PennState

NSF 2D Crystal Consortium
NSF Materials Innovation Platform

Scalable Growth, In-Situ Characterization and Processing of 2-Dimensional Crystal Materials for Future Generation Electronics….

An overview of the 2D Crystal Consortium - Materials Innovation Platform (2DCC-MIP)

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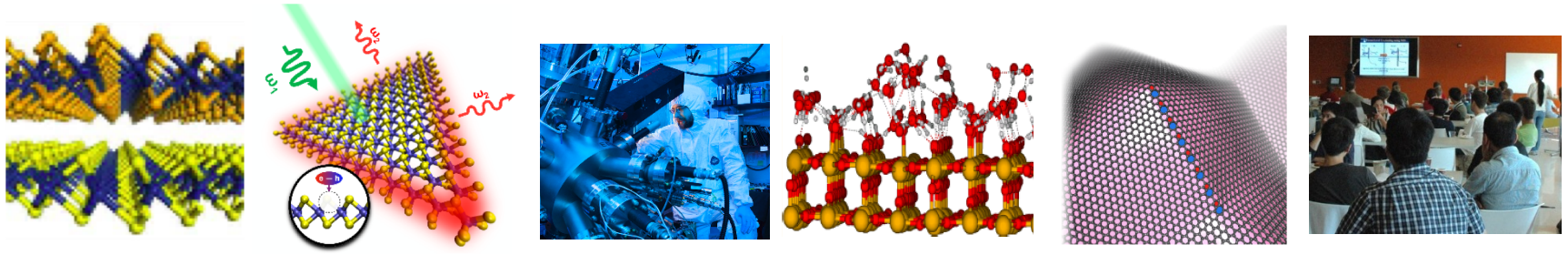
2DCC-MIP Bulk Crystal Growth Lead
Department Head, Electronic Materials and Devices
Penn State Applied Research Laboratory

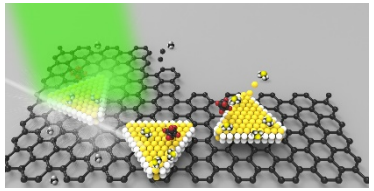


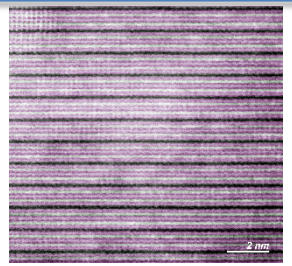
NSF Division of Materials Research:

Materials Innovation Platforms (MIPs)

MIPS are **national user facilities** - the first round (awarded in 2016) are focused on **bulk crystal growth and epitaxy** of hard crystalline materials using a **materials genome approach** (theory-synthesis-characterization).

2D Crystal Consortium
NSF Materials Innovation Platform





A 5-year, $17.8 million Platform at Penn State University to advance the synthesis of 2D layered chalcogenides for next generation electronics.

http://mip.psu.edu

Basic components of a MIP:

- National User Facility/Program
- In-House Research
- Education and Outreach

PARADIM
PLATFORM FOR THE ACCELERATED REALIZATION, ANALYSIS & DISCOVERY OF INTERFACE MATERIALS

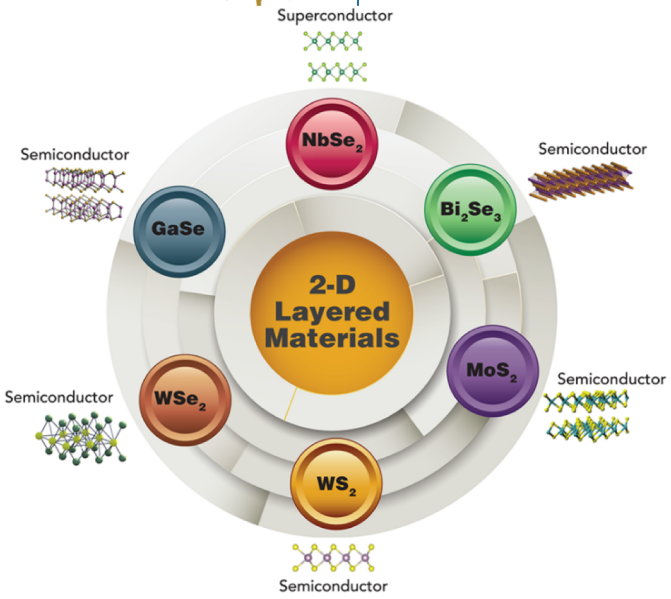
http://paradim.cornell.edu

Overview of the 2DCC-MIP Platform

Scientific Focus:

2D layered chalcogenides for next generation electronics

2D monolayers, surfaces and interfaces are emerging as a compelling class of systems with transformative new science that can be harnessed for novel device technologies.



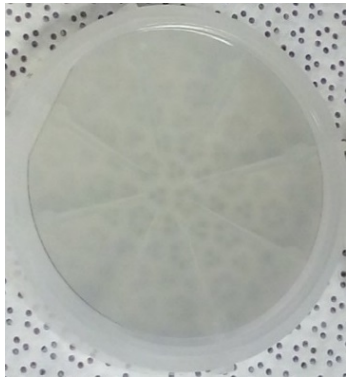
Advances in synthesis are needed to drive further developments in the field.

2DCC Platform Components

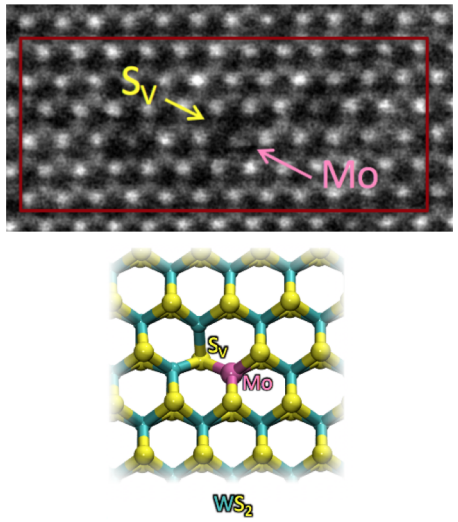
- National User Facility/Tool Development
- In-House Research
- External User Program
- Data Management/Data-Enabled Science
- Education and Outreach

Scientific Goals of the 2DCC

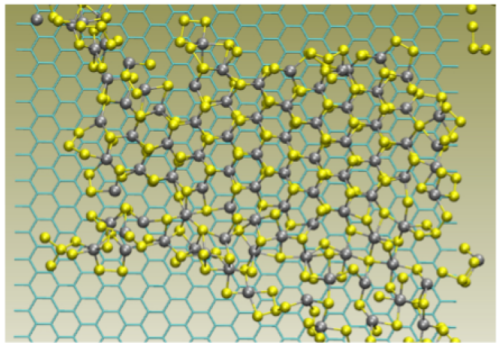
- Develop the science of 2D chalcogenide epitaxy to match level of established material systems such as III-V, II-VI, IV, oxides, Heuslers.
- Enable wafer scale growth of ‘electronic grade’ single layers and heterostructures.
- Develop new growth approaches, tools and techniques to advance the synthesis of layered chalcogenides.
- Benchmark and compare the properties of exfoliated bulk crystals and MOCVD/MBE films
- Utilize theory/simulation/data-enabled science tools to gain insight into growth processes and guide exploration of the multidimensional growth parameter space.



Wafer scale epitaxial growth of WSe_2 and WS_2 monolayers (Choudhury, et al.)



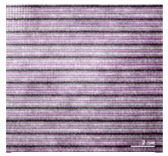
Coupling between Mo dopants and S vacancies in $Mo_xW_{1-x}S_2$ (Azizi et al.)



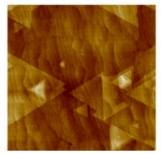
Force-biased MC simulation of MoS_2 growth on graphene (Lofti et al.)

