2D Crystal Consortium
NSF Materials Innovation Platform

STRATEGIC AND IMPLEMENTATION PLAN

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Executive Summary

The Two-Dimensional (2D) Crystal Consortium-Materials Innovation Platform (hereafter "2DCC-MIP" or "2DCC") focuses on the discovery and development of two-dimensional layered chalcogenides (2DLC) for fundamental science and applications in next-generation electronics and quantum technologies. These materials include transition metal dichalcogenide (TMD) films that are only a few atoms thick, topological insulator (TI) bismuth chalcogenide films that only conduct on the 2D surface, and multilayers of dissimilar chalcogenide films whose properties are dominated by 2D interfaces. The 2DCC-MIP is motivated by the potential of 2DLCs for new physics and high-impact technologies tempered by the significant challenges associated with their synthesis. The interplay between topology, dimensionality, and interactions in 2DLCs provides a rich landscape for studies of emergent quantum phenomena (such as Majorana zero modes) and transformative technology such as topological spintronic devices for non-volatile memory, triggered single-photon sources at room temperature and low-power nanoelectronics and sensor technology. Related 2D materials which form heterostructures with 2DLCs, such as graphene, hexagonal boron nitride and 2D metals, also fall within the purview of platform interests.

The 2DCC-MIP develops state-of-the-art epitaxial growth capabilities in molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD) of 2DLCs; novel synthetic methods for 2D materials synthesis via confinement heteroepitaxy; innovative bulk growth methodologies for multicomponent chalcogenide crystals including high-pressure and continuous feed approaches; and multiscale process modeling capabilities with direct simulation of reaction kinetics. This synthesis web is interconnected with a comprehensive suite of advanced spectroscopy, scanning probe and layer transfer/processing tools allowing sample exchange while maintaining vacuum or inert-gas environments, all feeding into a comprehensive sample data tracking system that embeds knowledge graph functionality. Knowledge graphs contain both data and an ontology describing relationships between the data which enables new relationships not explicitly provided to be inferred. This facilitates more natural modes of interaction with the data such as question-and-answer, recommendations, etc. enabling new modes of data-enabled materials discovery, informed by advanced materials simulation and modeling.

In addition to the on-going research, user program, knowledge transfer, outreach and training activities that continue to advance beyond the first five years of facility operation, additional **goals for year 6** of operation (June 1, 2021 – May 30, 2022) include:

(1) Acquiring and developing instrumentation: several new pieces of equipment will expand existing capabilities. This includes a Double Crucible Vertical Bridgman (DCVB) system for the Bulk Growth Facility; a high-pressure thermal evaporator with in-situ plasma source for confinement heteroepitaxy for the Thin Films Facility and a Glovebox Cluster Tool (GCT) layer transfer and alignment system which cuts across experimental facilities. As of September 1, 2021, purchase orders have been placed for all new equipment and shipment is expected within 6–12 months.

(2) Hiring 2DCC technical staff: technical staff have been recruited to work on two of the new pieces of equipment (high pressure thermal evaporator and glovebox cluster). A postdoctoral scholar will be hired at the beginning of year 7 to work on the DCVB system which will be delivered in that timeframe. A postdoctoral scholar with expertise in data science has been recruited to work on knowledge graph development in the Theory/Simulation/Data facility. Additional staff will be hired to fill open positions at the Assistant Research Professor and postdoctoral scholar levels in the Thin Films and Theory/Simulation facilities.

(3) Advancing synthesis science of 2DLCs and materials discovery goals include: 1) Use molecular beam

epitaxy to improve the crystalline perfection of magnetically-doped topological insulator heterostructures, develop control over interfacial/topological superconductivity, develop new chalcogenide topological semimetals, and develop new types of 2D van der Waals ferromagnets. 2) Synthesize intrinsic ferromagnetic TIs with controlled chemical potential using the flux method and assess their potential as novel topological quantum materials. 3) Identify the origin of step-assisted domain alignment in TMDs grown epitaxially on sapphire and determine optimum conditions to achieve wafer-scale inversion domain-free monolayers. 4) Use ReaxFF reactive potentials developed for TMDs to provide theory support for in-house and external user projects. 5) Discover and develop new 2D heterostructures enabled by combinations of current and new thin-film and bulk growth techniques as enabled by the GCT coupled to the integrated vacuum/inert gas environment.

(4) Advancing data management/data science: A data science working group has been established that meets monthly to coordinate activities between the existing data management team and the new data science researchers. Information in the existing Lifetime Sample Tracking (LiST) database will be made accessible to external users and curated datasets will be made available to the public. A knowledge graph framework and ontology for LiST 2.0 will be developed, and we will pursue development of a national DMR instrument database.

(5) Increasing training opportunities for external users – The Resident Scholar Visitor Program (RSVP) was initiated in year 5 to provide opportunities for extended stays at the 2DCC-MIP facility by graduate students and early career researchers to facilitate training of the next generation of crystal growers and tool developers. In year 6, we will increase the number of on-site RSVP participants from 4 to 8 to accommodate growing interest.

(6) Building partnerships to enhance impact and broaden participation. In year 6, we will be kicking off a 5-year Partnerships in Research and Education in Materials (PREM) program with Florida International University, a Hispanic-serving institution entitled “Innovations in Materials, Processes and Applications for Quantum Technologies (IMPAQT).”

(7) Increasing participation by industry and government labs users. An industry outreach coordinator has been identified for the 2DCC-MIP facility to assist in the development of outreach plans to potential industry users. We will pursue joint funding opportunities with industry (e.g. STTR) and begin initial discussions with the Pennsylvania Department of Community and Economic Development (PA DCED) on workforce development initiatives.

1.0 Facility Overview

1.1 Vision and Mission of the 2DCC

2DCC Vision
Advance discovery-driven research into the growth, properties and applications of 2D layered chalcogenide crystals and related 2D materials for next-generation technologies by innovating state-of-the-art synthesis, characterization and data/computational tools to foster a diverse scientific ecosystem of in-house experts and external users to drive international leadership by the US 2D materials research community.

2DCC Mission

1. Accelerate discovery in 2D chalcogenide materials by operating a world-class user facility that includes:
   a) a closed loop iterative collaboration of thin film and bulk growth synthesis techniques, *in situ* characterization, and predictive modeling of growth mechanisms and processes
   b) a community of practitioners that combines the expertise of an in-house research program and external users
   c) open sharing of knowledge, best practices, and publication-quality data

2. Provide access to synthesis, in-situ characterization and theory/simulation user facilities including instrumentation and expertise to users through a competitive proposal process

3. Maintain a vibrant in-house research program in synthesis, characterization, and theory/simulation of 2D chalcogenides to drive advances in the field

4. Engage a diverse user base from academia, government, and industry in the U.S. and internationally and increase participation of women and underrepresented groups in science and technology through diverse representation in staffing and research activities.

1.2 Five-year Goals

The following five-year goals are high-level objectives that reach across the facility. Progress toward these goals will be reported to the NSF on a yearly basis, tracked by the 2DCC leadership and the 2DCC External Advisory Committee, and evaluated regularly by external expert panels as designated by the NSF.

- **The 2DCC will be a worldwide example of a successful user facility devoted to the synthesis of 2D chalcogenides and will stimulate the revitalization of the science of crystal growth and epitaxy in the U.S.**
  Progress is monitored through regular review by an external panel of experts informed by quantitative statistics on the productivity, scope, and impact of the external user program and 2DCC-sponsored workshops, including metrics on co-authorship and acknowledgement of the 2DCC in publications and other research products.

- **The 2DCC will develop foundational knowledge in bulk and thin film crystal growth of 2D layered chalcogenide crystals to enable atomic-level control of composition and crystallinity in wafer-scale epitaxial films and heterostructures and realize novel chalcogenide phases and structures.**

Progress is monitored by the quality and reproducibility of materials produced by the facility, the quality of publications related to the synthesis and properties of 2DLCs and the number of new material compositions and structures made available to the userbase each year, as assessed through regular review by an external panel of experts.

- **The 2DCC will maintain a comprehensive database of synthesis and characterization data for all samples produced in the facility that is consistent with FAIR principles and will develop innovative data science techniques that use the data for prediction and discovery.**
  Progress is monitored through regular tracking of database content, user and public access and demonstration of data science related in-house and user projects and publications.

- **The 2DCC will continue to promote a materials genome approach to accelerated discovery and development of 2D thin films and crystals.**
  Progress is monitored through regular review by an external panel of experts that is informed by the percentage of user projects and publications supported by the 2DCC that employ a combination of theory/simulation and experiment, as well as the capability and impact of new theory and simulation tools and resources made available to the research community.

- **The 2DCC will continue to foster a community of researchers in 2D synthesis and promote the science of crystal growth and epitaxy through training, education, and knowledge transfer focused on the synthesis of 2D chalcogenides.**
  Progress is monitored through regular review that is informed by quantitative statistics on MIP equipment time allocations and user participation in 2DCC-sponsored workshops, seminars, professional development activities, user career development outcomes, and progress towards commercialization of 2DCC-derived technologies.
  - *A minimum of 50% of equipment time will be allocated for external users.*
  - *A minimum of 10% of equipment time will be allocated for users from non-R1 institutions.*

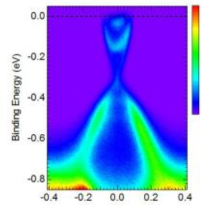
- **The 2DCC will continue to foster a robust external user base spanning academia, industry, and national labs including representation from early-career faculty and faculty from Non-R1 and/or facility-limited institutions .**
  Progress is monitored by user program participant statistics and on-site training as assessed through regular review by an external panel of experts.

1.3 User Program

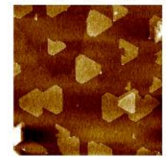
The 2DCC user program is focused on the synthesis of 2D chalcogenides for next generation electronics and quantum technologies and includes priorities that are accomplished by a community of practitioners that collaborate among the in-house research and external user programs. Over time, priorities will be adjusted by meritorious peer-reviewed proposals, user committee recommendations, and input from the 2DCC external advisory committee.

1.3.1 Science Drivers

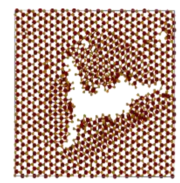
The 2DCC research priorities are organized by three science drivers that are motivated by the unique properties of layered materials that often emerge in ultrathin or few-layer films, necessitating atomic-level control of film growth mode, stoichiometry, point defects and structural imperfections.



Physics of 2D Systems (Phys2D) – provide enabling materials synthesis, characterization, and modeling capabilities to facilitate fundamental studies of new fundamental physical processes that occur in 2D systems, such as efficient spin-charge conversion and the quantum anomalous Hall effect in topological insulators, valleytronics in transition metal dichalcogenides, and quantum transport in 2D heterostructures.



Epitaxy of 2D Chalcogenides (Epi2DC) – understand fundamental mechanisms of 2D film formation in van der Waals bonded systems including the role of the substrate in nucleation and epitaxy, self-limited growth of monolayers, epitaxy in 2D heterostructures, miscibility and alloy formation, intentional doping, and native defects.

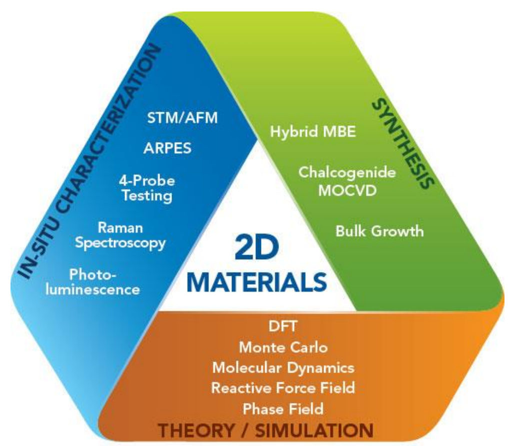


Advanced Characterization and Modelling (AdvCM) – develop techniques and tools to both probe and model 2D chalcogenide films in situ to study the evolution of surface morphology, lateral and vertical domain growth, growth-related defects and grain boundaries, electronic band structure, carrier transport, closely integrated with theory and simulation that targets key kinetic processes during growth, enables new insights on in situ characterization, and accelerates the process of identifying compelling synthetic targets and overcoming experimental obstacles to their synthesis.

1.3.2 2DCC Facility Components

The 2DCC's state-of-the-art synthesis and characterization facilities, located in the Millennium Science Complex and Davey Labs on the Pennsylvania State University campus, support a robust external user program and an in-house research effort focused on transformative advances in the synthesis and characterization of 2D chalcogenide layered materials.

The 2DCC user facility includes three main components:
(1) *Thin Films Facility*
(2) *Bulk Crystal Growth Facility*
(3) *Theory/Simulation/Data Facility*.



Closed Development Loop

The three 2DCC facility components and the additional leveraged facilities described in section 1.3.4 (which are independent of 2DCC governance) are all under the auspices of the Materials Research Institute which is part of the Vice President for Research Office at Penn State.

