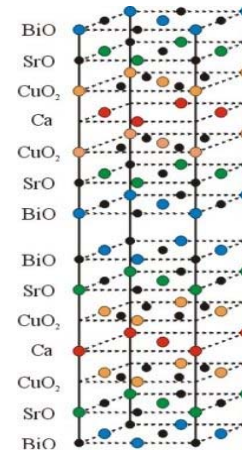
# IRG 1: Heterostructures of van der Waals Materials



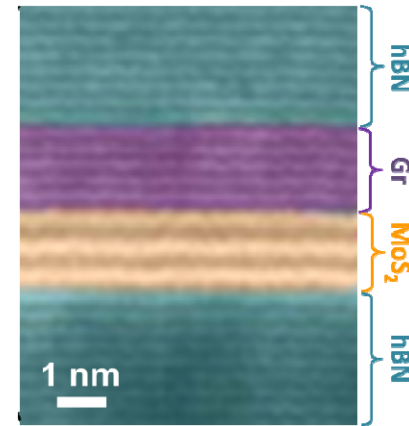
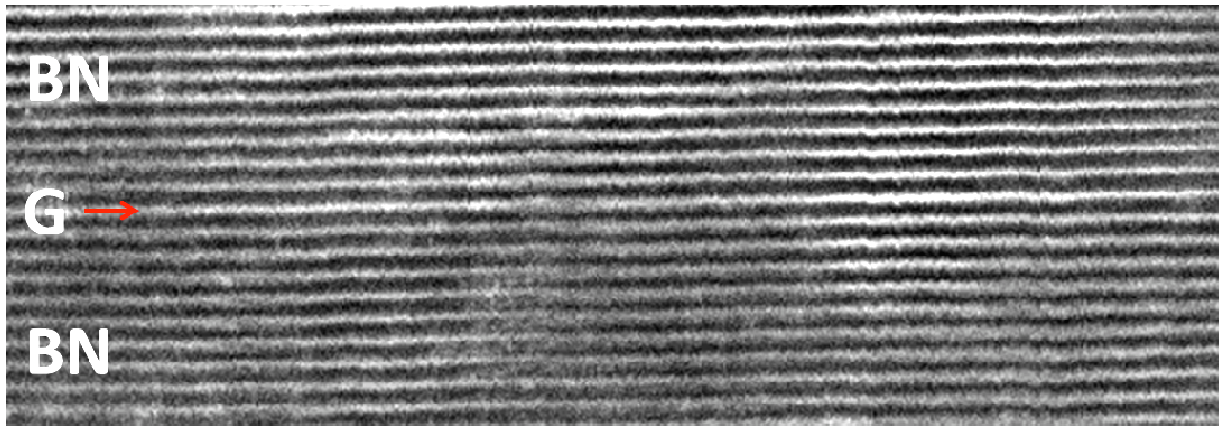
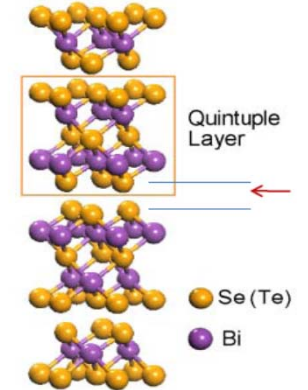
Dichalcogenides



Oxides



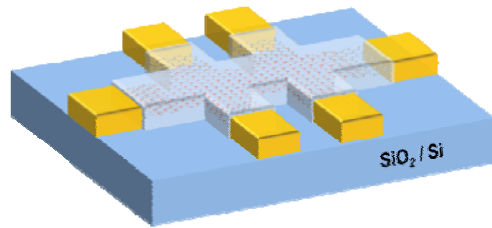
Topological Insulators



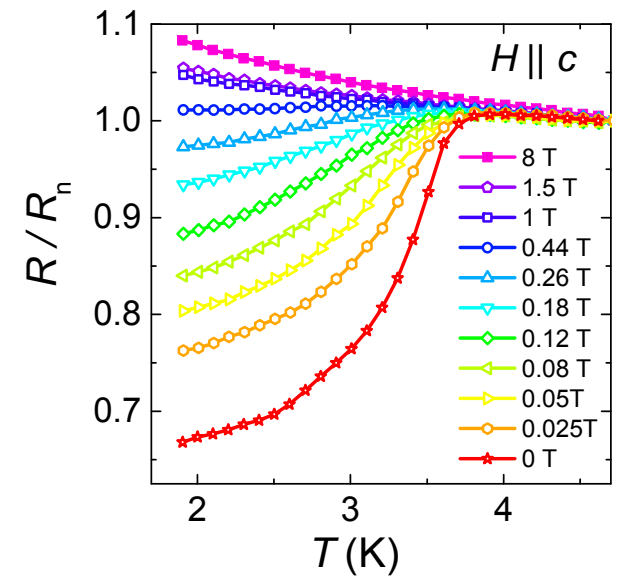
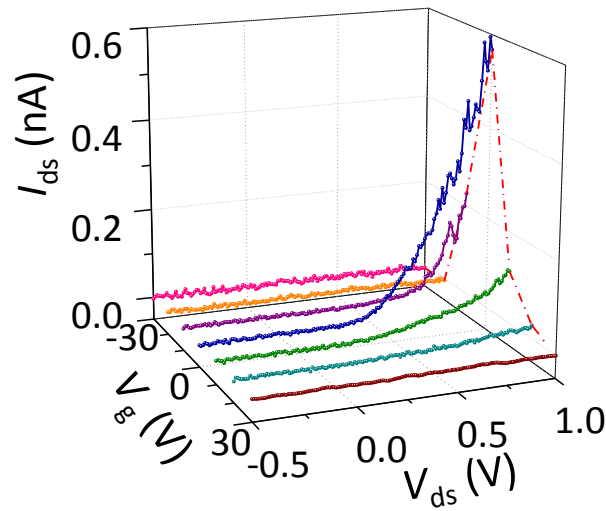
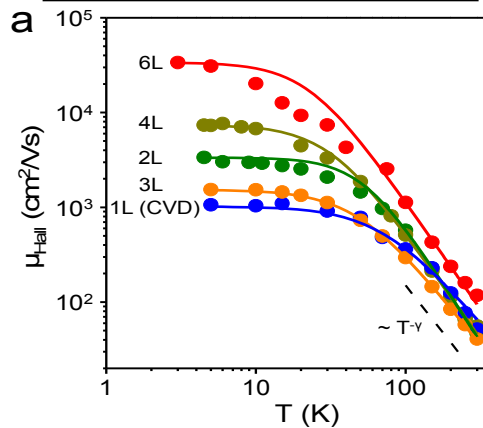
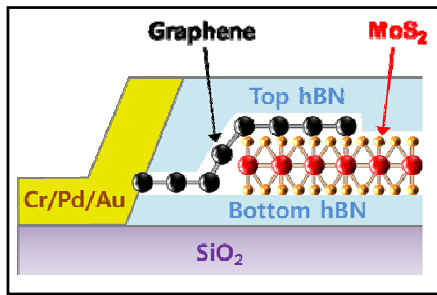
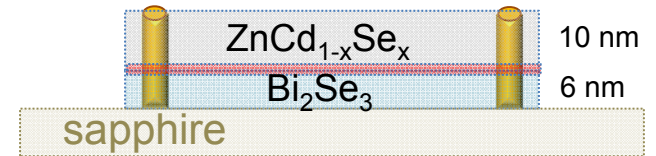
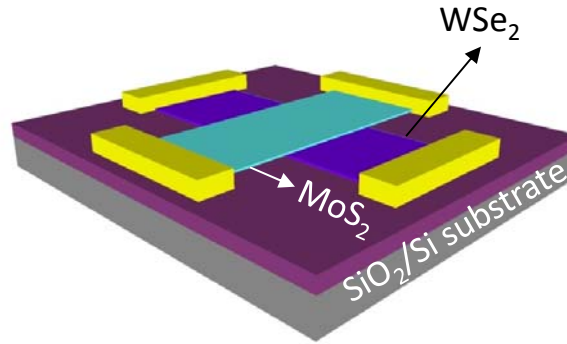
Polymer-free transfer achieves atomically clean heterostructures