2DCC User Facilities

Thin Films and In-Situ Characterization

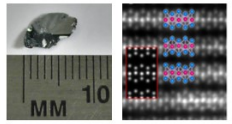


MBE grown $(Bi,Sb)_2Te_3$



MOCVD WSe_2

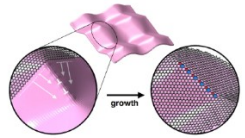
Bulk Crystal Growth



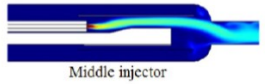
CVT grown WTe_2

Bridgman grown Bi_2Se_3

Theory and Simulation



Finite length grain boundaries on curved surfaces



Fluid dynamics simulation of MOCVD reactor

Millennium Science Complex – First Floor

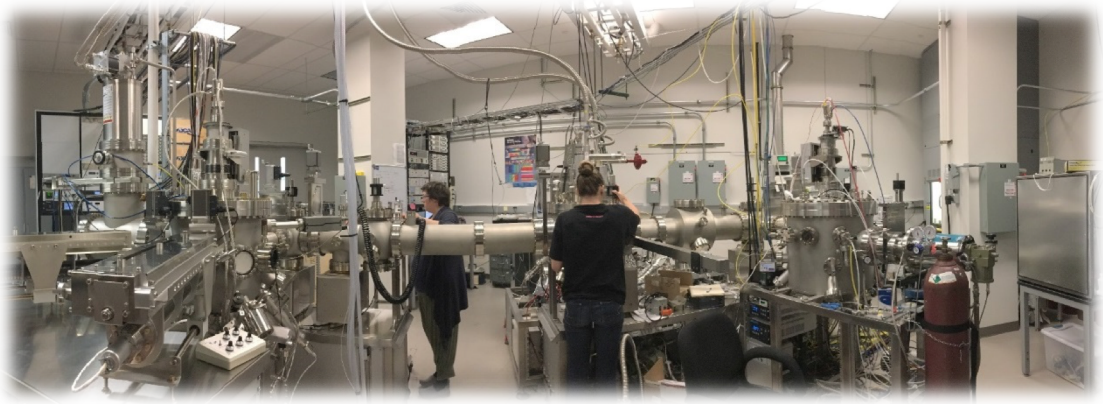
Bulk Growth Lab
Bridgman System
CVT Furnaces