(1) <u>Thin Films Facility</u>

The 2DCC-MIP Thin Films Facility includes state-of-the-art equipment for epitaxial growth of 2DLC thin films by molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD). A high-pressure thermal evaporator with integrated plasma source is under development for synthesis of 2D metals and related materials via confinement heteroepitaxy. A suite of advanced characterization tools are available for in situ, in vacuo and ambient controlled characterization including laser and vacuum ultra-violet (VUV) angle-resolved photoelectron spectroscopy (ARPES), four-probe scanning tunneling microscopy (STM), confocal Raman and photoluminescence (PL) spectroscopy and mapping and spectroscopic ellipsometry. Vacuum suitcase integration enables sample transfer between tools for multi-technique synthesis, processing and characterization of samples without air exposure.

Multi-Module UHV MBE Growth and Characterization System (MBE1)

A multi-module ultra-high vacuum (UHV) growth and characterization system for chalcogenide films is located in 35 Davey Laboratory. The cluster tool consists of an MBE system connected with in-situ cryogenic ARPES and four-tip STM tools. The cryogenic ARPES module features a high intensity helium plasma source and monochromator and is also equipped with a tunable-wavelength Y-Fi laser light source. Samples can be transferred directly into the characterization tools, without exposing them to atmosphere, allowing the properties of pristine surfaces to be studied. Ports for seven thermal effusion cells and a six-pocket e-beam evaporator allow a wide range of materials to be fabricated. In-situ Reflection High Energy Electron Diffraction (RHEED) and spectroscopic ellipsometry allow real-time characterization of films as they grow. The MBE system can grow on up to 2 inch wafers. An adaptor to flag style holders allows growth on up to 1 cm^2 substrates that can be transferred in the ARPES and STM modules. The nanoprobe STM features 4 independent tips that can be used for 4-point in-situ electrical transport measurements down to 4.5 K. The integrated scanning electron microscope (SEM) can be used to position each tip independently over chosen features of the sample with a resolution better than 1 micron. Each tip is capable of scanning tunneling measurements although currently only one tip can be used for STM at a time. A small superconducting coil under the sample stage can produce magnetic fields up to 200 Gauss. Argon sputtering is available for tip and sample cleaning and preparation.

Hybrid MBE (MBE2)

The 2DCC Hybrid Chalcogenide Molecular Beam Epitaxial (MBE) system is dedicated to the growth of chalcogenide thin films. The hybrid MBE approach enables the synthesis of chalcogenide materials from molecular precursors through the addition of a gas injector system giving access to a different growth kinetics, potentially favorable for transition metal elements with low vapor pressures. The MBE reactor is equipped with a series of state of the art *in-situ* monitoring capabilities, such as reflection high energy electron diffraction (RHEED), ion gauge beam flux monitor, residual gas analyzer, heated quartz crystal monitor, and a spectroscopic ellipsometer. The hybrid chalcogenide MBE can handle wafers up to 3 inches. The chalcogenide MBE reactor is connected via a UHV transfer line with an oxide MBE reactor and a sputter deposition system. The *in-vacuo* transfer between the components of the cluster enables the integration of chemically dissimilar materials, such as growth of chalcogenide films on oxide thin films, as well as capping chalcogenide thin films using sputter deposition tool or integration of top electrodes via shadow mask onto the film without breaking vacuum to minimize potential contamination of film surfaces. A port is available for connection of a vacuum suitcase for *in-vacuo* sample exchange between systems within the 2DCC facility.

Chalcogenide MOCVD System (MOCVD1)

MOCVD1 includes a horizonal cold wall MOCVD quartz tube reactor with induction heating and is equipped for growth on substrates up to 2 inch diameter. Gas foil rotation of the wafer holder is used to improve uniformity. The reactor loads and unloads through a nitrogen-purged glovebox which prevents exposure of the reactor and sample to ambient air. The gas panel includes pneumatic valves, mass flow controllers and pressure controllers and separate pressure-controlled run/vent manifolds for the metal and chalcogen sources. Six bubbler stations are available for solid or liquid precursor and four gas source connections are available. A separate connection is available for chloride precursors. A chemically resistant rotary vane pump enables operation from 10 to 700 Torr. System operation is automated through a recipe driven LabView program and is equipped with interlocks to enable safe system shutdown in the event of a loss of carrier gas, toxic gas alarm or reactor failure. A water scrubber equipped with a sodium hydroxide neutralization system treats the reactor effluents to safe limits.

Multi-Module MOCVD Growth and Characterization System (MOCVD2)

MOCVD2 is a custom designed multi-module system from CVD Equipment Corporation. The system includes a load lock and high vacuum robotic transfer stage. The stainless-steel MOCVD chamber consists of temperature-controlled wall and flanges and a rotating, resistively heated 2" diameter substrate holder for substrate temperatures up to 1000 ^{o}C. The MOCVD reactor includes two purged optical ports for *in situ* spectroscopic ellipsometry and a third for sample viewing. A chemically resistant rotary vane pump enables system operation from 10 to 700 Torr. The gas manifold is comprised of welded stainless-steel tubing with metal gasket seal fittings, pneumatically controlled valves, pressure controllers and mass flow controllers. Six bubbler manifolds are available for liquid or solid precursors two of which include double dilution and two which can be maintained at elevated temperature (up to 200^{o}C) for low vapor pressure sources. Three pressure balanced vent/run manifolds are available for metal, chalcogen and dopant precursors. System operation includes recipe-driven control and data logging. The system has an interlocked safety system including toxic gas monitoring, H_2 detection and other alarms for safe operation. A pyrolyzer/water scrubber equipped with a sodium hydroxide neutralization system treats the reactor effluents to safe limits. The robotic transfer stage enables transfer of samples directly from the MOCVD growth chamber into a custom designed glovebox for optical characterization. A WITec apyron confocal microscope is housed in the glovebox to enable ambient-controlled Raman and photoluminescence measurements.

(2) Bulk Crystal Growth Facility

The 2DCC-MIP Bulk Crystal Growth facility is focused on the growth of layered chalcogenide bulk crystals through chemical vapor transport (CVT) and melt growth techniques. The bulk crystal growth facility includes multiple CVT furnaces, a vertical Bridgman (3-zone) furnace, a compounding furnace, six muffle furnaces, an arc-melting furnace for metallic tube sealing, a diamond saw, ampoule sealing and chemical transport stations, and a glove box. The furnaces have automated temperature control and the capability to simultaneously anneal multiple sample tubes to enable rapid analysis of a larger parameter space. Several glove boxes are available for sample preparation without air exposure.

(3) Theory/Simulation/Data Facility

The 2DCC-MIP Theory/Simulation/Data Facility is used to develop key simulation capabilities of general use by in-house and external users and the broader community in modeling and understanding growth of 2DLCs and related 2D materials. Reactive force field development, guided by first-principles expertise, expands the capabilities to handle precursor chemistry and substrate interactions. Additional efforts enable macroscale simulation of the thermal-fluid environment in process chambers and development of theoretical and data-driven tools and results for the interpretation of characterization data, identification of new synthetic targets, and optimization of growth conditions. Data-driven discovery oriented around materials growth integrates theory and computation with comprehensive experimental growth protocols and characterization data that is acquired, curated, and analyzed across the diverse growth tools and sample types of the 2DCC. Knowledge graphs which define relationships between data and machine learning techniques are further employed to accelerate materials discovery.

1.3.3 Penn State Facilities Leveraged by the 2DCC

Materials Characterization Laboratory (MCL) (https://www.mri.psu.edu/materials-characterization-lab) The Materials Characterization Lab (MCL) is a fully staffed, open access, analytical research facility at Pennsylvania State University's Materials Research Institute. Current MCL capabilities include microscopy, surface chemical spectroscopies, X-ray scattering, molecular spectroscopy, thermal analysis, particle characterization, electrical characterization, and materials processing. Access to the MCL facilities is available through the user research proposal process.

Nanofabrication Laboratory (Nanofab) (https://www.mri.psu.edu/nanofabrication-lab)

The Nanofabrication cleanroom facility is a fully staffed, open access, clean room facility at Pennsylvania State University's Materials Research Institute. The Nanofab encompasses class 1000/100 space and sub-fab support space, with capabilities in lithography, deposition, etch and "bottom-up" nanofabrication. Access to the Nanofab facilities is available through the user research proposal process.

Materials Computation Center (MCC) (https://www.mri.psu.edu/materials-computation-center), The Materials Computation Center (MCC) in partnership with the Institute for Computational and Data Sciences (ICDS), provides broad licensing and technical support for a diverse suite of advanced materials simulation software and associated computational hardware platforms. MCC staff support materials computation efforts across the university on a broad range of materials systems and complement the activities of the 2DCC-MIP Theory/Simulation/Data facility which focuses on layered chalcogenide systems and related 2D materials. 2DCC users have access to MCC capabilities in computational methods including first-principles techniques at the density functional level (Quantum Espresso, VASP, etc.) and powerful empirical methods that can model complex reaction pathways over long time scales and length scales at both atomistic (ReaxFF) and phase-field levels.

Institute for Computational and Data Sciences (ICDS) (https://www.icds.psu.edu/). ICDS is Pennsylvania State University's computational hub and supports high performance computing solutions campus wide, providing access to the Roar supercomputer, a high-performance computing cloud network. 2DCC in-house researchers and users access the Roar computational network for projects associated with the Theory/Simulation/Data facility.

Physics User Facilities (https://www.mri.psu.edu/2d-crystal-consortium/user-facilities/related-facilities). The Pennsylvania State University's Physics Department has user facilities for low temperature magnetometry and magnetotransport measurements. This includes a multimode atomic force microscopy (AFM) / magnetic force microscopy (MFM) / STM system, two superconducting quantum interference device (SQUID) magnetometers, three physical property measurement systems (PPMS) / magnetic property measurement systems (MPMS) systems for magneto-transport measurements over a temperature range from 50 mK - 300 K and magnetic fields from 0 - 8 T.

1.4 Education/Training/Broadening Participation

The 2DCC offers programs that address:

- Engagement of a diverse user base from academia, government and industry in the U.S. and internationally; and
- Broadening participation of women and minorities underrepresented in science technology engineering and mathematics through diverse representation in staffing and research activities.

1.4.1 Website (http://www.mip.psu.edu)

The 2DCC website provides an online resource for engagement with the broader community and is specifically directed at providing information for current and potential users. The 2DCC website is a portal for hosting of educational and knowledge transfer materials such as webinars, tutorials, user facility information, proposal submission portal and procedures, news and upcoming events, the facility data management tool and available sample information and general information regarding the 2DCC Facility. *Target audience*: All academic levels, government, industry, potential and current users, general public

1.4.2 Webinar Series

The webinar series was established in June 2016 and includes technical talks from internal and external speakers as well as topics concerning the science related to broadening participation in research. The webinars are operated as live broadcasts on the web and are recorded for broader dissemination via the

website, post session.
Target audience: All academic levels, government, industry, potential and current users

1.4.3 Graphene and Beyond Workshop

The Graphene and Beyond Workshop brings together participants from academia, government and industry to enhance synergy within the community and build toward a strong future in 2D crystal science and technology. The workshop topics focus on 2D material synthesis, characterization, processing, properties, theory/simulations and applications and includes seminars on recent results from the 2DCC and other institutions. The workshop also features focused discussions on intellectual property and commercialization opportunities of 2D materials.
Target audience: All academic levels, government, industry, potential and current users

1.4.4 Resident Scholar Visitor Program (RSVP)

RSVP is an on-site training and professional development activity for graduate students and early career researchers. The program provides travel and housing support for extended visits at the 2DCC-MIP facility ranging from 2 weeks to 6 months. The purpose is to enable participants to become independently trained to operate complex synthesis equipment and carry out more extensive research projects than would be feasible in a shorter period of time.
Target audience: Graduate students, postdoctoral scholars and early career faculty.

1.4.5 Research Experiences for Undergraduates (REU)

An NSF REU site award entitled "Nanomanufacturing of Complex Nanomaterials" has provided additional resources enabling 2DCC-MIP to host undergraduate students in the facility in-person during the summer of 2019 and virtually during the summers of 2020 and 2021 in collaboration with the Penn State Nanofab. The current REU award will support undergraduates in summer 2022 and funding will be sought to continue the program for an additional three years.
Target audience: Undergraduate students, particularly those associated with user research groups, Non-R1 institutions and institutions with limited facilities to conduct research.

1.4.6 Science Travel Extension Program for Outreach Representatives Working to Advance Research Diversity (STEP FORWARD) for all career levels and institutions

The STEP FORWARD program aids faculty with travel plans to identify nearby institutions with limited research facilities or instrumentation and/or early career faculty that may be interested in the 2DCC research or access to the facility. This program assists in making contact with those institutions and potential users to arrange a visit, and provides funding to cover travel expenses incurred by 2DCC personnel for this activity to ensure the broadest participation of interested potential users and dissemination of 2DCC outcomes to the community.
Target audience: Junior and senior faculty, postdocs, graduate and undergraduate students

2.0 Knowledge Sharing

The "Platform" in Materials Innovation Platform has several aspects. First, activities within the 2DCC are *synergistic*. Examples of synergy include cross-fertilization of the User Program and in-house research, tight iterative coupling of experiment to theory and computation, *in vacuo* and inert-ambient sample exchange across the platform, and multiuser collaborations sparked by the annual User Meetings. Second, platform offerings reach outward in a series of expanding circles of interaction and support (Fig. 2.1) that provide *multiple entry points* for members of the materials community to utilize 2DCC resources whether samples, reactive potentials, data curation services, research consultation, tutorials, reviews and roadmaps, visitor programs, etc. Third, the 2DCC has a mission to develop and maintain pioneering *user-serving data infrastructure*, specifically the LiST data curation tool and its proposed transformative extensions. This multilayered array of interaction points for users, visitors, personnel, data clients, and others across career stages is designed to accelerate discovery and application of new materials phenomena.