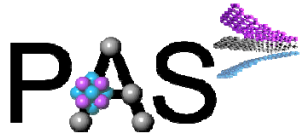
# Examples

hBN-encapsulated MoS<sub>2</sub>



atomically thin p-n Junction Interfacial superconductivity

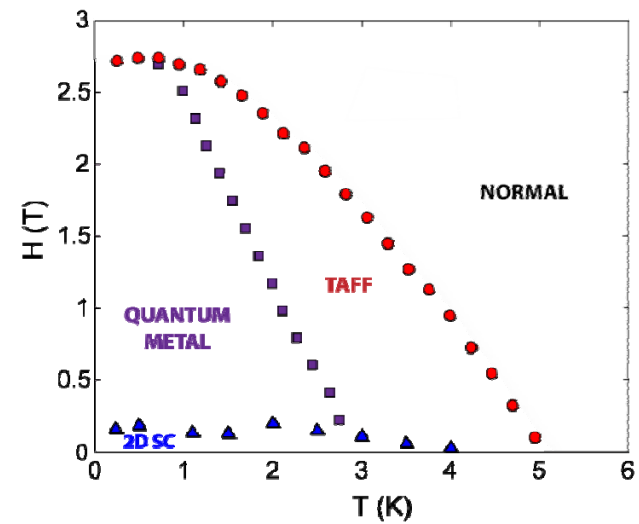
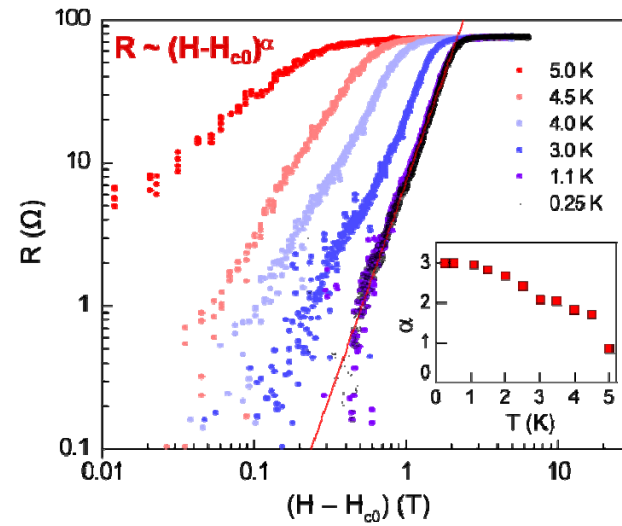
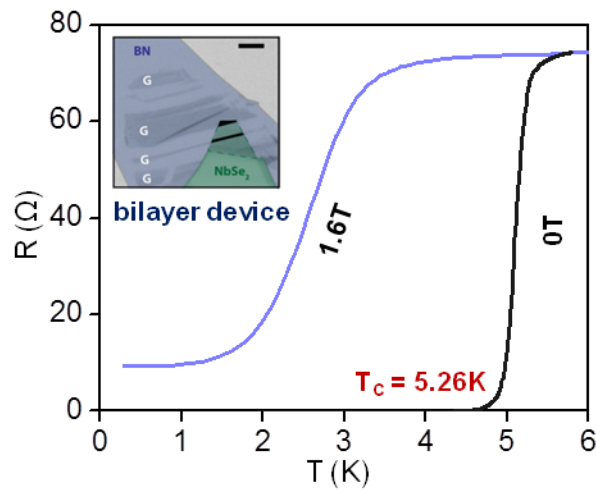
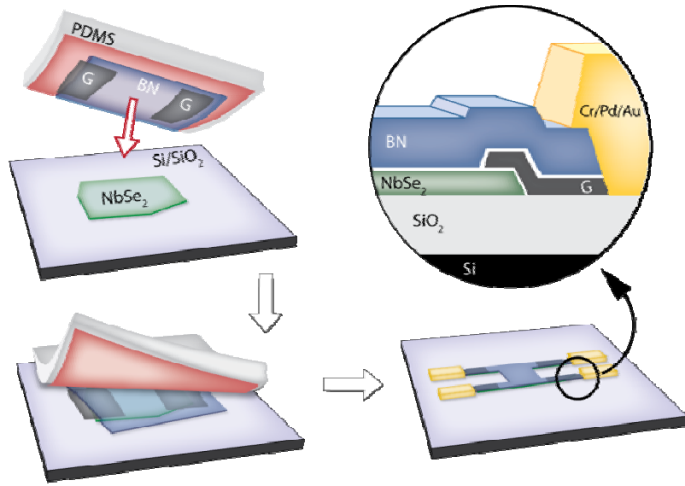