MBE System 2 located in basement of Davey Lab

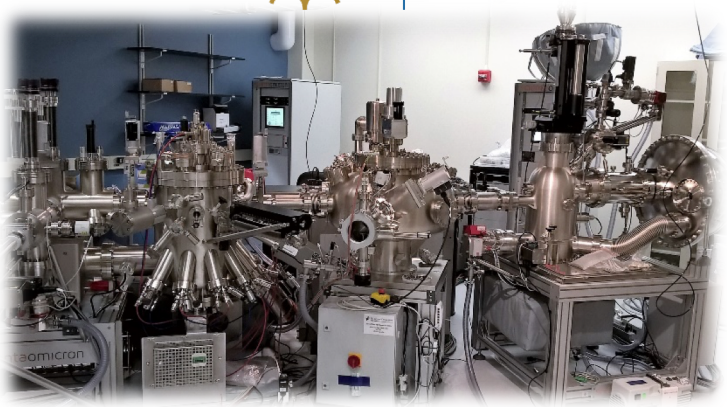
MBE Lab
MBE System 1

CVD Lab
MOCVD System 1
MOCVD System 2

2DCC Facilities - Experimental

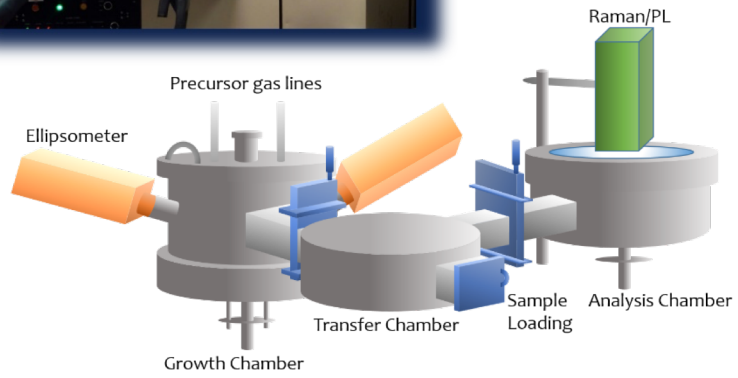


Hybrid MBE for Chalcogenides and Oxides



Multi-Module UHV System
Solid Source MBE + Cryo ARPES
and 4 probe STM

Chalcogenide
MOCVD



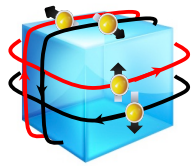
Multi-Module MOCVD + ellipsometry and Raman/PL

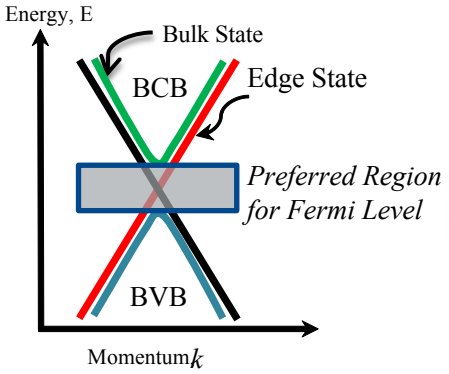
CVT

Vertical Bridgman

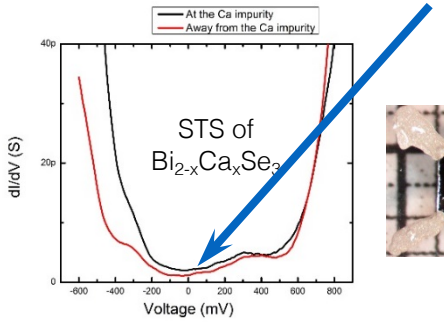
Compounding
Furnace

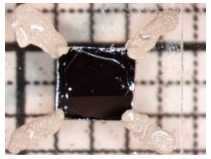
Vertical Bridgman Synthesis of Bulk Bi_2Se_3 Topological Insulating Single Crystals