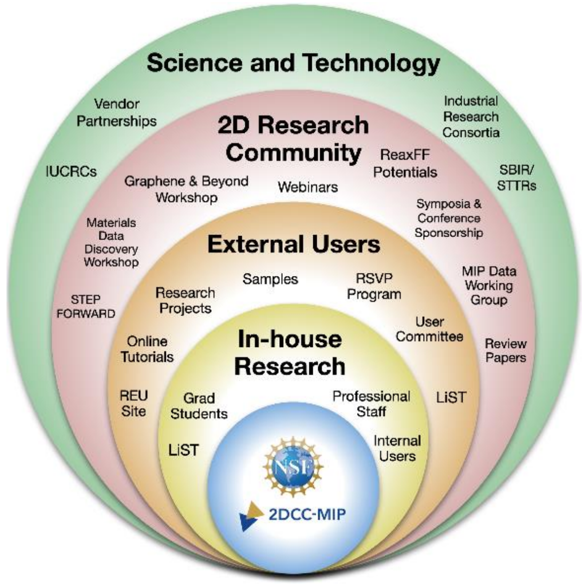


Figure 2.1. 2DCC provides multiple layers of engagement as part of a growing NSF-MIP-supported ecosystem for materials synthesis.

Note: Knowledge sharing aspects cross-related to education and training such as Graphene and Beyond, Webinars, RSVP program, REU Site are described in the Education/Training and Broadening Participation sections of this strategic plan. This section focuses specifically on the data and infrastructure of LiST 1.0, List 2.0 and ReaxFF potentials.

2.1 LiST 1.0

The Lifetime Sample Tracking Tool (LiST) version 1.0 was created in the first five years of the platform (March 2016 – February 2021). LiST is a capture and curation tool for growth and characterization data on all samples produced by the Platform (5000+ thus far) to share with users upon request and to build up a comprehensive communal data resource to enable new modes of discovery. The LiST 1.0 interface is depicted in Figure 2.2. The organization and availability of sample data within the LiST framework facilitated a new mode of knowledge sharing – the data request mechanism – which was added to the 2DCC User Program in 2019 to enable users to access experimental and computational data for data science projects.

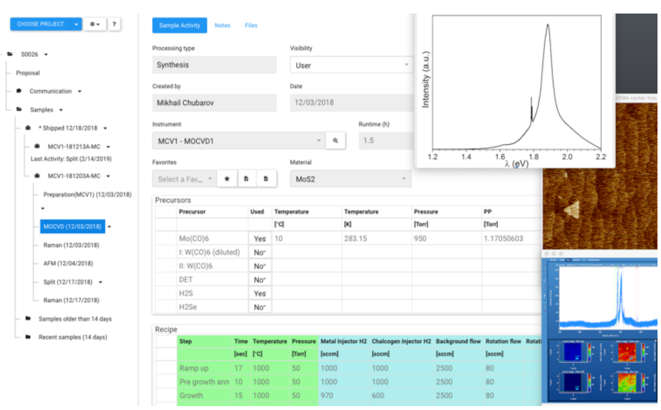


Figure 2.2. LiST captures and curates comprehensive growth protocol and characterization data on all samples produced in the 2DCC, both user and in-house.

We refer to LiST 1.0 as the capture and curation core infrastructure of the tool and LiST 2.0 as the data science extension, or module, of the tool. LiST 1.0 will continue to be maintained and targeted for upgrades for data access:

Goals

- Upgrade authentication
- Enhance data accessibility to both public and users
- Upgrade day-to-day operational aspects for ease of end-user use
- Capture and curate archive quality simulation data

Milestones and Timeline

Year 6

Shibboleth Authentication

- Use Shibboleth as an alternative for authentication to let users log into LiST using their institution account
- Allows to grant access to the community (for public data) while still being able to track who is accessing the data

Data Only Projects

- Enhance software for personnel to self-select samples to a data-only project and configure access through that project

Public Data Sets

- Configure publication related data sets
  (synthesis and/or characterization data on samples, simulation setup and/or result)
- Make such data sets accessible via publications, and/or create DOIs for such data sets

Year 6-7

Alignment to Community Standards

- Review community data standards
- Develop and further align to community efforts in emerging data standards and vocabularies for synthesis and characterization

Year 7

Communication and File Exchange

- Provide a web form directly in LiST where users can create their reports (as opposed to using a word template)
- Enhanced user data access efficiency (e.g. download zip files of selectable grouping of files)

API Access to LiST

- Make LiST API accessible for other tools (other than the web frontend)
- Allow fine granular authorization for API users
- Generate documentation automatically from the source code

Tighter integration with synthesis software

- Enable synthesis machine software that controls experiments to capture basic sample data (ID, user, material, substrate, etc.)
- Have LiST import those data automatically, assuring that all samples are known in LiST
- Attach / import recipe and log files automatically

Year 8

File storage backends

- Implement additional backends to ensure long-term data storage and access (e.g. currently SharePoint)

Synthesis Recipe Configurator

- Create a frontend tool that allows researchers to configure and test their synthesis recipe templates

Years 9 and 10

- Receive feedback in Year 8 from Users on future enhancements focusing on usability and analysis, etc
- Ongoing software maintenance
- Integration of LiST 2.0 data analytics, machine learning tools and Jupyter Notebook

Anticipated Outcomes

LiST 1.0 enhancements are expected to increase user access and ease of use to accelerate the route to discovery. Additionally, the software enhancements will reduce day-to-day workloads of facility personnel via automation of ingestion routines for machine read-out as well as make significant contributions to the efforts of LiST 2.0. The further development of LiST to align to community efforts in emerging data standards and vocabularies around diverse categories of characterization and synthesis data will ensure advancing goals in interoperability and reuse of data. LiST 1.0 already represents a significant effort in knowledge sharing with users and among facility personnel and the planned efforts above will ensure the same is true for the broader scientific community at large.

2.2 LiST 2.0

LiST 2.0 was inspired by the success of the LiST 1.0 capture and curation tool in the first five-year performance period. It is a new aspect to the 2DCC in-house research as of the renewal. Once completed, LiST 2.0 will provide 2DCC researchers and users unprecedented insight into the data gathered through the LiST interface using data analytics and machine learning tools. This will require interdisciplinary research efforts bridging state-of-the-art machine learning and materials science.

Goals

- Develop applications for both scientific insight and practical quality of life improvements for the LiST database using state-of-the-art machine learning and data science methods.
- Demonstrate those applications (i.e. LiST 2.0) through 2DCC in-house research projects to build competence and a portfolio of case studies to share with the public.
- Deploy those applications to solve logistical and scientific problems for the 2DCC user base.
- Share insights and know-how gained from development of AI tools for our 2D materials problems among 2DCC users, fellow MIPs, and scientific community at large.

Milestones

- Design a 2D materials ontology for use with the LiST Knowledge Graph. This will describe relationships between personnel, instruments, samples, and data currently in LiST schema.
- Implement a graph database using ArangoDB to support all document types in LiST. This will facilitate the use of graph-based learning on the data stored within the SQL version of LiST.
- Perform data imputation and record completion using generative models. Validate on held-out data and benchmark scientific and logistical advantages of the data-driven tools.
- Contextualize the results stored in LiST using natural language processing of 2D materials literature. Demonstrate by automatically identifying relevant papers for material samples.
- Demonstrate active learning on sparse data using adaptive Design of Experiments.

- Predict a suitable synthesis procedure for a new material using the AI pipeline in LiST 2.0. Compare to predictions by human experts to evaluate insight gained by the models.
- Share LiST 2.0 applications with one other community (e.g. MIP) and assist with implementation to test transferability to new domains.

Timeline

Year 6: Knowledge graph software framework and ontology
Year 7: Completion and data imputation models using unsupervised representation learning
Year 8: Query prediction and context from literature using Natural Language Processing
Year 9: Active process learning and sparse data inference using Bayesian optimization
Year 10: Design advice for new synthesis protocols using generative deep learning

Anticipated Outcomes

Tool Development

The most direct outcome from this effort will be the suite of data analytics tools built to interact with the LiST database. These tools will provide two types of advantages to users interacting with LiST. First, they will make the database easier to access through quality-of-life improvements such as more intelligent searches, query autocomplete, and automatic provision of contextual information. Second, the tools will provide new mechanisms for scientific insight by identifying previously unknown patterns in the historical data and accelerate discovery through efficient design and optimization of new processes. This software stack will be integrated with LiST but also built to integrate with other SQL databases.

In-House Research

It is anticipated that LiST 2.0 will enable new modes of materials discovery and accelerate our in-house research efforts related to synthesis. The tools are expected to dovetail with existing research projects to provide additional insights and accelerate scientific progress once they are deployed. However, we also plan to develop a unique line of data science research to develop the tools themselves. Our database is qualitatively different than most other materials databases currently available in that all samples are grown in our facility by a relatively small number of staff and users yet represent a wide array of materials and characterization techniques. The first aspect ensures reliability and repeatability of observations, which is essential for machine learning models to accurately capture the behavior of the physical systems. The second aspect allows us to explore learning on few-shot and sparse samples, which are active areas of research in the machine learning community; in the 2010's much focus was directed towards supervised learning on "big data" problems, while more recently it has become apparent that deployment to technical and scientific domains requires more flexible approaches to deal with the reality of data sparsity.

Knowledge Sharing

The LiST 2.0 project is expected to yield scientific insights in materials science and provide a case study in applied data science for solving domain-specific problems. We will seek to share these insights with the 2DCC community through distribution of open-source software and a variety of educational programs to build competence with data science and machine learning in our user base. In addition to the codes themselves being shared, we will produce didactic Jupyter notebooks to illustrate common use cases of the software and provide examples of the syntax and capabilities. These will be shared at workshops and user meetings which will encourage user engagement with the tools and build buy-in for the data-driven discovery paradigm.

Beyond the codes themselves, we will seek to share our experiences in data analytics with other communities of materials science practitioners (e.g. other MIPs). This will be achieved through retrospective analysis and participation in community forums (e.g. MaRDA and 2DDF).

2.3 Integration of ReaxFF Distribution and User Requests with LiST

The ReaxFF reactive force field method is a powerful and attractive computational tool for 2D-material synthesis as it allows for large-scale (>> 10,000 atoms), long-time (> 1 nanoseconds) simulations on complex chemical systems – thus providing a key connection between Density Functional Theory and experiment or meso/macroscale simulations. Over the last five years, a number of ReaxFF parameter sets have been developed for key 2DCC material targets – including MoS_2, $MoSe_2$, WS_2, WSe_2, Ga/In/graphene and hBN. These parameter sets are currently distributed through the Material Computation Center (MCC) website and have attracted a significant level of requests, leading to around 50 parameter file distributions a year (Figure 2.3). We now seek to integrate this parameter distribution more closely with 2DCC and increase the user support through access to key ReaxFF in- and output files and tutorials. Furthermore, we want to encourage new theory user requests by facilitating users to define projects requiring the development of new ReaxFF parameter sets.

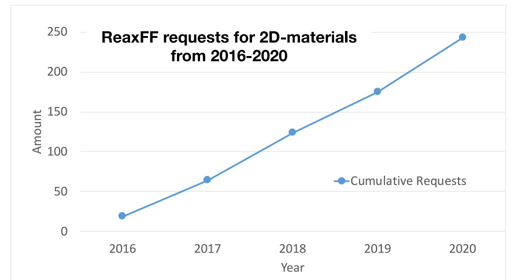


Figure 2.3: External user requests for ReaxFF parameter sets for 2D-materials through the Material Computation Center website.

Goals

We want to increase the accessibility of the ReaxFF 2D-material parameter sets by connecting the MCC requests to LiST – thus enabling external users not only access to the force field parameters, but also to key ReaxFF in- and output files. Furthermore, we intend for every 2DCC related ReaxFF parameter set to set up a brief tutorial, using the AMS software, with key screenshots showing system building and system response during ReaxFF simulations (Figure 2.4). Going beyond support for existing ReaxFF parameter sets, we also want to facilitate the formulation of external user projects that require new ReaxFF development – like combining existing ReaxFF parameter (e.g. TiO_2/MoS_2) interactions or ReaxFF development for new materials (e.g. WTe_2).

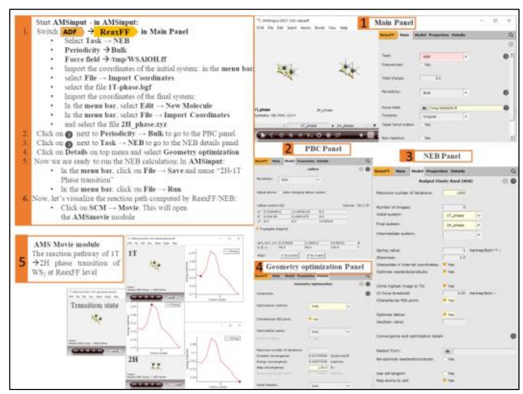


Figure 2.4: Example of a ReaxFF tutorial using AMS Graphical User Interface snapshots.

