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)

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

Basic components of a MIP:
- National User Facility/Program
- In-House Research
- Education and Outreach

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
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.
2DCC User Facilities

Thin Films and In-Situ Characterization
- MBE grown (Bi,Sb)$_2$Te$_3$
- MOCVD WSe$_2$

Bulk Crystal Growth
- CVT grown WTe$_2$
- Bridgman grown Bi$_2$Se$_3$

Theory and Simulation
- Finite length grain boundaries on curved surfaces
- Fluid dynamics simulation of MOCVD reactor

Millennium Science Complex – First Floor

- Nanofab
- 2DCC-MIP
- MBE Lab
- MBE System 1
- CVD Lab
- MOCVD System 1
- MOCVD System 2
- Bulk Growth Lab
- Bridgman System
- CVT Furnaces

MBE System 2 located in basement of Davey Lab
2DCC Facilities - Experimental

- Hybrid MBE for Chalcogenides and Oxides
- Multi-Module UHV System
  - Solid Source MBE + Cryo ARPES
  - 4 probe STM
- Chalcogenide MOCVD
- Multi-Module MOCVD + ellipsometry and Raman/PL
- Vertical Bridgman
- CVT
- Compounding Furnace
Vertical Bridgman Synthesis of Bulk Bi$_2$Se$_3$
Topological Insulating Single Crystals

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”:

  - First-principles Methods
  - Reactive empirical force fields
  - Continuum modeling
  - Topological properties
  - Catalysis at surfaces
  - Kinetic processes at surfaces
  - Phase diagrams

People:
- Yuansi Wang
- Vin Crespi
- Susan Sinnott
- Ji-Kui Liu
- Kasra Momeni
- Long-Qing Chan
- Sulin Zhang
- Mike Janik
- Kristin Reichenbecher
- Jorge Sofo
- Chaosong Liu
- Adri van Duin
- Susan Sinnott
- Kristin Fichthorn
- Mike Janik
- Yuanxi Wang
2DCC Research and Publication Highlights


**In-House Research:**
Atomically thin stripes in Mo$_x$W$_{1-x}$S$_2$ monolayers

![Image of atomically thin stripes in Mo$_x$W$_{1-x}$S$_2$ monolayers]


**External User Project:**
Room temperature spin-orbit torque switching induced by a topological insulator

![Image of spin-orbit torque switching induced by a topological insulator]


**In-House Research:**
Epitaxy of MoS$_2$ on h-BN without mirror boundaries

![Image of epitaxy of MoS$_2$ on h-BN without mirror boundaries]


**Review Article:**
Quantum materials discovery - a synthesis perspective

![Image of quantum materials discovery]

Data Management/Data-Enabled Science

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

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
Outreach and Education

Monthly Webinars

Graphene & Beyond Workshop

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