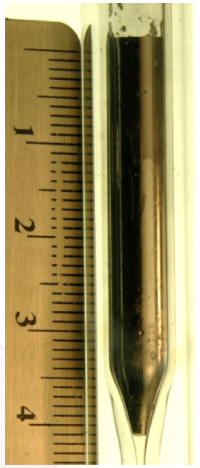




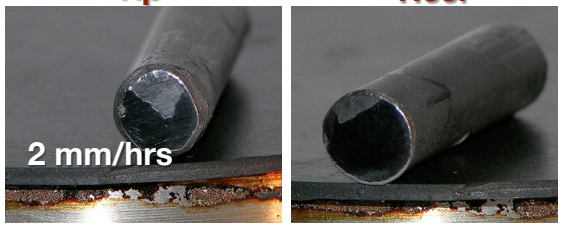
Fermi level tune into the bulk gap

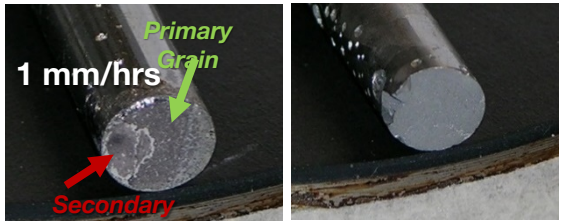


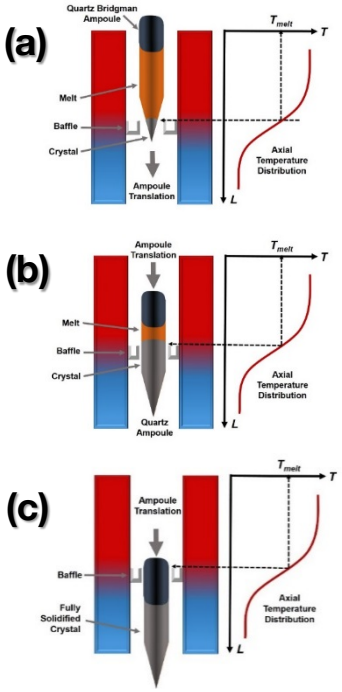


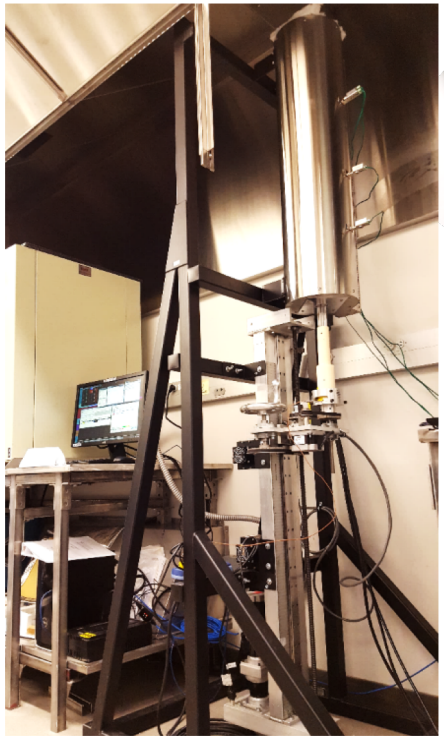


Grown Rate

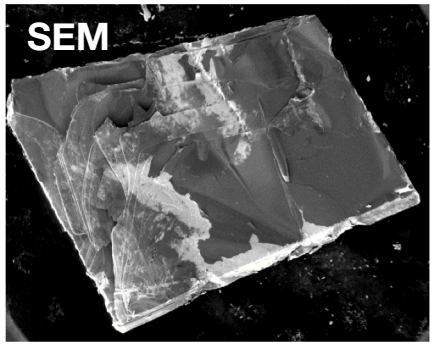


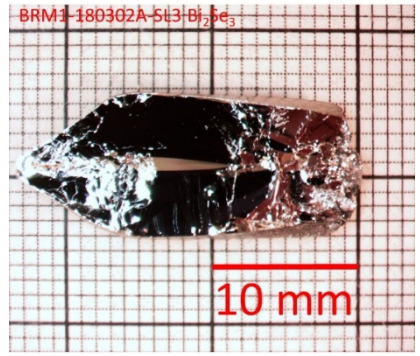






Growth rate optimized to maximize size of primary grain

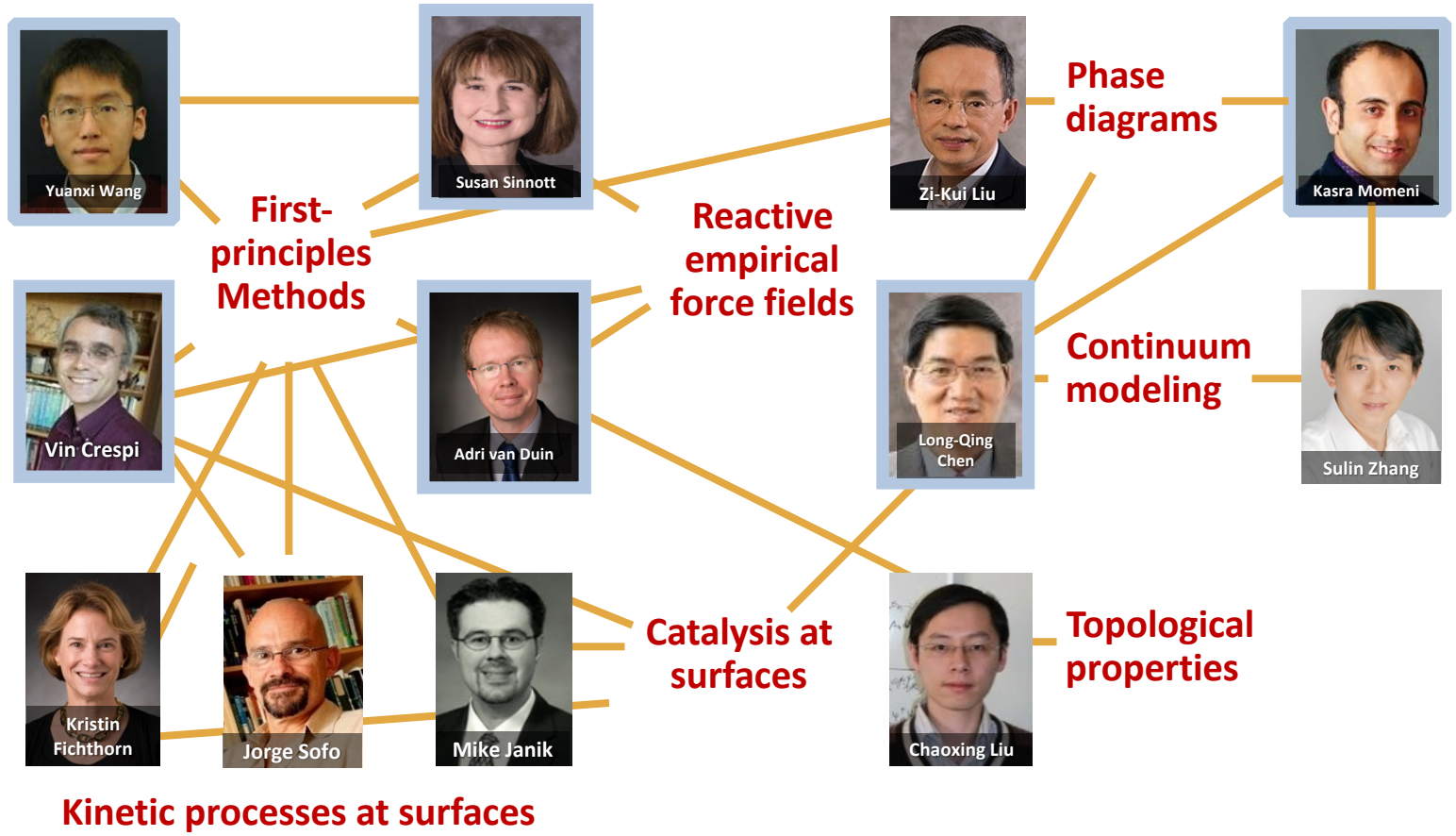




Desire for high quality single crystal with Fermi level located in the bulk bandgap

The 2DCC Theory/Simulation "Facility" is Hardware + Software + People

- High memory + Low memory compute nodes and storage
- Reactive force fields, phase field models, first-principles codes
- Theory "bullpen" :

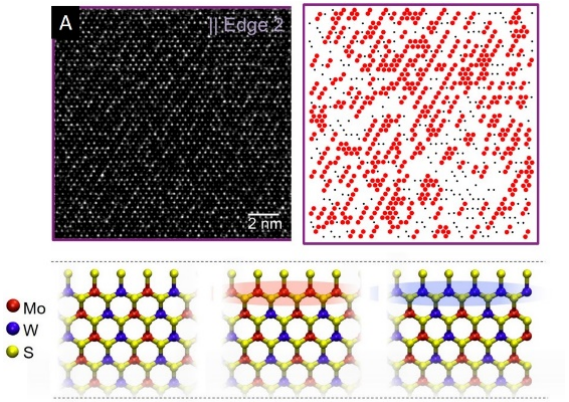


2DCC Research and Publication Highlights

2DCC publications: 2 (2016), 13 (2017), 6+ (2018)

In-House Research:

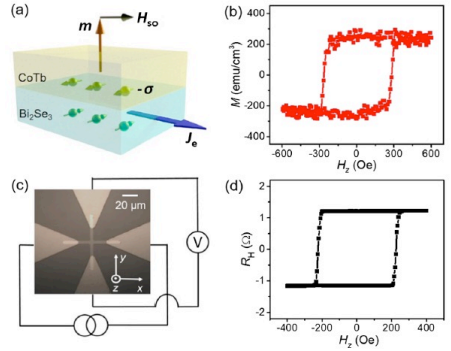
Atomically thin stripes in $Mo_xW_{1-x}S_2$ monolayers



A. Azizi, Y.X. Wang, Z. Lin, K. Wang, A.L. Elias, M. Terrones, V.H. Crespi and N. Alem, Nano Lett. 16, 6982 (2016)

External User Project:

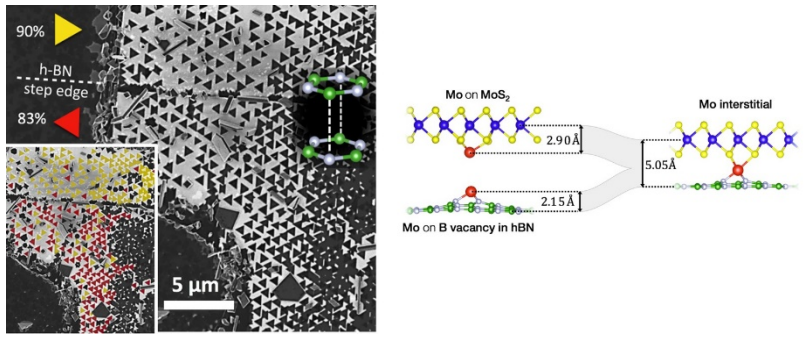
Room temperature spin-orbit torque switching induced by a topological insulator



J. Han, A. Richardella, S.A. Siddiqui, J. Finley, N. Samarth and L.Q. Liu, Phys. Rev. Lett. 119, 077702 (2017)

In-House Research:

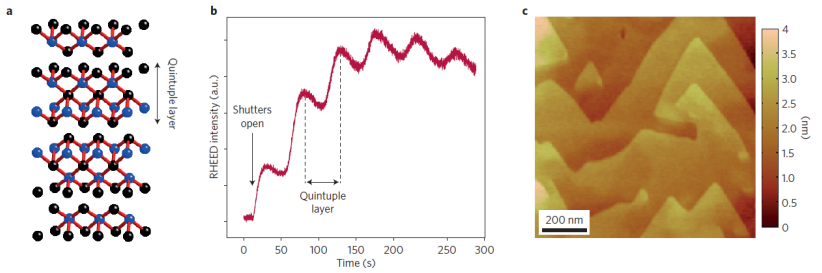
Epitaxy of MoS_2 on h-BN without mirror boundaries



F. Zhang, Y.X. Wang, V.H. Crespi and N. Alem, arXiv:1801.00487

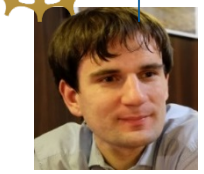
Review Article:

Quantum materials discovery - a synthesis perspective



N. Samarth, Nature Materials 16, 1068 (2017).

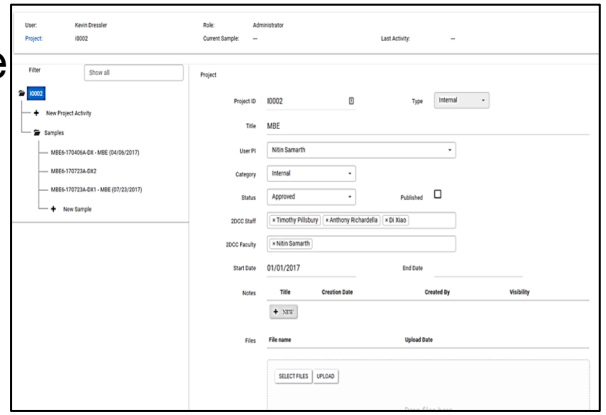
Data Management/Data-Enabled Science



Konrad Hilse
Data Mgmnt Spec.