Milestones and Timeline

Year 6

- MCC/User Proposal Portal connection:
  We will include a link in the MCC website questionnaire that links these user requests to the User Proposal Portal.
- Archive existing 2DCC-relevant ReaxFF parameter sets:
  For each of the 12 currently published ReaxFF parameter sets associated with 2DCC we will archive the parameter file itself, its training set data and key in- and output files associated with published ReaxFF simulations. For large ReaxFF trajectories we may limit their size but provide guidelines for the user to re-create these trajectories.

- ReaxFF tutorials:
  For each currently published ReaxFF parameter set we will put together a tutorial including AMS screenshots- which will help new users to follow the simulation setup.

Year 7

- Develop ReaxFF parameter request portal:
  This portal will allow users to formulate requests for ReaxFF development. This will be integrated with the functionality of the MetaData Explorer tool. The users can select chemical elements and will be given a direct response indicating the required development time – based on the current existence of ReaxFF parameters and their transferability to the elemental combination selected by the users. After this initial step, we will discuss with these users potential synergies with existing 2DCC efforts. If, after this, the users want to go forward with a proposal we will provide a proposal template – typically 2 pages – and assist these users with putting together and submitting a user request.

Anticipated Outcomes

We anticipate that the integration of the ReaxFF distribution into LiST and the streamlining of user request will greatly reduce the barriers for new ReaxFF users – especially for undergraduate students and for users with limited computational chemistry experience. As such, this will lead to a significant expansion of potential ReaxFF users. This will increase the interest in ReaxFF development for new materials – which connects to the ReaxFF request portal, which facilitates for these users to estimate parameter development time. By these means we will both grow the ReaxFF user community and the ReaxFF parameter library, thus increasing its relevance for the materials simulation community.

3.0 In-House Research

In its first 5 years, the 2DCC-MIP's in-house research was broadly framed by four science drivers including *Physics of 2D Systems, Epitaxy of 2D Chalcogenides, Next Generation Devices and Advanced Characterization and Modeling*. Significant advances in all these areas played an important role in developing a strong and diverse user base. Over the next five years, in-house research will continue to be aimed at developing foundational knowledge in bulk and thin film crystal growth of 2D chalcogenide crystals to enable atomic-level control of composition and crystallinity in epitaxial films and heterostructures and realize novel chalcogenide phases and structures. The complementary advantages of different growth methods available within the 2DCC-MIP facility will be harnessed to synthesize hybrid materials and heterostructures that are beyond the reach of individual synthetic approaches. Complete integration of bulk crystal-MOCVD-MBE synthesis, exploiting bulk crystal growth for tailored substrates, also provides a new foundation for fundamental studies of van der Waals epitaxy and novel heterostructure synthesis. Theory and data-driven discovery tools – employing comprehensive tracking of synthetic protocols and resulting sample properties across the platform – are deployed in a tightly integrated theory-computation-measurement-synthesis loop that targets the understanding of both key kinetic growth processes and the results of in situ and ex situ characterization, following the vision of the Materials Genome Initiative.

The scope of the in-house research continues to focus on advancing the fundamental synthesis science of chalcogenide-based van der Waals crystals to improve the crystalline perfection of films and bulk crystals and enable discovery of new phases and structures. These advances, enabled by state-of-the-art synthesis and characterization tools and data resources, foster transformative new materials systems with broad impact on compelling issues at the rapidly developing frontiers of quantum science and technology, next-generation electronics, and optoelectronics.

The specific goals, milestones and anticipated outcomes for in-house research are outlined below based on science driver.

3.1 Physics of 2D Systems

3.1.1 Molecular Beam Epitaxy

Over the past decade, chalcogenides such as Bi_2Se_3, Fe(Se,Te), and $(Mo,W)(S,Se,Te)_2$ have emerged as a rich playground for discovering exciting emergent phenomena created by the nexus of topology, relativistic quantum mechanics, fundamental symmetries, and crystalline order. Certain topological quantum materials such as Bi_2Se_3, have already shown attractive characteristics such as efficient spin-charge conversion at room temperature that are of immediate technological relevance in quantum electronics applications (e.g. energy-efficient non-volatile magnetic random access memory). Others such as Fe(Se,Te) and $Bi_2Se_3/NbSe_2$ heterostructures are topological superconductor candidates, relevant for a more long ranged quantum electronics vision (topological quantum computing). The strategic plan for in-house research on molecular beam epitaxy (MBE) builds on our established strengths in the well-controlled synthesis by MBE of thin films and heterostructures derived from magnetic topological insulators (Cr- and V-doped $(Bi,Sb)_2Te_3$) and exotic chalcogenide-based superconductors (ultrathin Fe(Se,Te) and $NbSe_2$), as well as our developing expertise in the synthesis by MBE of topological semimetals (e.g. $ZrTe_2$) and two-dimensional (2D) ferromagnets (e.g. $CrTe_2$). We aim to pursue new families of topological quantum materials that can serve as platforms for the discovery of emergent phenomena and for the development of quantum electronic devices. The integrated Scienta-Omicron multimodule MBE tool provides a strong focus on characterization of both structural and electronic properties since it allows *in vacuo* four probe electrical measurements at μm scales, scanning tunneling microscopy (STM), and angle resolved photoemission spectroscopy (ARPES) using both Helium lamp and laser excitation.

Goal: Motivated by the research interests of the in-house team and by queries from existing and potential users, we propose to expand the scope of our exploration of synthesis of topological quantum materials in four complementary and uncharted directions.

1. We will use MBE and *in vacuo* reflection high energy diffraction and STM and *ex situ* x-ray diffraction to study the epitaxial growth (kinetics, nucleation, defects) to improve the crystalline perfection of magnetically-doped topological insulator heterostructures with the aim of uncovering emergent quantum behavior currently hidden by disorder. Currently, even though quantization of the anomalous Hall effect is about 0.1 ppm, the samples are highly disordered with x-ray double crystal rocking curves of typical width 0.1^0 and a low temperature Drude mobility around 0.02 m^2/V.s. We will work with our theory colleagues to model the MBE growth of these materials.
2. We will use MBE and *in vacuo* STM and ARPES to develop new material candidates for interfacial and topological superconductivity. This will include exploiting the unique 2DCC oxide-chalcogenide dual MBE system to explore and understand novel interface-controlled quantum phenomena such as high temperature superconductivity in single layer FeSe on $SrTiO_3$ (STO) and related oxides.
3. We will use MBE and *in vacuo* ARPES to discover new chalcogenide topological semimetals that harbor surface Fermi arcs. One approach to realizing this is by interfacing a Dirac semimetal with a ferromagnet, thus achieving a Weyl semimetal by breaking time-reversal symmetry while still preserving inversion symmetry. We will also be guided in our search by first principles and model Hamiltonian calculations by 2DCC theorists.
4. We will use MBE to develop new types of 2D van der Waals ferromagnets that can be epitaxially integrated with chalcogenide topological quantum materials for novel spintronic devices.

Milestones

- Magnetically-doped $(Bi,Sb)_2Te_3$ heterostructures with narrow x-ray double crystal rocking curves ($< 0.03^0$) and Drude mobility > 0.1 m^2/V.s.
- Chalcogenide Dirac or Weyl semimetal exhibiting surface Fermi arcs.
- Single layer FeSe on STO or a related materials with an *in vacuo* four probe zero resistance state at a critical temperature $T_C > 77$ K.
- Chalcogenide 2D ferromagnet with a Curie temperature > 300 K.

Timeline

Year 6: Systematic STM study of nucleation and defects in quantum anomalous Hall insulator heterostructures and modeling of observations with theory; all epitaxial growth of interfacial superconductors by dual chamber oxide-chalcogenide MBE; definitive ARPES demonstration of Dirac and Weyl band structure in MBE-grown chalcogenide semimetal thin films.
Year 7: Improvement of XRD linewidths and Drude mobility in quantum anomalous Hall insulator heterostructures; control over interfacial superconductivity using interfacial engineering of epitaxially grown oxide; ARPES study of changes in band structure of Dirac semimetal interfaced with a ferromagnetic substrate; development of new families of 2D chalcogenide ferromagnets and antiferromagnets (in concert with theorists).
Year 8: Search for emergent quantum phenomena in quantum anomalous Hall insulators with improved crystallinity; enhanced superconducting T_C using interfacial engineering of epitaxially grown oxide; search for signs of surface Fermi arcs in Weyl semimetal thin films via ARPES and quantum transport; search for high Curie temperature in 2D chalcogenide ferromagnets.
Year 9: Development of alternate strategy for quantum anomalous Hall insulators with superior crystallinity by interfacing topological insulators with insulating ferromagnets and antiferromagnets; development of new interfacial superconductors with band structure necessary for topological

superconductivity; search for new families of Weyl semimetals (guided by theory); integration of 2D chalcogenide ferromagnets and antiferromagnets with topological materials.
Year 10: Further development of quantum anomalous Hall insulators by interfacing topological insulators with insulating ferromagnets and antiferromagnets; further development of interfacial topological superconductors; search for new families of Weyl semimetals (guided by theory); integration of 2D chalcogenide ferromagnets and antiferromagnets with topological materials.

Anticipated outcomes

(a) Quantum anomalous Hall insulator with fractional Chern number.
(b) Epitaxial Weyl semimetal thin films showing Fermi arcs in ARPES and quantum transport.
(c) Interfacial superconductor with high Tc above 77 K.
(d) Credible evidence for a chalcogenide topological superconductor.
(e) Ambient temperature topological spin-orbit torque device using 2D chalcogenide ferromagnet/topological heterostructure.

3.1.2 Bulk Growth

Topological quantum states in materials have high potential to revolutionize information and energy technologies. The in-house bulk crystal research in the past a few years has focused on the growth of an intrinsic antiferromagnetic (AFM) topological insulator (TI) $MnBi_2Te_4$ and the investigation of a long-sought, ideal type-II Weyl semimetal state in this system. The bulk growth research over next five years will not only expand to materials relevant to $MnBi_2Te_4$ [i.e. $MnBi_2Te_4(Bi_2Te_3)_n$ (n=1 & 2)], but also explore other new magnetic topological materials. Theory predicts $MnBi_2Te_4(Bi_2Te_3)_n$ can host a variety of topological quantum phases, including high temperature quantum anomalous Hall insulator, axion insulator, and Weyl semimetal states driven by spontaneous ferromagnetism, which can be realized if the FM phases of $MnBi_2Te_4(Bi_2Te_3)_n$ can be synthesized.

Goals: The central goal of the bulk crystal research is to synthesize FM $MnBi_2Te_4(Bi_2Te_3)_n$ and other novel magnetic TIs and seek novel topological quantum phases in them. Functional properties enabled by band topology in materials is critically dependent on materials' compositions, which are hard to be controlled using conventional crystal growth techniques. We will establish a new crystal growth facility – double crucible vertical Bridgman (DCVB) furnace (the 1st of its kind in academia) and develop crystal growth capacity with precisely controlled chemical stoichiometry using this technique. In search for new intrinsic magnetic TIs, we will combine synthesis guided by theoretical predictions with exploratory synthesis. Through data mining in topological databases, many promising candidate materials could be identified for synthesis. The other approach is to introduce magnetism and band topology to trivial insulators close to the critical point through chemical substitutions. For instance, we have recently found a trivial insulator $BaSc_2Te_4$ can be turned to a possible magnetic TI via rare earth element substitution for Ba. Additionally, another focused direction of bulk growth is to discover and grow new nonlinear optical chalcogenides with large nonlinear coefficients and low absorption.

Milestones

- Develop DCVB crystal growth capacity of chalcogenides.
- Grow FM $MnBi_2Te_4(Bi_2Te_3)_n$ and seek novel topological quantum phases in them.
- Discover and grow novel intrinsic magnetic TIs.
- Discover and grow new nonlinear optical chalcogenides.

Timeline

Year 6: Grow FM $MnBi_2Te_4(Bi_2Te_3)_n$ with controlled chemical potential using the flux method.
Year 7: Develop DCVB crystal growth capacity for magnetic topological chalcogenides.
Year 8: Demonstrate novel topological quantum phases in bulk crystals and 2D thin layers of

$MnBi_2Te_4(Bi_2Te_3)_n$ and search for new intrinsic magnetic TIs and nonlinear optical chalcogenides via flux and chemical vapor transport crystal growths.

Year 9: Grow new intrinsic magnetic TIs discovered in year 3 using the DCVB technique and continue the search for new magnetic TIs and nonlinear optical chalcogenides.

Year 10: Explore novel topological quantum phases among the magnetic TIs discovered in years 8 & 9 and grow nonlinear optical chalcogenides using DCVB.

Anticipated Outcomes

- Establishing the DCVB bulk growth facility for chalcogenides crystal growth
- Demonstration of novel topological quantum phases in $MnBi_2Te_4(Bi_2Te_3)_n$ and other new magnetic TIs.
- Discoveries of new nonlinear optical chalcogenides with large nonlinear coefficient.