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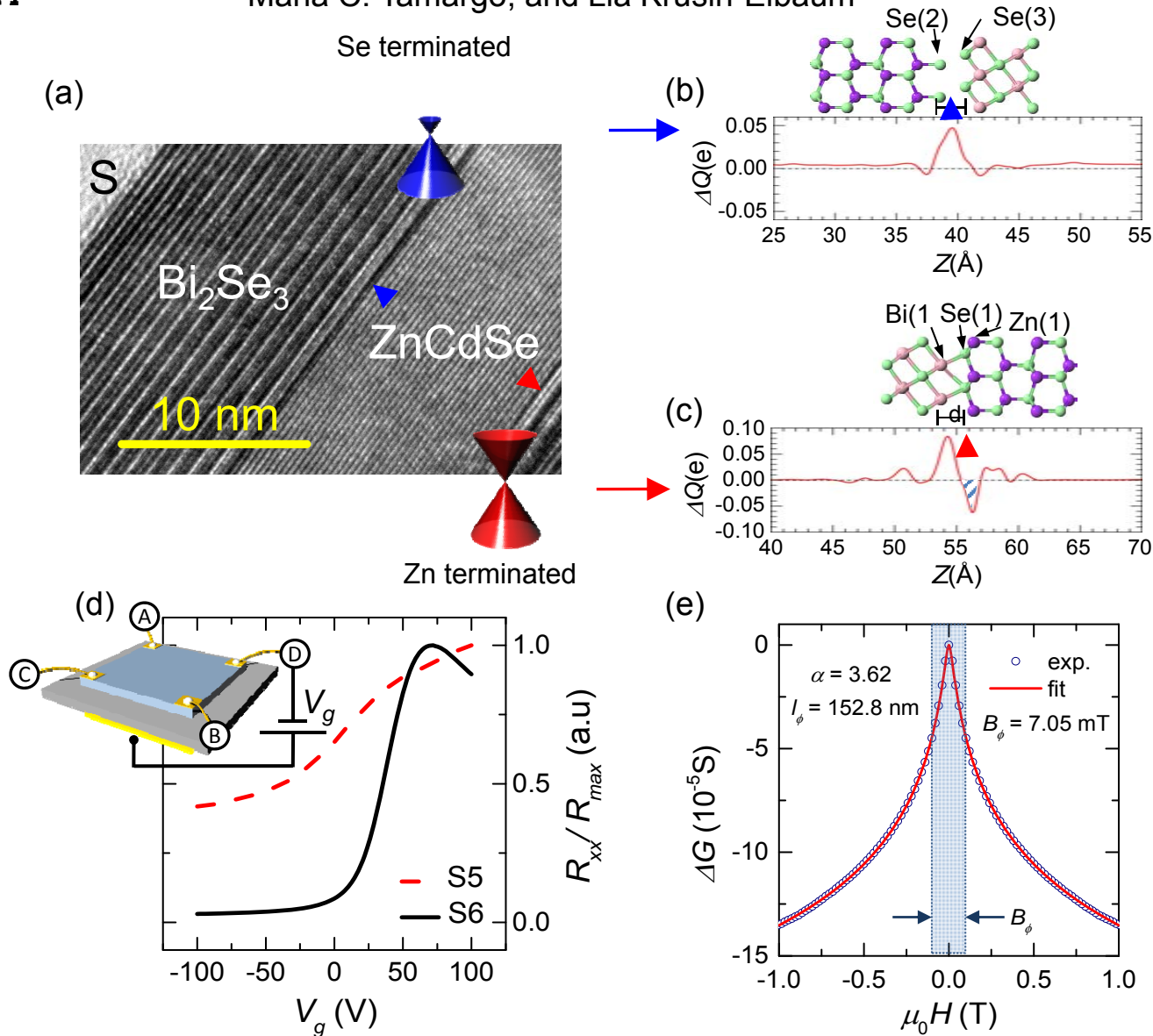
# Magnetic field tuned quantum metal in 2D NbSe<sub>2</sub>

A. W. Tsen, B. Hunt, Y-D Kim, J. Hone, P. Kim, C. R. Dean, A. N. Pasupathy

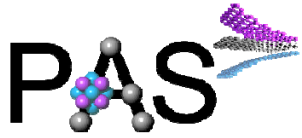


# Robust topological interfaces and charge transfer in epitaxial $\text{Bi}_2\text{Se}_3$ /II-VI semiconductor superlattices (NanoLetters 2015)

Zhiyi Chen, Lukas Zhao, Kyungwha Park, Thor Axtmann Garcia,  
Maria C. Tamargo, and Lia Krusin-Elbaum

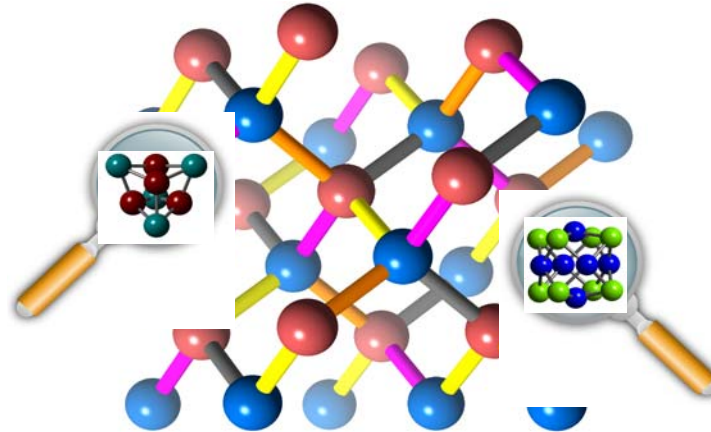






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# Creating Multifunctional Materials From Superatoms



## Materials

Thermoelectrics

Novel Superconductors

Magnetic Memory

Photovoltaics

Ferroelectrics

.....

## Control

Band Structure

Spin/Magnetism

Dimensionality

Phonon Properties

Length Scale

.....

## Strategy

SA Composition

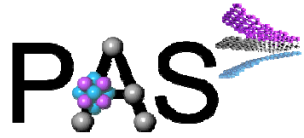
SA Size

Inter-SA coupling

SA Structure

SA Interface

.....