Lifetime Sample Tracking (LiST) Database Development

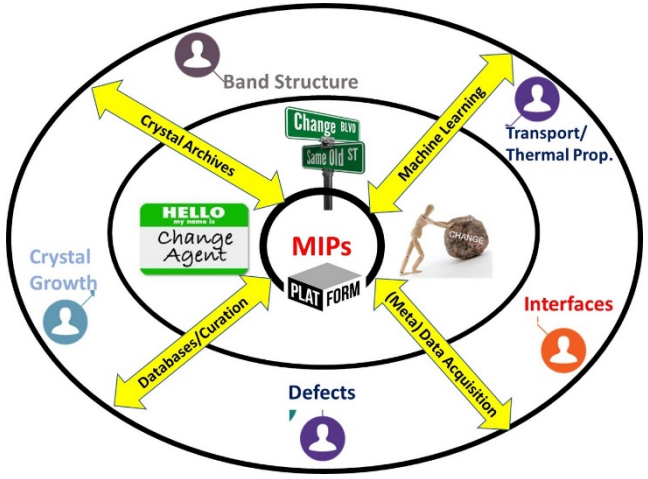
- Centralized database for sample tracking and curation
- Designed to capture all information associated with sample production, characterization, usage, storage
- Organized based on user project/in-house research
- Web interface personalized for each facility
- Accessible to external users



Example of LiST interface for MBE sample tracking

NSF DMR 2D Data Framework

- Working group focused on application of data science to 2D materials
- 2DCC-related activities:
  - High throughput modeling
  - Machine learning for materials discovery
  - Metadata acquisition and curation



2D Data Framework (courtesy of Eva Campo, NSF)

Outreach and Education

Monthly Webinars

~42 external participants each month
(19 unique institutions)

Graphene & Beyond Workshop

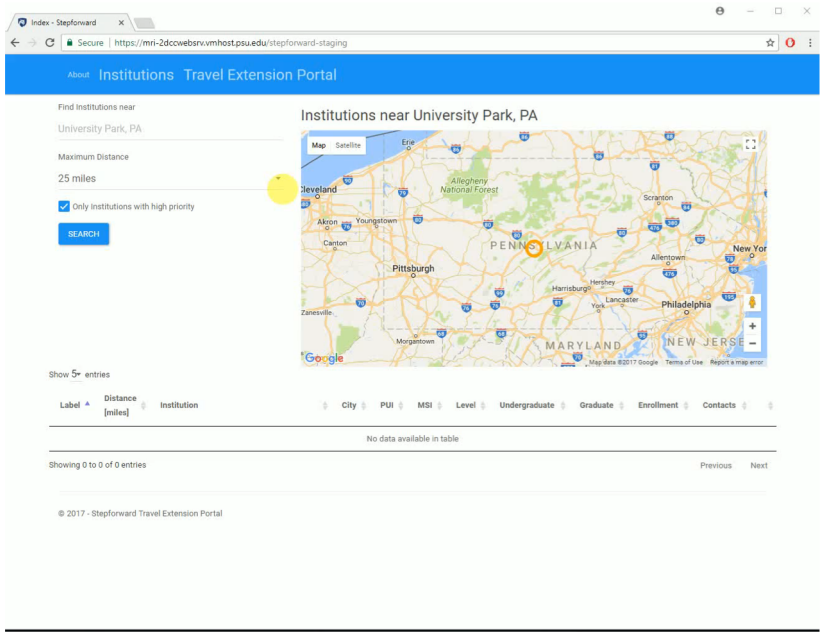
2018 meeting – 6th consecutive year

~175 attendees at workshop held May 9-12, 2018

STEPFORWARD Program

Outreach visits by 2DCC faculty/staff to PUIs & MSIs

(5 visits in 2016-2018)



Want more information?

Check out our website

www.2dcc.psu.edu