3.2 Epitaxy of 2D Chalcogenides

TMD Heterostructures

In-house research during the first 5 years of the 2DCC-MIP was directed at developing epitaxial growth of wafer-scale transition metal dichalcogenide (TMD) monolayers by metalorganic chemical vapor deposition (MOCVD). This involved studying fundamentals of nucleation and lateral growth of TMD domains, the role of substrate type and structure on domain orientation and the type of grain boundaries and defects present in the epitaxial films. Over the next 5 years, synthesis efforts on TMD epitaxy will build on this work to focus on synthesis of vertical and lateral heterostructures to discover fundamental rules of heteroepitaxy in van der Waals systems.

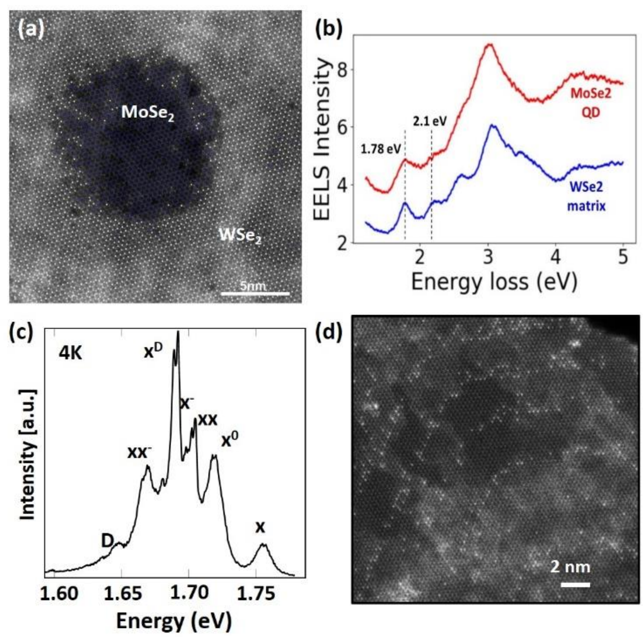


Figure 3.1. (a) $MoSe_2$ dot in WSe_2 monolayer matrix; (b) Low temperature high resolution EELS indicating the presence of excitons in the $WSe_2/MoSe_2$ film, with peak shift and broadening suggesting quantum confinement; (c) 4K PL of WSe_2 monolayer grown by MOCVD showing emissions associated with neutral (x, xx), charged (x^- xx^-) bright (x^o), dark (x^D), and defect-related (D) excitons. (d) Periodic pulsing of W during MoS_2 growth produces "rings" which mark the extent of lateral domain growth.

Goals

Synthesis efforts will tackle the growth of vertical TMD heterostructures, where epitaxial layer-by-layer growth can produce clean and strongly coupled 2D interfaces that are key to maximizing emission from interlayer valley excitons and Moiré bilayers. Studies will also be aimed at the creation of quantum dots (QDs) in TMD lateral heterostructures (Figure X) that can serve as sites for single photon emission (SPE). Aberration-corrected scanning TEM and electron energy loss spectroscopy (EELS) will be used to characterize the structure and composition of the QDs. Theory efforts will focus on prediction of suitable defects in TMDs that can serve as ideal SPEs with minimal decoherence.

Periodic pulsing of a different metal precursor during growth in combination with ultra-high-resolution TEM provides a unique approach to study fundamentals of growth at the atomic level using metal "markers", informed by first-principles calculations. The range of TMDs investigated will be expanded to include the tellurides (WTe_2, $MoTe_2$) and group-V and group-VII transition metal dichalcogenides (e.g. $NbSe_2$, ReS_2, etc.), materials that are all relevant to the previously described research plans on topological quantum materials. These additional precursors will also enable studies of dilute substitutional doping (e.g. Re and V in WSe_2) and miscibility and ordering in ternary or quaternary alloys.

Milestones

- Determine the effect of substrate step structure on the epitaxial orientation of TMD monolayers and use this as a method to achieve monolayers with very low density of inversion domains.
- Develop processes for MOCVD growth of transition metal tellurides (e.g. WTe_2 and $MoTe_2$)
- Investigate fundamentals of nucleation and lateral growth in mixed metal (e.g. MoS_2/WS_2, etc.) TMD vertical heterostructures
- Investigate fundamentals of QD and lateral heterostructure formation in mixed metal TMD lateral heterostructures (e.g. $MoSe_2$ quantum dots in WSe_2 matrix).
- Develop in situ spectroscopic ellipsometry as a viable method to monitor monolayer and bilayer growth of TMD films during MOCVD.
- Study the growth of mixed chalcogen TMD vertical and lateral heterostructures (e.g. $MoSe_2/MoS_2$) and understand limits imposed by chalcogen exchange.
- Expand the suite of TMD materials grown by MOCVD to include Re, Nb and V-based chalcogenides.

Timeline

Year 6: Domain alignment on stepped substrates and MOCVD growth of Te-based TMDs.
Year 7: Vertical and lateral mixed metal TMD heterostructures.
Year 8: In situ spectroscopic ellipsometry for real time thickness measurements of TMDs.
Year 9: Vertical and lateral mixed chalcogen TMD heterostructures.
Year 10: Re-, Nb and V-based TMDs and heterostructures.

Anticipated Outcomes

The research is expected to provide new insights into fundamental mechanisms of nucleation, orientation and lateral growth of TMDs on van der Waals surfaces, the effect of lattice mismatch on heteroepitaxy in lateral and vertical heterostructures and the limits of interfacial abruptness and defect formation. The work will also assess the feasibility of using spectroscopic ellipsometry to monitor TMD growth particularly at the sub-monolayer level in real time under typical growth conditions. The optical properties of epitaxially grown vertical TMD heterostructures will be characterized and compared to structures formed by layer transfer and stacking. The formation and optical properties of embedded TMD quantum dots will also be determined.

3.3 Advanced Characterization and Modeling

Goals

Growth outcomes for 2D or layered materials are often dominated by kinetic events of nucleation and growth that are rare in both space and time, in a manner that depends critically on the specific characteristics of deviations from the translational symmetries of the final growth targets. As such, theory/computational efforts to assist in understanding and optimizing growth often aim to understand the idiosyncrasies of a specific material grown by a specific method, with limited ability to attack growth challenges at-scale. Valuable theory/modeling efforts along these system-specific lines should and will continue, balanced with more generalized investigations as outlined next. A common experimental challenge in growth is when an overriding synthetic requirement (e.g. the retention of volatile chalcogen species during MBE growth) drives a growth parameter (e.g. substrate temperature) to the edge of a "growth window" beyond which materials quality degrades unacceptably along an orthogonal axis. One high-level goal of the 2DCC is to advance towards more general theory-led methodologies that facilitate expansion of the growth window for high-quality outcomes for both known and yet-to-be-synthesized material targets. Specific goals here include the computational identification of possible "hidden actors" in growth, meaning elemental or chemical species whose relative energetics of incorporation onto the growth edge versus the interior of a 2D material suggests that they may "ride the growth edge" and thereby modulate the kinetics of growth, potentially improving crystallinity by facilitating surface or edge mobilities of constituent species of a target 2D material. Such efforts could also help to identify deleterious impurities whose presence at very low levels may impede high-quality material growth but are otherwise difficult to identify directly. The same tool can also identify promising new candidates for substitutional doping by an inversion of the selection criteria, in a manner that is applicable to both thin-film and bulk growth of layered materials across a range of target properties (magnetism, charge carrier compensation, etc.). By extending these investigations to more complex multi-dopant configurations, it may also be possible to gain further insights into kinetically controlled limits on experimentally achievable dopant concentrations and push boundaries in this domain as well. Related efforts which quantify at-scale the precursor/substrate binding interaction near a growth edge may be able to exploit trends similar to the volcano plot in catalysis to identify especially promising moderately binding substrate/precursor combinations that enable high-quality growth, where the growth edge+substrate plays the role of "catalyst" informed by gas-phase simulations of precursors impinging on the substrate in realistic experimental conditions. These explorations are a natural domain of theory when operating in a survey/exploratory mode, as experimentalist are justifiably hesitant to intentionally introduce novel species into growth chambers without a strong basis to anticipate positive outcomes. In these investigations, reactive force fields will continue to be advanced in capability and material/substrate coverage to the advantage of both internal research and the larger community, married closely with first-principles and data-driven methods, including integration with the List 2.0 capabilities described elsewhere. Note that the approaches outlined above also apply to bulk growth outcomes where impurities may assist or degrade growth outcomes.

Milestones

- Develop computational methodology for rapid assessment of "volcano-plot" precursor/substrate assessment.
- Connection of this methodology to experimental synthetic systems.
- Development of computational means to assess roles of minority species in diverse 2D materials growth processes, connected to materials systems of interest.
- Integration of computational efforts with List 2.0 data/analysis engine.

Timeline

Years 6–10: In addition to targeted long-term theory/modeling goals described above, ongoing theory/simulation efforts will also couple to emergent experimental advances in an agile manner, including studies of nucleation, alignment, and heterostructures.
Year 6: Initial development of methodologies for precursor/substrate assessment, minority species dynamics, and more capable reactive force fields.
Year 7: Initial integration of computational methodologies with the developing List 1.0/2.0 data tool.
Year 8: Computational screens for optimization of successful growth conditions across a plurality of materials and growth approaches of experimental interest.
Year 9: Further integration of computational methodologies with the List 2.0 data tool.
Year 10: Precursor/substrate screen and minority species analysis methodology sufficiently mature for sustained deployment.

Anticipated Outcomes

These efforts are anticipated to provide new means of optimizing materials growth conditions for a broad swatch of emerging 2D materials of interest to the community, including both the quality of known high-interesting, high-impact materials and facilitating target identification and successful growth of new materials as well. Insights into nucleation and the growth of more complex heterostructures and interfaces will also be obtained, in alignment with the goals and outcomes of other components of the strategic plan.

4.0 Tool Acquisition and Development

The 2DCC has successfully installed and commissioned for external users, local users and in-house research efforts a range of synthesis and in situ characterization instrumentation as well as theory and simulation tools. Descriptions of existing tools are provided on the 2DCC website here including 3D virtual tours of the experimental facilities. This section below is a description of the plans for new instrumentation to be developed, installed and made availability to the community over the first two years of the 2DCC renewal period.

4.1 Goals

- Add synthesis capabilities for incongruent melting materials in bulk growth
  Double Crucible Vertical Bridgman (DCVB)
- Add synthesis capabilities in thin films
  Confinement Heteroepitaxy (CHet): in situ defect generation (ion and plasma sources), evaporation sources for intercalation of alloys and multilayers, accommodate 4" substrates, optical ports for in situ spectroscopic ellipsometry
- Add capabilities for development of hybrid structures and devices for air-sensitive materials
  Glovebox Cluster Tool: exfoliation and transfer stacking on air-sensitive van der Waals flakes and hybrid structures from MOCVD and MBE thin films
- Add ambient-controlled characterization capabilities
  AFM Module: enable ambient-controlled characterization of surface and correlation of surface morphology with Raman/PL maps
  457 nm Excitation Laser Module: better spatial resolution imaging and higher excitation efficiency; enable resonant Raman of wide bandgap 2D materials

4.2 Milestones and Timeline

The following is a milestone timeline plan for tool acquisition and development. Quarters are defined as: Q1 = June 2021 – August 2021; Q2 = September 2021 – November 2021; Q3 = December 2021 – February 2022; Q4 – March 2022 – May 2022; etc

Instrumentation	Milestone	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8
DCVB	Purchase								
	Vendor Build and Test								
	Arrival								
	Process Development								
	Available for Users								
CHet	Purchase								
	Arrival								
	Process Development								
	Available for users								
GBox Cluster	Purchase								
	Arrival								
	Process Development								
	Available for Users								

AFM & 457nm Laser	Purchase								
	Arrival								
	Process Development								
	Available for Users								

4.3 Anticipated Outcomes

The 2DCC Thin Films facility has developed a unique suite of equipment for epitaxial growth of 2D chalcogenides by MBE and MOCVD which enable monolayer-level control of growth with *in situ* and *in vacuo* studies of film growth and properties. These tools are ideally suited for both the proposed in-house research on TI, superconducting and TMD-based heterostructures and also the broader needs of the user community in this area. However, the search for new quantum materials is better suited to bulk growth methods that can rapidly screen a wider range of compositions. This section outlines the anticipated new capabilities/outcomes for new instrumentation acquisition and development for thin film and bulk crystal synthesis as well as characterization and device functionality.

DCVB: To enhance capabilities in this area and address growing interest from users, the 2DCC will implement a double crucible vertical bridgman furnace for the Bulk Growth facility. This system will:

- Enable continuous feed of source material by utilizing the two crucibles design
- Enable control of chalcogen volatilization under high pressure environment
- Enable growth of large homogeneous crystals and precise control of stoichiometric compositions of chalcogenides crystals

CHet: This system will add new capabilities to produce large-area 2D materials by combining plasma etching and thermal evaporation for controlled intercalation of a wide range of elements at a scale and flexibility that can serve growing user needs. The new instrument will enable control over each process variable under *identical* environmental conditions by incorporating the most critical steps into a single instrument. This instrument will enable controlled introduction of defects into the graphene surface using either directed plasma or ion beam exposure to enable precise control over defect chemistry just prior to metal deposition and intercalation. The system will be capable of substrate heating to 1000°C during metal deposition, which is critical to realize long-range intercalation of metals to create uniform 2D films, coupled to the ability to co-deposit and co-intercalate metals to form alloys or heterostructures *within* the confines of the graphene/SiC interface.