# IRG-2 Team & Management

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COLUMBIA-CCNY

## Synthesis



Colin  
Nuckolls



Xavier  
Roy



Michael  
Steigerwald



Luis  
Campos

## Structure, Electronics, and Magnetism



Theo  
Siegrist  
(FSU)



Erich  
Stach  
(BNL)



Katayun  
Barmak



John  
Hill  
(BNL)



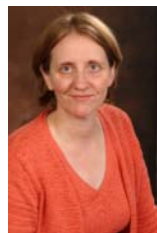
Jim  
Misewich  
(BNL)

IRG  
Leads

## Spectroscopy



Xiaoyang  
Zhu



Ann  
McDermott



Andrew  
Crowther  
(Barnard)



Louis  
Brus



Jonathan  
Malen  
(CMU)



John  
Kymissis

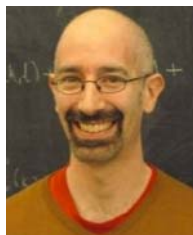


Philip  
Kim



George  
Tulevski  
(IBM)

## Theory



David  
Reichman



Angelo  
Cacciuto



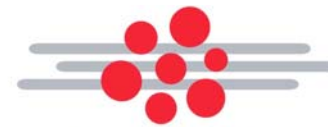
Andrew  
Millis

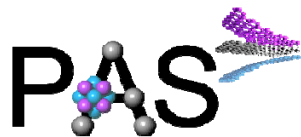


Timothy  
Mueller  
(DuPont)



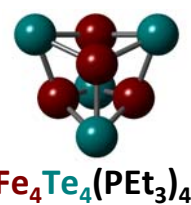
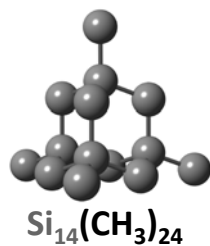
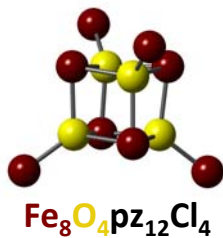
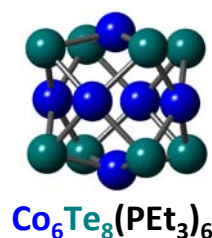
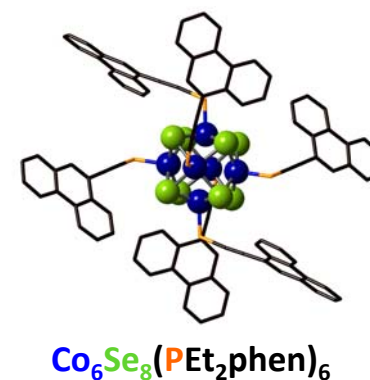
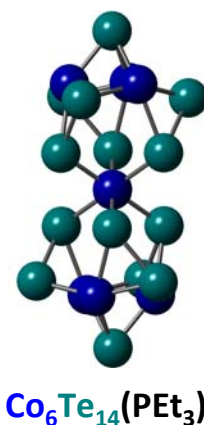
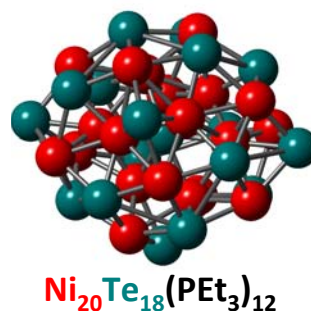
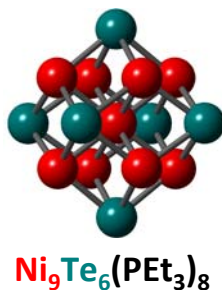
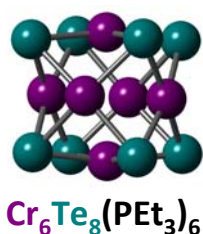
Center for Functional Nanomaterials  
Brookhaven National Laboratory





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# Design & Synthesis of Superatoms



phen = 9-ethynylphenanthrene

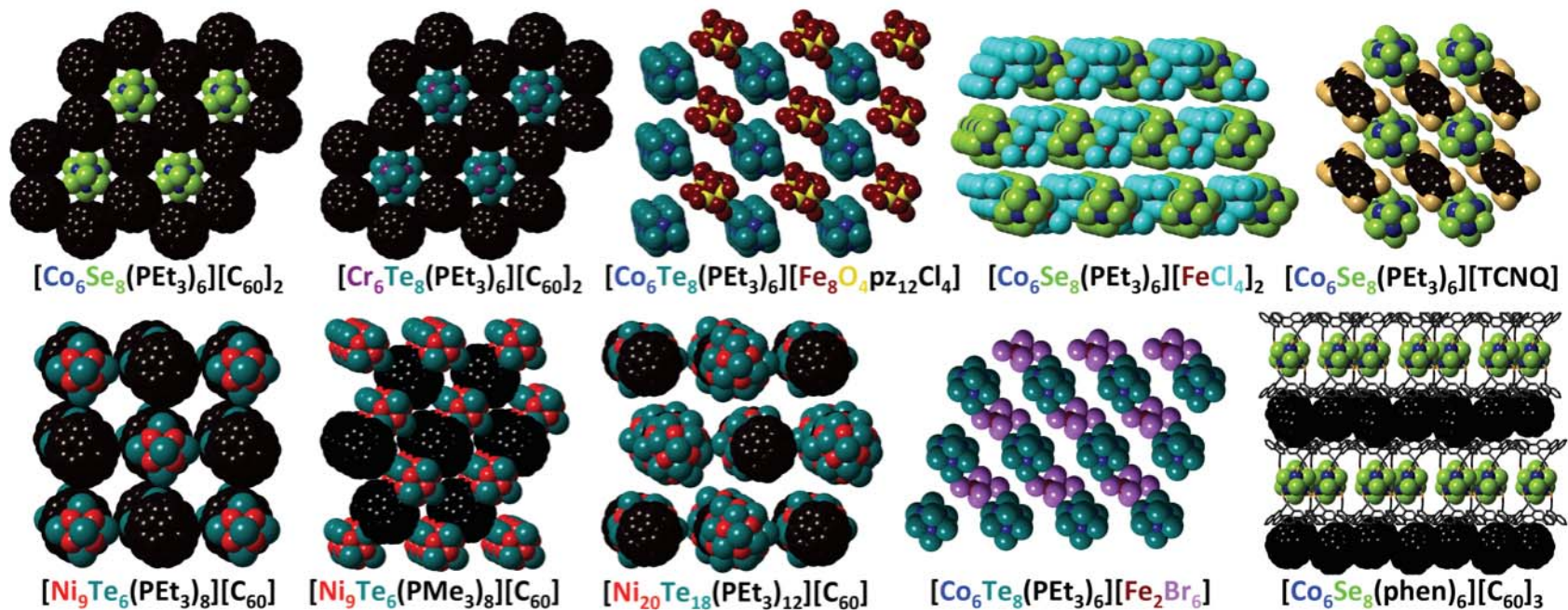
pz = pyrazolate

- Tunable size, shape, & composition with Atomic precision (XRD, TEM, PXRD)
- Surface control for strong inter-SA interactions.
- Programmable properties: DOS, oxidation/reduction potential, electronic/magnetic, thermal, photochemical...
- First principles theory (e.g. DFT)  $\Leftrightarrow$  Spectroscopy

Design and Synthesis: Nuckolls, Roy, and Steigerwald

M. L. Steigerwald et al., *Inorg. Chem.* **1994**, 33, 3389; *Inorg. Chem.* **1993**, 32, 5165; *JACS* **1989**, 111, 9240.