Glovebox Cluster Tool: A set of tools inside a chain of vacuum compatible gloveboxes (designed for air-sensitive materials) will perform exfoliation, controlled transfer, AFM characterization and lithography-free device fabrication on atomically thin flakes of layered crystals and thin films or heterostructures synthesized by MBE, MOCVD and CHet. This tool will enable the 2DCC to push the envelope on unprecedented hybrid structures, better understand novel phenomena at the interface, and realize new device functionalities all while contributing to feedback in improving synthesis.

AFM and 457 nm Excitation Laser Module: This upgrade to the MOCVD2 system will enable ambient-controlled characterization and correlation of surface morphology with Raman/PL maps via the AFM and enable better spatial resolution imaging and higher excitation efficiency to allow for resonant Raman of wide bandgap materials (e.g. hBN).

5.0 User Facility Operation

Directors
Synthesis – Joan Redwing; ***In situ Characterization*** – Nitin Samarth; ***Theory/Simulation*** – Vin Crespi
User Programs – Joshua Robinson; ***Operations and User Facilities*** – Kevin Dressler

Vision: Empower pioneering advancements in the science and technology of 2D materials.

Mission: To develop the synthesis science of 2D materials via unique instrumentation and processes that utilize *in situ* and ambient controlled characterization, modelling and data, and partner with a diverse set of researchers across the United States to develop the foundational understanding of the unique properties that 2D materials have to offer.

The 2DCC User Facility enables cutting edge research and discovery on the synthesis and characterization of 2D chalcogenide materials by a national user community guided by three science drivers (described in section 4.1): *Physics of 2D Systems*, *Epitaxy of 2D Chalcogenides* and *Advanced Characterization and Modeling*.

5.1 Goals

Operational Goals

- Operate a facility focused on providing an outstanding user experience.
- Staff the user facility with a diverse set of skilled scientific and operational support personnel.
- Establish and maintain an up-to-date user portal that educates and encourages potential users, provides user resources, and enables facile methods for proposal submission.
- Maintain policies and procedures that effectively guide use of the facility.
- Provide timely notice of award/decline to 2DCC proposers
- Expand programming for the annual users meeting

Instrumentation Goals

Develop and maintain a state-of-the-art facility for 2D materials synthesis, characterization, and theory

- Develop and continually expand the palette of "standard" samples.
- Develop routes to scale-up successful synthesis recipes to two-inch (or larger) wafers.
- Continually advance next generation, *in situ* and ambient-controlled characterization techniques on MIP-based instrumentation as a means to provide insight into growth fundamentals and prepare the highest quality 2D materials for high-impact research projects.

Infrastructure Goals

Provide state-of-the-art facility with cost-effective and safe infrastructure.

- Collaborate closely with building facility coordinators and environmental health and safety personnel to continually monitor the performance of safety monitoring instrumentation and abatement systems.
- Evaluate annually the effectiveness of building infrastructure to enable increased complexity of next generation instrumentation and instrumentation upgrades.

5.2 Milestones and Timelines

- Facility renovations for new instrumentation (e.g. DCVB, CHet, GloveBox Cluster, AFM & 457 nm Laser) completed – Q4-Q5
- All new signature instrumentation installed and available to users (see Section 4 timeline)
- Improve user access to LiST 1.0 (see Section 2.1)

- Improve user access to existing ReaxFF reactive potentials and requests for new potentials (see Section 2.3)
- Provide new opportunities for user-user interaction by expanding the annual users meeting to a full day symposium style meeting including the User Committee meeting

5.3 Access Modes

Local and external users of 2DCC capabilities obtain access via three proposal types: **Sample request, Data request** and **Research Project** proposals, all submitted through a proposal submission portal. The 2DCC is now adding a fourth mechanism for **reactive potential requests**. Research proposals are accepted on a rolling basis or in response to topical solicitations, while sample and data requests are entirely rolling. All proposals are evaluated by the User Proposal Review Committee (UPRC) consisting of external scientific and technical experts in thin films, bulk crystal and theory/simulation from the US. The Operations Director coordinates reviews and manages conflicts of interest. Reviews are conducted in strict confidence, including content and reviewer identity, and are only shared with the ELT for feasibility decisions.

Once selected to move forward, a proposal is then approved/awarded and the users access the facility. See Section 6.6 for more information on access modes (e.g. remote, visiting, independent) of approved/awarded users.

5.4 Staffing

Scientific Staff: The facility is staffed with full-time PhD level scientists in each facility (i.e. four assistant research professors, two in MBE and one in MOCVD thin film activities, one for theory/simulation, and one for Bulk Crystal Growth), a full-time postdoc for MBE, two postdocs for MOCVD thin film activities, two for Bulk Synthesis, one for Confinement Heteroepitaxy, one for heterostructures and layer transfer, and two postdocs in the Theory/Simulation facility.
Operational Support Staff: The facility is staffed with a full-time Operations and User Facility Director, Data Manager and Programmer/Analyst and part-time personnel such as Administrative Support Coordinator, an External Evaluator for assessment efforts, web and IT support staff, and MRI Facilities Coordinator.

5.5 User Training

Extensive training programs within the core facilities enable users to become knowledgeable and proficient with both general lab safety protocols and specific equipment operation. Training procedures begin with an overall university-wide safety course followed by specific laboratory safety courses and then typically multiple levels of hands-on equipment training by the technical staff responsible for the equipment in the case of independent users. If the staff member deems the user capable, they authorize their independent use of the equipment. If not, the users will require more training time. For equipment like the MOCVD and MBE systems, it can take several weeks of training to acquire the knowledge to effectively run the tools independently, requiring a significant training commitment. The 2DCC operates some specific programs centered around intensive training in the facilities. Special training programs are outlined in Education/Training section of this strategic plan (e.g. Resident Scholar Visitor Program and REU Site).

Note also that the 2DCC has made available virtual 360º video tours of its facilities to enable users to familiarize themselves with the equipment and laboratory layout. The videos are posted on the User Facilities tab of the 2DCC website. This is not only useful for initial training steps for user but it is also useful for the general public and potential new users to tour the facilities in an efficient, informative and safe manner.

5.6 Safety, including the Safety, Operation and Access Action Plan

Executive Summary: Safety in the 2DCC is managed primarily by the Operations and User Facility Director in collaboration with the Millennium Science Complex Facilities Director and laboratory safety managers for each facility instrumentation location. All participate in various university safety committees. The Operations and User Facilities Director manages direct feedback from users and communicates concerns to the safety managers and the Millennium Science Complex Facilities Director. ***No safety violations have occurred in the 2DCC facility to date.*** Content and implementation of safety training protocols and procedures for 2DCC instrumentation are filed in each facility location, managed by the lab safety managers. Protocols and procedures are reviewed on a yearly basis by lab managers.

This period brought on new challenges to maintain a safety and healthy work environment for students, staff, and faculty. Due to COVID-19, the 2DCC Operations and User Facility Director worked closely with the Millennium Science Complex Facilities Director, among others, to develop a COVID-19 Safety plan that is posted for all that work in the MRI (https://www.mri.psu.edu/covid-19-info). Details of the COVID-19 Safety, Operation and Access Action Plan are described below.

Safety, Operation and Access Action Plan

Overview

Safety is an important aspect of working in the 2DCC. The development, synthesis and characterization of next generation materials requires the use of hazardous and complicated material combinations. It is extremely important that everyone working on these systems be expertly trained in chemical safety and safe lab practices.

Safety Mission

Create and promote safety in the 2DCC by encouraging a culture of safety through education.

User Access Modes

Remote: *Offsite* users that request standard samples, data, and computational time or choose to have experiments fully executed by 2DCC staff. Off-site users are not required to complete training as they will not be personally accessing the facility or using the equipment.

Visiting: ***Onsite*** users that work jointly with 2DCC staff typically and are in residence for days to weeks. The User must complete all required pre-requisite training in order to gain access to equipment.

Independent: ***Onsite*** users that are fully trained by staff to operate equipment and are in residence for weeks to months. The User must complete all required pre-requisite training in order to gain access to equipment.

For complex instruments like the MOCVD, MBE and *in situ* characterization systems, it takes weeks of training to acquire the knowledge to run the tools safely and independently. Attaining independent user status on these tools requires a significant commitment of time for hands-on training. It is anticipated that the 2DCC staff will take on the majority of the responsibility of running these complex experiments under the direction of external users.

*Safety in the Materials Research Institute**

The 2DCC is under the auspices of the Materials Research Institute (MRI) at Penn State University, the physical home of the facility. The MRI has a long track record of managing core user facilities (e.g. the Materials Characterization Lab and the Nanofabrication Lab) and training people on the safe and responsible use of equipment infrastructure, which is monitored by the Penn State Environmental Health and Safety (EH&S) office, which is responsible for the development and implementation of environmental and all occupational health and safety programs throughout Penn State's multi-campus system. Extensive training programs are in place within the core facilities to enable users to become knowledgeable and proficient with both general lab safety protocols and specific equipment operation. This practice is employed by the 2DCC.

*Note new procedures were put in place as of May 2020 to address COVID-19 safety operations, and they are described in Appendix D **(**MRI – MSC Building COVID-19 Supplemental Procedures). They are subject to change.

A. User Training and Safety Procedures

2DCC Facilities

Users that will be onsite and only observing will only be required to complete step 1. Those who will be operating equipment either independently or jointly with 2DCC staff will be required to complete all three steps:

STEP 1: University-wide safety training and certification completed online, administered by Penn State Environmental Health and Safety (EHS), plus a 30 minute in-person session with EHS conducted in the Millennium Science Complex.
*Note, the user will provide a copy of the EHS certificate to the Operations Director and the assigned safety manager before going to laboratory-specific safety training
STEP 2: Laboratory-specific safety training and certification (Lab Safety Managers)
STEP 3: Equipment-specific training (Technical Staff)

Other specific EHS training may be required depending upon the lab to be used. A 2DCC technical contact will provide additional information as needed. Individual equipment training will be required and can be scheduled by contacting the appropriate technical or administrative staff for each facility.

Note: If the technical staff member responsible for a piece of equipment deems the user capable, they authorize their independent use of the equipment. If not, the users will require additional training time.

Equipment Access

On-site users must complete all required pre-requisite training in order to gain access to the Millennium Science Complex or Davey Lab and the equipment within. The facility instrumentation is accessible only by electronic card swipe outside the hours of normal operation when staff are not present. Facility access authorization for users needing to operate outside of these hours (e.g. an independent user) are determined on a case-by-case basis depending on the equipment use that is desired. For example, operation of growth and processing equipment outside the hours of normal operation typically requires the presence of a lab "buddy" who is knowledgeable of the process and safety issues. Users must be familiar with the after-hours policy of the equipment/facility that they wish to use and obtain the necessary approvals.

Standard Operating Procedures

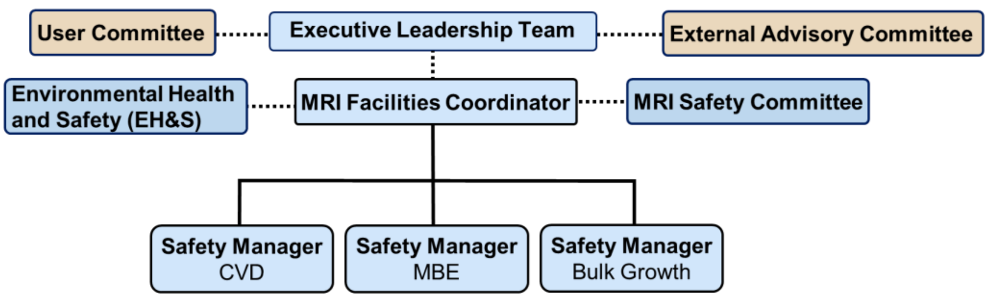
Standard Operating Procedures (SOPs) will be developed by the safety managers for MIP equipment after installation and will be reviewed periodically by the MRI Facilities Coordinator to ensure they are up to date and complete. SOPs will be introduced to users during equipment specific training.

MRI Core Facilities

Users may use equipment and tools within the MRI core facilities as a part of their research projects. Onsite users who wish to personally operate equipment in the core facilities must undergo safety training at all appropriate levels as for 2DCC facilities. Where complicated processing equipment and chemical use occurs, there are additional levels of training requirements. Each lab in the core facilities has a safety officer whose responsibility it is to keep training records for that lab, educate the lab users, and police the lab to ensure user safety. MRI maintains a Safety Committee with faculty, staff and student representatives to provide education and oversight of safety issues within its user facilities and shared research laboratories.

B. Safety Management Structure

Safety oversight in the MRI facilities is managed by the MRI Facilities Coordinator who is the central point of coordination for MRI safety and compliance with regulations administered by the Penn State University's EHS. The MRI Facilities Coordinator works with the 2DCC ELT to implement facility wide procedures and oversee safety managers that represent each 2DCC experimental facility. The 2DCC Operations and User Facilities Director represents the 2DCC on the MRI Safety Committee and collaborates with the MRI Facilities Coordinator to ensure that safety concerns brought forward by feedback of the User Committee and the EAC are addressed in a timely manner. Safety managers are responsible for safe operation of instruments in their facility inclusive of all user training and instrument operation and meet monthly with the MRI Facilities Coordinator.



Safety Organization. 2DCC safety management structure. Brown boxes are the conduit for external feedback to the ELT and the safety managers.

5.6 Allocation

Instrument time/resource allocation: The 2DCC accepts as many top-ranked proposals as the capacity of the facility will allow. Time allocation on awarded projects is determined by proposal-specific needs to execute the project plan and is balanced by future time that is available on the equipment for scheduling. A minimum of 50% of the time allocation on signature MIP equipment is set aside for external user projects. The remaining time is available for in-house research and internal (PSU) users. The Operations and User Facilities Director works with the relevant 2DCC experimental or theory staff to determine time allocation needs that include instrument and staff time. Allocations are reviewed by the 2DCC Executive Leadership Team (ELT). Additional considerations for priority are given to PIs from MSI and PUI institutions, members of underrepresented groups in STEM, first time users and prior users in good standing.

5.7 User Committee and User Meeting

The user committee leadership consists of a chair and vice-chair that serve in succession to form two-year rotations for completed service. The chair and vice-chair are solicited by the 2DCC from active or former users. Membership of the user committee is informal being based on attendees at the annual users meeting and therefore changes year to year. The user committee meets in a private session with an external evaluator during a portion of the annual user meeting. The user committee and the broader user meeting provides a foundation for developing a robust user community that closely interacts and shares data to advance the synthesis science and properties of 2D materials at a more rapid pace than otherwise possible. The increasing attendance (45 users participated from 34 projects including 11 non-R1 and 2 government institution projects in May 2021) at the 2DCC user meetings has outgrown the former half-day format. To accommodate additional users and increase impact for and among users, the meeting will be expanded to a full-day symposium coordinated with the annual Graphene and Beyond workshop. The symposium will be dedicated to highlighting user success stories and plans/outcomes for user projects in a manner that inspires users to team across projects. Our goals here are to create bridges between projects to enable discovery of new phenomena, generate new (internal and external) proposal ideas, and enable users to attract external funding to support larger projects than otherwise possible. The symposium will include an overview of facility capabilities and breakthroughs, a research keynote, user highlights and poster presentations. Community bridges will be encouraged through the overall program presentations and also through breakout clustering centered around collaboration for specific research inquiry in theory/simulation/data science, characterization and synthesis.

5.8 User Fee Structure

For users from U.S. academic institutions and government laboratories, the 2DCC covers all fees including equipment operating expenses, consumables, general laboratory materials and supplies, time with faculty and staff experts, technicians, graduate students, etc. The Platform also covers a limited amount of fees associated with training and equipment usage in the Materials Characterization Lab (MCL) and Nanofabrication Facility as appropriate. Users from industry with propriety research and international users are charged fees based on full cost recovery for equipment usage covering operational expenses, general consumables, regular maintenance, etc. and fees for computational time. *User rates* follow Penn State's administrative policy AD-15 (Fees and Rates for Facilities and Services). Equipment usage is managed through a web-based reservation and management system – Laboratory Equipment Operations (LEO). LEO is a reservation and billing system that allows for equipment to be accessed only by fully trained authorized users (controllable by 2DCC technical staff), with an active budget. Academic rates are based on the direct cost to operate the facility while industrial and international user rates are based on the commercially available costs to operate the equipment which typically includes capitalization and profit.

6.0 Education/Training/Broadening Participation

Over the past five years we have developed a number of education, training and outreach activities, including:

User-centric Activities

- **Monthly webinars**. ~90 participants (45 local/45 online), including instrument/technique tutorials, frontier science overviews and science of equity, broadening participation in research talks
- **Research Experience for Undergraduates (REU)**. Partnering with the Penn State Nanofab, hosted diverse cohorts of undergraduates (~12/summer starting 2019) for summer research, in some cases connected to existing user projects
- **Resident Scholar Visitor Program (RSVP)**. This training and professional development opportunity for graduate students and early career researchers has now trained two cohorts of scholars.
- **User Committee Meetings**. These annual half day events have consistently drawn a large fraction of our users (32 projects represented in our 2020 meeting) to present their research, develop collaborations and share their thoughts on the direction of the 2DCC
- **Proposal Partnerships**. We have joined external users in the development of other research proposals including, for example, a successful NASA MUREP with Florida International University in 2019.

Community-Wide Activities

- **Online Resources & Review Articles**. We are developing a "tools of the trade" library of short training videos. 2DCC participants (in-house researchers and externals users) have also taken a leading role in publishing relevant review articles and perspectives.
- **Data Sharing and Collaboration Tools**. Our STEP-FORWARD tool allows members of the community to identify programs for potential collaboration opportunities, while LiST currently enables better understanding of potential collaborations with the 2DCC and will in the near future extend that to individuals and groups across the community.

Enhancing Participation

We have also worked to ensure the broadest demographic participation in our personnel and user base and, as possible, in the above-listed activities.

- The demographic distribution of both our **senior personnel and external users -** 30% women, 15% URM **-** are better than but comparable to the pools from which we draw (e.g. materials science and physics PhDs)
- We met or exceeded our **usage goals** from the first 5 years (>50% external users, >10% from non-R1 universities)
- **Users that contribute to our heterogeneous institutional ecosystem also contribute to our excellence**. For example, over the past 5 years, non-R1 users comprised 18% of our overall user base but produced 35% (9 out of 26) of external user publications and contributed to half (2 of 4) of the joint in-house/external user publications. 2 of the 9 non-R1 publications were from faculty at MSIs (8% of all external user publications).

6.1 Goals

Our goals are, as they have been from the beginning, to provide a wide variety of 2DCC-related educational opportunities and training to as broad a professional audience as possible. In particular, over the next five years our goals are to

- help our local participants – graduate students, postdoctoral scholars and research faculty – to develop the skills and external visibility that facilitate their progress in the field through robust

professional development opportunities

- increase **onsite training** of our users, in particular of graduate students and junior faculty
- expand our **outreach** into the broader materials community to develop **new collaborations** both between external users and the 2DCC and between individuals and groups outside of the 2DCC
- continue to **diversify** both our groups of local participants and users with the aspiration that these group demographics will move towards those of the broader U.S. population

6.2 Milestones & Timeline

User-centric Milestones

- Expand the **Webinar Experience** (Y1)
    - Enable zoom break-out room "snack sessions" to extend the local pre-webinar discussion experience to our online participants
    - Expand the range of webinar speakers to include more of our external users, including those at non-R1 institutions, to promote sharing of expertise throughout the broader 2D community
    - Co-host high profile speakers, for example, honorary colloquia speakers, with academic units on campus. By encouraging these visitors to give a webinar in addition to their colloquium, we have the opportunity to introduce the 2DCC to them and, by extension, to webinar participants who were otherwise unfamiliar with our MIP
- Double the number of **RSVP** participants by naming two cohorts per year (Y1)
- Provide more opportunities for our users to present their research and initiate collaborations by extending our **Annual User Meeting** to a full day to allow more user presentations and by creating other presentation opportunities for example at the concurrent **Graphene and Beyond Workshop** or at MIP-organized symposia and workshops (Y1)
- Involve users more closely with the development of new synthesis targets through **Materials Data Discovery Workshops** (Y2,4), which will bring together growers, data scientists, and materials theorists around the challenge of using advanced data-driven techniques to predict pathways to transformative new materials, using a virtual format to enhance access across career stages. As a mechanism for engendering discussion and interaction, each data/theory team will initially propose a data-driven synthetic goal which will then focus group discussion towards potentially viable experimental routes to fruition.
- Strengthen research collaborations and student training with our **new PREM partner, FIU**, focusing in particular on the mentoring of underrepresented minorities and women. All participating PSU faculty will participate in mentor training with this emphasis (by Y2)

Community-Wide Milestones

- Expand our **"Tools of the Trade" Library** to include educational modules on the theory and practice of bulk crystal growth and thin film epitaxy (ongoing)
- Our most prominent expansion is that of our **LiST tool** (for timing details, see section 2), where we are working to make it easy for researchers to
    - access existing 2DCC-generated data (boosting our new proposal type – data requests)
    - add their own characterization data, expanding the depth of information available for mining
    - obtain information not only about theoretical, computational and experimental results, but also about the people involved in these lines of research, in order to improve collaboration-finding
- Continue to grow our **publication** rate (ongoing), sharing with the community not only the results of in-house and external research, but also the fact that much of this research is being done at or in collaboration with non-R1 institutions and/or institutions with limited facilities to carry out research.

Local Participant Milestones

- Strong **mentoring**, both *of* and *by* our early career local researchers (ECLRs), is a crucial part of their professional development.
    - All ECLRs will have mentees who have participated in mentor training (Y2)
    - They will also themselves participate in mentor/mentee training (ongoing)
- Our ECLRs will also have annual meetings with their mentees to check on their professional development and chart paths forward toward their eventual career goals (starting Y1)

External Participant Milestones

- 2DCC leadership participates in and shares information about the 2DCC at the major conferences of societies across a broad array of institutions to engage potential new users and existing users alike in the research of the 2DCC national facility
- 2DCC will also continue more personal interactions with early career faculty and institutions that do not have advanced facilities to carry out their research to enable collaboration to advance the science and impact of the 2DCC.

6.3 Anticipated Outcomes

The 2DCC education, training and outreach activities will expand and diversify collaborations not only between members of the broader materials community and the 2DCC, but also between our users. Further development of the LiST tool will both contribute to this and will expand our data-centered partnerships, building new opportunities for collaboration between data scientists and machine learning experts with our experimentalists, focused on synthesis, characterization and device physics, and more traditional theorists, focused on the same. Another anticipated outcome is the enhancement of professional development opportunities for our students, postdocs and early career faculty, in particular as related to mentor training. We anticipate that, at a minimum, all of our internal participants will participate in a mentoring workshop on this topic, gaining or improving these important skills.

7.0 Collaboration with Industry and National Labs

The 2DCC has historically engaged industry and national labs through a variety of mechanism including 1) Knowledge sharing through the annual Graphene and Beyond workshop, collaboration with 2D Research centers (e.g. the NSF I/UCRC named ATOMIC), inclusion of industry for industry-led tutorial-style webinars, international partnerships for workshops (i.e. Graphene Flagship) and research collaboration and personnel exchange (i.e. IMEC); 2) Tool development (e.g. CVD Equipment Corporation, DCA, Scienta Omicron, KM Labs, Witec) for new synthesis instrumentation and advanced characterization tools paired with synthesis instrumentation, all of which were commissioned for users in the first five years of the 2DCC's operation, and 3) Research partnerships on industry-sponsored research, small business user projects (e.g. SBIR/STTR), and a variety of national lab user projects for sample requests and research projects including synthesis, characterization and theory/simulation components.

In the next 5-year period, the 2DCC will continue to engage on the aforementioned areas but also further expand that engagement such as pursuing opportunities for joint funding with industry for feasibility assessment and technology development. An additional avenue for industry engagement that is being investigated is to pursue training opportunities for undergraduates and early career scientists from Pennsylvania schools (i.e. state universities and community colleges) as a workforce training component that may be attractive to the Pennsylvania Department of Community and Economic Development (PA DCED) for advancing the professional development of the next cadre of professional scientists for Pennsylvania-based industries. The PA DCED seeks to both attract companies into Pennsylvania and support those companies by enabling training initiatives to close job-skill gaps. The 2DCC is in a unique position to assist with this gap for crystal growth, semiconductor thin films and processing and advanced characterization.

The 2DCC has engaged and will form a tight collaboration with David Fecko, MRI Industrial Relations Coordinator to not only ensure enhancement of existing programs but to expand into the new areas mentioned.

7.1 Goals

- Enhance knowledge sharing programs (e.g. Graphene and Beyond, collaboration with 2D Centers, industry and national lab led tutorial webinars, international partnership and exchange).
- Expand tool development to new capabilities in larger area 2D materials, incongruent materials and controlled stoichiometry in bulk crystals, advanced characterization, heterostructure development and new device functionalities, and machine learning tools via LiST 2.0.
- Expand to more opportunities for industry sponsored research and small business-related user projects to capture expertise and interest from start-up and small companies in the user program.
- Cultivate opportunities in the feasibility and technology development space by encouraging and participating in joint funding with industry large and small.
- Cultivate strong relationships with the state of PA DCED by formalizing recruitment of students and early career scientists into 2DCC onsite training programs for professional development and formalizing a sub-cohort within the RSVP effort.

7.2 Milestones

- A marketing campaign to draw in new industrial, government, and academic lab usership at market-specific expos and conferences that involve 2D and electronic materials content.
- Promotion of facility capabilities and associated programmatic funding support at PSU site-specific 2D and materials conferences such as "Graphene and Beyond" and "Materials Day."
- Involvement of industry partners in webinar series
- Collaboration and partnerships with industry in specific sectors targeting joint funding

opportunities (e.g. electronics and quantum, sensors/transducers, coatings, manufacturing)

- Industry and national lab use of newly developed synthesis tools (e.g. DCVB, CHet)
- Build awareness of the 2DCC's training and advancement opportunities with local and state agencies such as PennTAP, the IRC network, and the regional chambers of commerce; a trained workforce will bring high tech jobs to the region.