# Superatom assembly via charge transfer



X. Roy et al. *Science* 2013, 341, 157.

## Multi-scale modeling $\leftrightarrow$ Experiment

- Parameterize inter-SA interactions (*ab initio* & semi-empirical calculations)
- Assembly dynamics as function of interactions (long-range electrostatics, CT, short-range anisotropy, van der Waals, polarization, etc...).
- Phase diagrams (Monte Carlo simulations...)

### Synthesis and Assembly:

Nuckolls, Roy, and Steigerwald

### Structure:

Barmak, Siegrist (FSU), Stach (BNL) and Stephens (BNL)

### Theory:

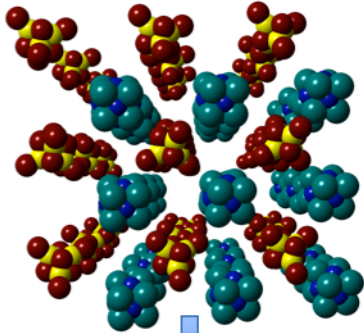
Cacciuto and Reichman

# PAS Superatom Assembly

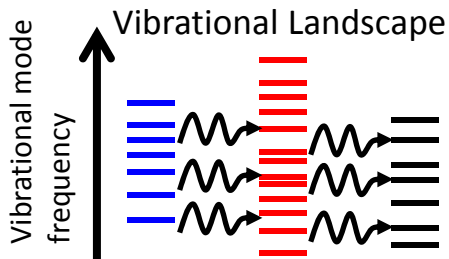
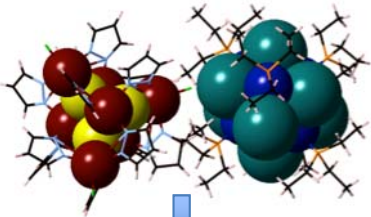
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## Thermal Conductivity

Superlattice structure



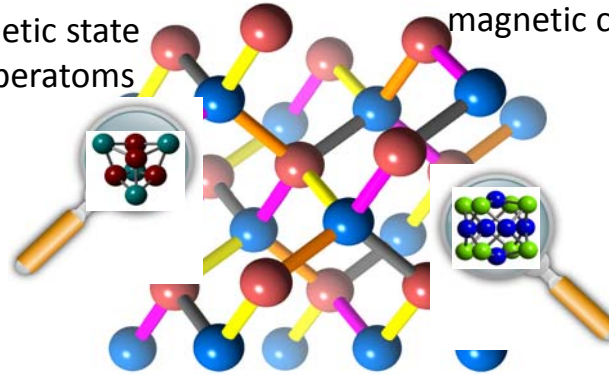
Superatom and Interface atomic precision



Cluster 1 Interface Cluster 2

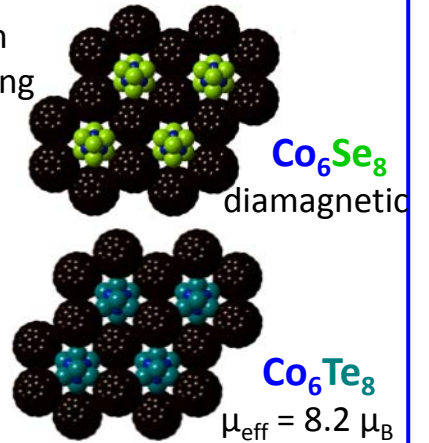
## Magnetic Properties

Magnetic state of Superatoms

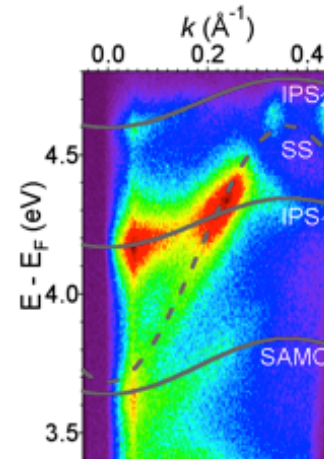
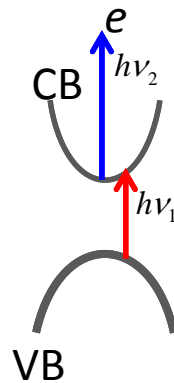


Inter-Superatom magnetic coupling

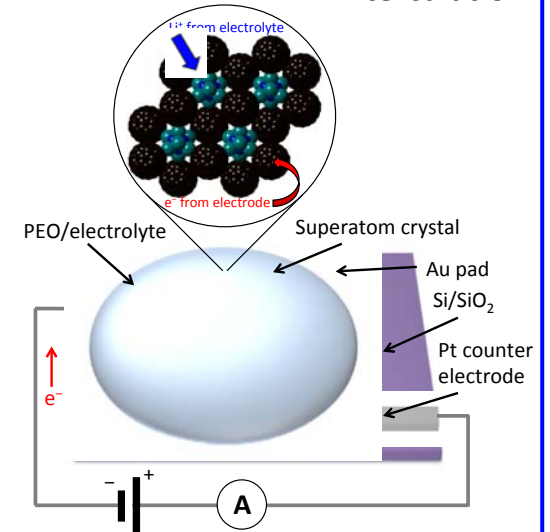
Example

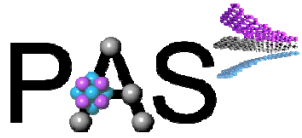


## Electronic Properties



Intercalation



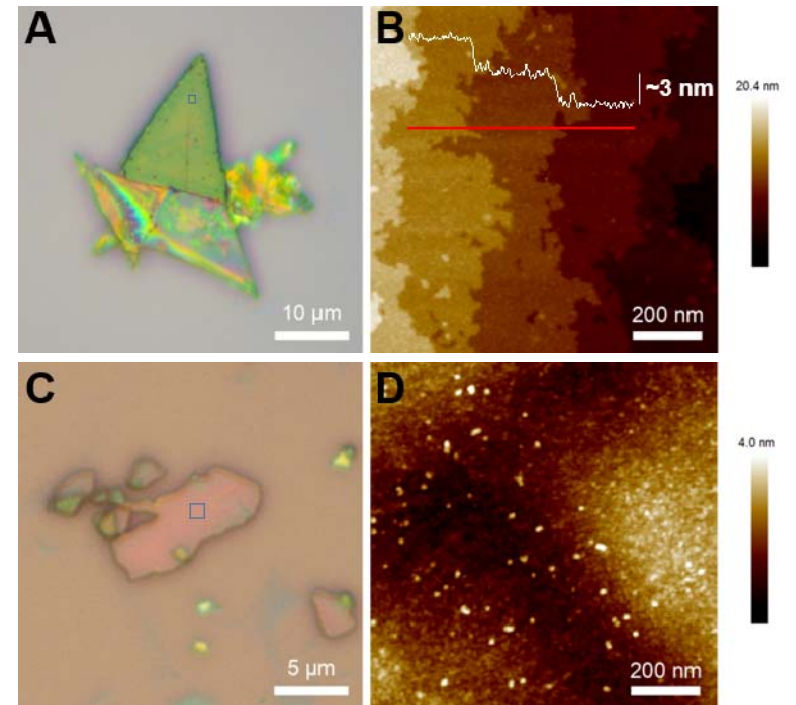
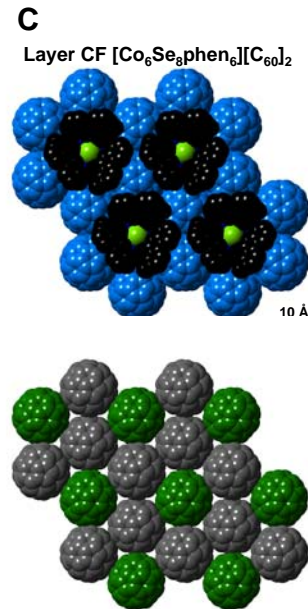
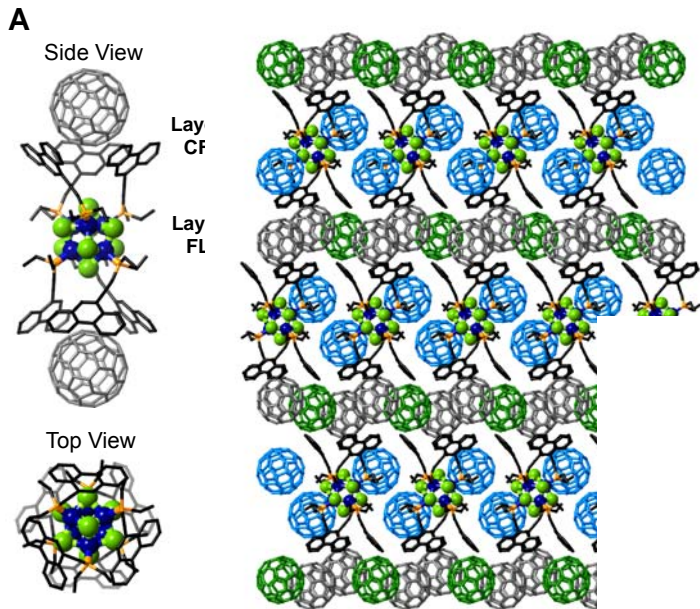
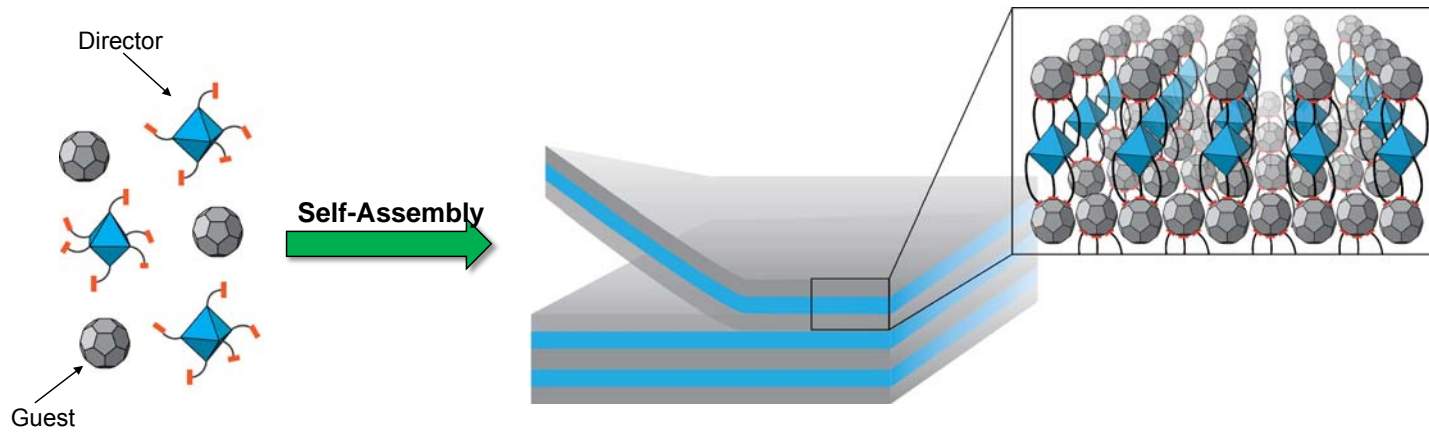


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SUPERSTRATIC AND SUPERA  
COLUMBIA-

# Van der Waals Solids from Self-Assembled Nanoscale Building Blocks

B. Choi, D. W. Paley, J. Yu, C. H. Lee, P. Kim, M. L. Steigerwald, C. Nuckolls, X. Roy

Submitted



# PAS Shared Materials Characterization Lab

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COLUMBIA-CCNY

- New Space: 240 Havemeyer (renovated) and 540 Havemeyer
- Manager: Dan Paley
- (1) SuperNova Single Crystal Diffractometer
- (2) Panalytical Powder X-ray Diffractometer
- (3) Bruker Fastscan AFM
- (4) Thermal Analysis DSC and TGA
- (5) XPS (refurbished)
- (6) SQUID Magnetometer

Other major new equipment to be purchased:

1. He liquifier for 2 magnet cryostats
2. Cryostat system at CCNY
3. UV-vis spectrometer

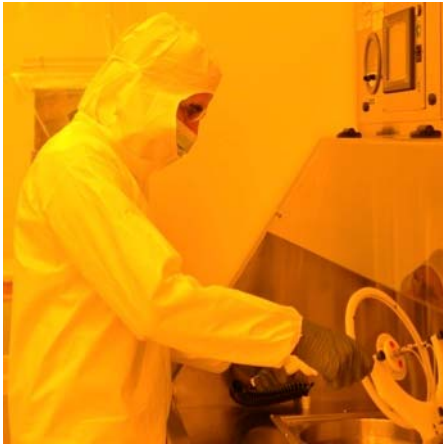




# PAS CUNY ASRC NanoFabrication Facility

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COLUMBIA-CUNY

The new NanoFab: 5,000 ft<sup>2</sup> of ISO 6 (Class 1,000) and ISO 5 (Class 100) cleanroom space; additional lab space for back-end processing and support areas; 6-inch wafer handling capability; CUNY funded technical staff.



photolithography



e-beam lithography



e-beam / thermal  
evaporator



inductively coupled  
plasma (ICP) etcher

Other major tools: ▪ SEM, ▪ PECVD, ▪ RIE ▪ ALD ▪ sputtering and evaporation tools, ▪ an advanced metrology suite, and ▪ a true 3D laser lithography, ▪ LPCVD, TOES, and Oxidation furnaces.

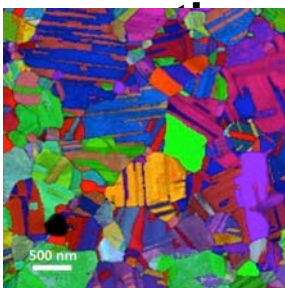
# PAS Electron Microscopy at CU and CCNY

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COLUMBIA-CCNY

Columbia

CCNY

820 sq. ft. space under



Katayun Barmak



FEI Talos  
F200A

Additional capabilities at BNL  
(+Rutgers/BNL)

CUNY

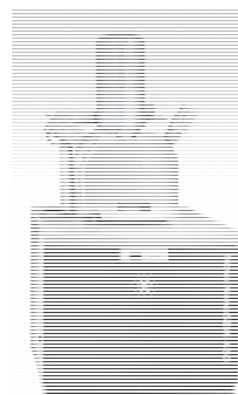
Titan Themis 200 (S)TEM

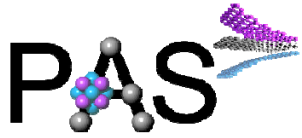


Tecnai G<sup>2</sup> Spirit BioTwin:  
Advanced 120 kV TEM



Nova NanoSEM 450 Helios NanoLab 660 (FIB/SEM)





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COLUMBIA-CCNY

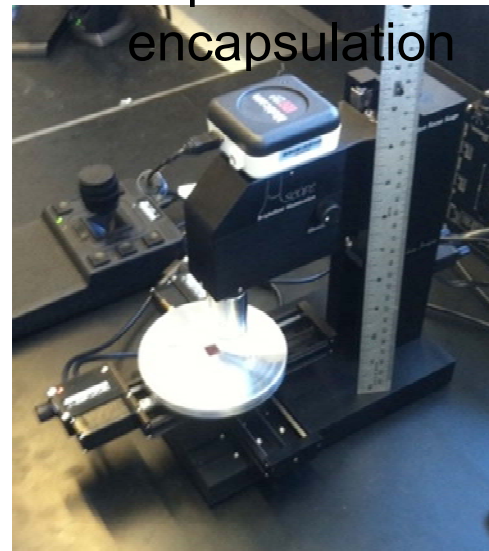
# Instrument Development: Inert Atmosphere Assembly System



- User facility for MRSEC
- Combines auto-finder and transfer stage
- AFM/Raman for characterization
- Metal evaporation / Parylene deposition for large-scale encapsulation



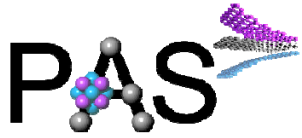
Transfer stage



Compact Auto-Finder

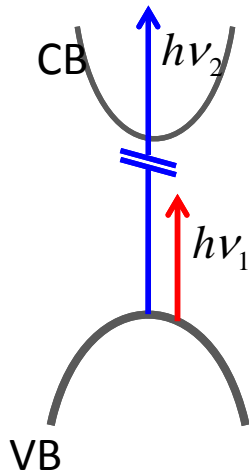


Combined AFM/Raman



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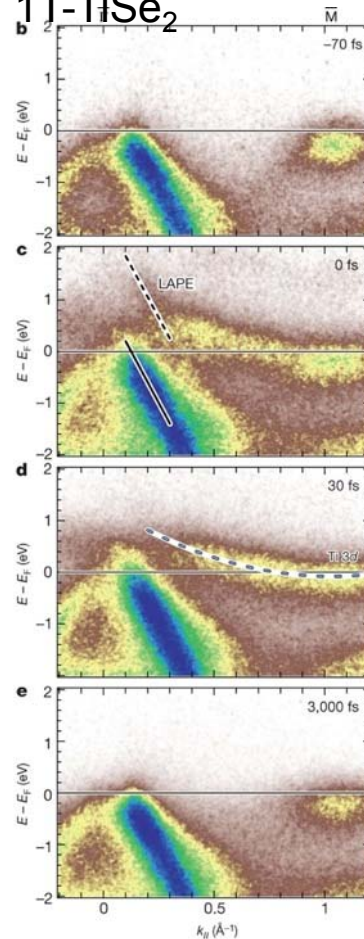
# INSTRUMENT DEVELOPMENT. TIME-RESOLVED ARPES WITH VUV laser source for complete mapping of valence and conduction bands



- \* Two femtosecond laser ARPES setups in XYZ lab ( $h\nu \leq 6$  eV).
- \* Extending to VUV  $\rightarrow$  complete mapping of VB & CB structure

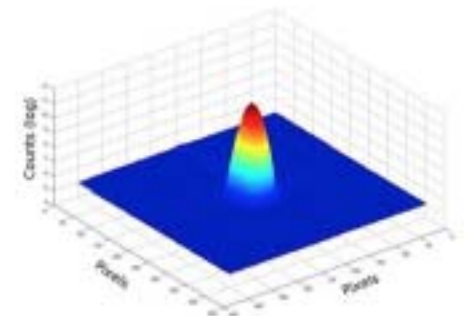
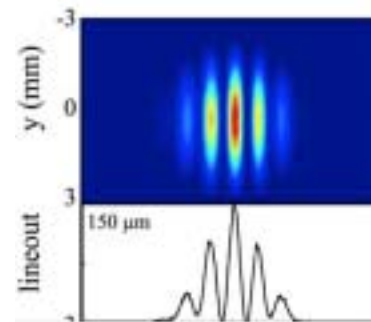


e.g., electronic phase transition in  $1T\text{-TiSe}_2$



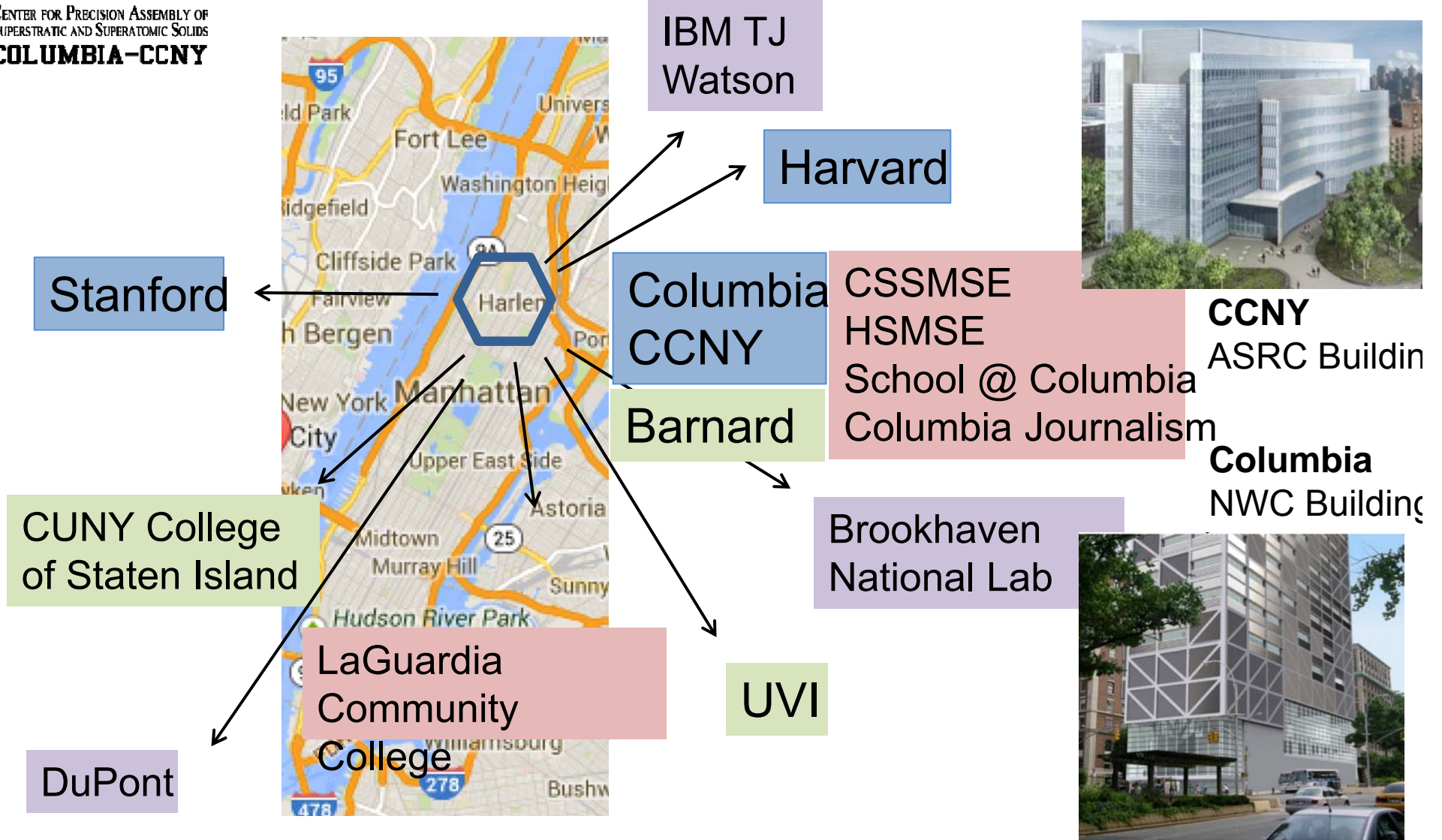
*Nature* **471**, 490 (2011)

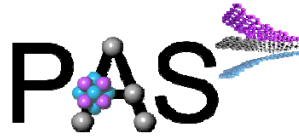
Extreme UV laser source: 47-13 nm (26-95 eV)



Profs. Henry Kapteyn & Margaret Murnane

# MRSEC INSTITUTIONS and Partners





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**COLUMBIA-CCNY**

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**Associate Director** Colin Nuckolls

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Xiaoyang Zhu  
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Diversity Committee

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Student Leadership Council

External Partners and Collaborators

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Lia Krusin

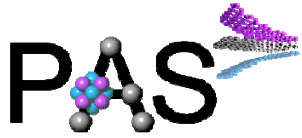
**IRG 2**  
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Xiaoyang Zhu

Catherine Tissot – MRSEC administration  
Dario Vasquez – outreach, seminars, website  
Xiomara Perez-Betances: CNI DO  
Emily Ford – SEAS outreach director

# PAS Integrated Education / Outreach Program

CENTER FOR PRECISION ASSEMBLY OF  
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COLUMBIA-CCNY

Level	Activities
<b>Primary</b>	Integrated Project Week at TSC
<b>Secondary</b>	RET program Science Honors Program – Nano course HS research program: CSSMSE partnership
<b>Undergraduate</b>	LaGuardia Community College partnership Curriculum development REU program Undergraduate research
<b>PhD/Postdoc</b>	Curriculum Workshops and Seminars Short Courses Student Leadership council
<b>Public</b>	Science celebration, Materials open house Journalism school pilot



# Summer MRSEC outreach and education programs at Columbia University / CCNY

CENTER FOR PRECISION ASSEMBLY OF SUPERSTRATIC AND SUPERATOMIC SOLIDS  
**COLUMBIA-CCNY**

The Columbia / CCNY MRSEC inaugurated its summer research education program in 2015 by hosting 44 summer researchers, including teachers, undergraduates, community college students, and high school students

Research Experiences for Teachers (RET)

Research Experiences for Undergraduates (REU)

Engineering the Next Generation (ENG)

LaGuardia Community College

Columbia Secondary School (K-12 school)



ENG trip to Brookhaven National Laboratory



REU Symposium Day