7.3 Timeline

In the next 6 months we don't expect to be able to travel and attend conferences, so we will focus on

- Developing promotional materials such as a marketing brochure and capabilities catalog
- Social media awareness and marketing campaign
- Developing promotional videos on user success stories to post on website

Once the pandemic has passed and fully unrestricted travel is possible (6 months and beyond)

- Attend 2 trade show/expos each year to market our capabilities in specific markets
- Visit local and state development agencies to promote the regional capabilities and draw businesses in to consider locating a research center or manufacturing plant nearby
- Invite large and midsize businesses into the center to tour the facility and meet with faculty and staff to develop deeper relationships and discuss collaboration opportunities

7.4 Anticipated Outcomes

Opportunities for joint funding with industry for feasibility assessment and technology development stem from the shared need of industry and the 2DCC regarding:

- Reproducibility & uniformity of material properties
- Process scalability
- Benchmarking of materials & devices
- Data science to accelerate process development

It is expected that joint funding efforts will contribute to closing the technology gap that exists in technology readiness levels (TRLs) between academic entities like the 2DCC (TRL 1-2) and industry interest and needs (TRL 4-9). Joint funding is expected to address the gap shown in figure 7.1.

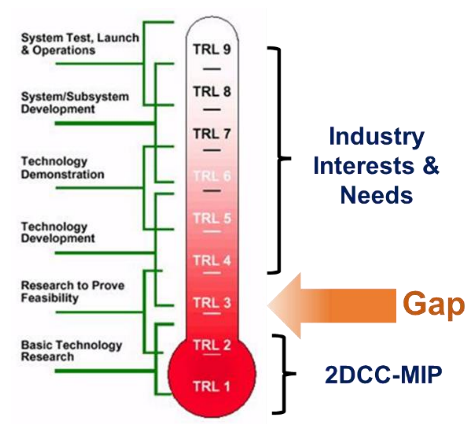


Figure 7.1: The gap between 2DCC materials and process development and industry needs.

2DCC efforts in building relationships with state agency initiatives (e.g. PA DCED) are expected to produce two major outcomes. First, agencies such as DCED are well connected to businesses at all levels, including marketing to attract new business into PA, which is a great resource to the 2DCC for potential direct users of the facility. Second, intentionally including PA-based students in 2DCC training initiatives such as RSVP shows a commitment to DCED for training workers likely to reside in PA. This is the basis for a mutually beneficial relationship that could lead to state-based funding in the future. Aligning with state priorities (also synergistic with Penn State University initiatives) contributes to the long-term sustainability of the 2DCC by not only potentially expanding the funding and user portfolio but also by increasing the regional relevance as a "go to" place for workforce training on state-of-the-art equipment in a diverse and inclusive environment.

8.0 Long-term Sustainability Plan

The 2DCC sustainability strategy is built upon platform components that mutually support each other. The platform elements and synergistic mission are aligned with Penn State University's goal of transitioning the 2DCC to a permanent core facility at Penn State in the future. Long-term sustainability rests on a number of factors which includes funding support (internal + external sponsor) and partnership with not only industry and national labs but also with national and international consortia and more broadly, workforce development. We are preparing for its evolution beyond a user facility to a national resource dedicated to promoting and rebuilding U.S. expertise within academia in the science and practice of crystal growth of thin films and bulk material. The goal is to be realized as a worldwide center of excellence for the synthesis of crystalline materials with a strong emphasis on training of the next generation of crystal growers, tool developers and simulation/data scientists. To achieve this goal, we envision a balanced portfolio of support from the University, state government, federal agencies, private industry and non-profits that will sustain us in the long term while managing (and helping to guide) shifts in technologies and national priorities.

Over the long-term, the 2DCC-MIP was originally envisioned as the nucleus of a new user facility at Penn State, one that completes the Synthesis–Processing–Characterization–Theory/Simulation/Data tetrad with a primary focus on synthesis and envisioned as a future *Materials Growth Laboratory*. The three other arms of the tetrad already exist within the Materials Research Institute (MRI) at Penn State, operating with ongoing institutional support: the Materials Characterization Lab (MCL), Materials Computation Center (MCC) and Nanofabrication Facility (Nanofab). MGL would close the loop (Figure 8.1) through provision of advanced tools for thin-film deposition and epitaxy, *in situ* characterization, bulk-crystal growth, and related materials synthesis techniques. It is anticipated that the MGL in the long term will have a broader material focus than the 2DCC, to respond to changing user needs and research priorities/opportunities. In addition, the scope of MGL will likely expand beyond research to include scientific services (e.g. production of non-standard samples, equipment and process consultation) and pre-commercial development in partnership with industry and government laboratories.

Figure 8.1: The Materials Growth Lab will complete the synthesis-processing-characterization-theory/simulation tetrad with interconnected data infrastructure.

Any transition from NSF support to self-support will be challenging, but risks will be mitigated with careful planning and continual evaluation and adjustment This will be done while keeping in mind the needs and aspirations of users and stakeholders of the current 2DCC facility. We will engage the 2DCC User Committee in these discussions to better understand the long term needs of users and the potential impact of moving to a fee-for-use model. Penn State has a successful example in the recent transition of the Nanofab which had been receiving federal support under the NSF National Nanotechnology Infrastructure Initiative. Elements to evaluate for the transition include the user portfolio mix of in-house (local) research and non-proprietary external user projects from academia and government labs versus income from proprietary projects. In the early years of the 2DCC, the vast majority of use was generated from non-proprietary academic PI projects with increasing portions of the portfolio emerging from National Lab PIs and industry in 2018-2021. We envision an adjustment period to acclimate researchers to a fee structure with initial candidate targets such as consumables to start developing a base of core internal and external users to sustain what would become the MGL.

Aggressive marketing to industry and an earnest effort to seek out partnerships and collaborations to encourage proprietary research on a fee-for-use basis needs to occur early on in transition. The 2DCC has already begun this effort by focusing on some small company opportunities (i.e. SBIR/STTR), industry-funded consortia (e.g. IMEC), NSF IUCRCs, equipment manufacturers, and device/systems manufacturers. However, a deeper relationship with industry is desired in which early career researchers (e.g. undergraduates, graduates) from external institutions and within Penn State are trained in the facility and then spend time in industry applying the skills learned in the facility for future industry pipelining of a skilled workforce. The 2DCC has already participated on proposals with this focus to begin this effort but we envision doing more as companies have shown genuine interest through letters of support for such initiatives.

More broadly, the 2DCC has a tremendous opportunity in cultivating funding interest from the state of Pennsylvania in terms of its Department of Community and Economic Development for similar activities but related to the workforce in Pennsylvania specifically. The state funding portion of the MGL portfolio shows promise in the area of workforce training and development that draws students from state-funded undergraduate institutions and colleges as well as other state-related higher education institutions to train and recruit students for the future Pennsylvania industry workforce in materials synthesis. Having an established, trained workforce in crystal growth is attractive to industries to locate in the PA region and with a DCED objective to cultivate economic development the opportunities are robust and have direct impact on the 2DCC's long-term sustainability in part due to its alignment with state priorities.

The 2DCC is also focusing on leveraging staff expertise and computational/data infrastructure, the 2DCC's Theory/Simulation facility and Data Science activities, including maintenance and upgrades of LiST, to merge with another arm of the tetrad, the MCC. The 2DCC has been an active partner in plans to expand cyberinfrastucture within MRI to enable growth and processing recipes and associated characterization data to be readily uploaded and tracked as samples and users move throughout the facilities, a function ideally suited to LiST. This is critical for accelerating discovery and development of new materials and for attracting users focused on data science methods for discovery.

The continuing legacy of the 2DCC is guided by a set of principles that will contribute to sustainability. They include, but are not limited to:

- Maintain U.S. competitiveness in 2D materials synthesis
- Advance in situ characterization and processing methods
- Promote technology development by industry by leading the way for synthesis & processing feasibility
- Propel the next generation of crystal grower/tool developers who embrace MGI principles and use of data science methods
- Demonstrate a culture of knowledge sharing that contributes to accelerate discovery and development

Appendices

Appendix A: External Committees

A.1 External Advisory Committee

The EAC is a standing committee that consists of external representatives from academia, industry, and national user facilities. The committee meets annually to assess the overall performance, safety, policies, objectives and mission of the MIP and to recommend changes and review new directions as appropriate.

Dr. Christopher Palmstrøm (Chair)
Department of Electrical and Computer Engineering
University of California Santa Barbara

Dr. Timothy Murphy
Director, DC Field Facility, National High Magnetic Field Laboratory

Dr. Stefano Curtarolo
Department of Mechanical Engineering and Materials Science
Duke University

Dr. Keith Evans
President & CEO & Co-Founder
Great Lakes Crystal Technologies

Dr. Anupama Kaul
PACCAR Professor of Engineering, Director of PACCAR Technology Institute
University of North Texas

A.2 User Committee

The user committee is described in Section 5.7 of this Strategic Plan.

A.3 User Proposal Review Committee

User Proposal Review Committee: The User Proposal Review Committee (UPRC) is a standing committee that consists of external committee members, and it is populated among the 3 main facility user areas (i.e. Thin Films, Bulk Crystal Growth, Theory/Simulation). Adhoc reviewers are only used when necessary (e.g. not enough reviewers because of UPRC conflicts on specific proposals). The 2DCC Operations and User Facilities Director identifies reviewers for each proposal and implements the review process.

UPRC members are appointed 1 year at time, renewable on a yearly basis: The reviewer pool currently includes 18 members. Names are not shown here for confidentiality purposes. UPRC membership is supplied to NSF upon request.

Appendix B: Postdoc Mentoring Plan

Scholar Responsibilities

Postdoctoral scholars serve multiple roles in the 2DCC. Scholars are expected to pursue novel research directions in in-house research, often in collaboration with 2DCC affiliate faculty; however, roughly half of the full-time scholars' effort will be spent interacting with users and serving as the primary mentor for students (undergraduate and graduate) working in the 2DCC. Publications and presentations are another crucial part of the research process, and the scholars work on this not only for in-house research, but also work with 2DCC users, helping them pull together and think about sample data.

Mentoring Structure

Because of the interdisciplinary and multi-faceted nature of their positions, all postdocs receiving any 2DCC monetary support also receive multiple levels of mentoring. First, each scholar has a primary mentor with whom they meet frequently, for example, in weekly group meetings. Beyond this somewhat traditional advisor-postdoc model, however, the postdocs also partner with other mentors and take advantage of other resources. For example, 2DCC personnel Eric Hudson (Director for Education/Training Programs) and David Fecko (lead for industry and national lab collaboration) provide support for research-specific educational and knowledge transfer initiatives respectively. Penn State's Office of Postdoctoral Affairs offers frequent professional development workshops—for example, Hudson has run several workshops for them on effective mentoring for postdocs working with graduate students and undergraduates, and help is available for writing publications as well. Postdocs attend facility-wide bi-weekly technical meetings (often presenting) and are specifically involved in many aspects of platform-level efforts such as feedback for the Lifetime Sample Tracking (LiST) tool development.

Postdoctoral mentoring and training changes with time across the postdocs career. For example, although it is expected that the scholars in these positions have a strong technical research background related to some aspect of materials growth or 2D material properties, the desire is for the scholars to be able to interact broadly with facility users, consequently, training in unfamiliar techniques is often required initially. Mentoring graduate students and undergraduates is also often a new role for these scholars, so as mentioned above this skill is also discussed. Finally, as the scholars' terms near completion, mentoring shifts toward promoting career advancement, including CV development and research proposal/grant writing skills. Scholars are encouraged to assist in the preparation of scientific grant proposals based on their research activity, with particular attention paid to best practices in proposal preparation, including identification of key research questions, definition of objectives, description of approach and rationale, and construction of a work plan, timeline, and budget.

Assessment

At the beginning of the performance review period they complete a Goal Setting Worksheet (i.e. an accomplishments, metrics and implementation plan) with their primary mentor. Their performance is assessed annually (minimum of beginning of year goal setting, mid-year check-in and an end of year review) and refined as necessary. Performance evaluations are based on previously specified goals, and tailored, in part, to the needs of the scholar.

Appendix C: Data Management Plan

Last updated June 25, 2020

Overview: The 2D Crystal Consortium - Materials Innovation Platform (2DCC-MIP) team includes experts in synthesis, characterization theory and data science. The 2DCC-MIP aims to accelerate discovery-driven research into the growth, properties and applications of 2D quantum materials and related chalcogenide crystals for next-generation technologies by innovating state-of-the-art synthesis, characterization, computational facilities and data infrastructure to foster a diverse scientific ecosystem of in-house experts and external users to drive international leadership by the US 2D materials research community. Data resources are a central component of supporting that vision.

Primary and secondary data will be generated from diverse sources (e.g. materials synthesis, simulation, characterization, data models/protocols/metadata, workshop materials and public presentations). Project personnel are dedicated to an operating principle of timely accessibility to the products of the research and data standards activities for the broader scientific community according to Findable Accessible Interoperable Reusable (FAIR) principles. PI **Redwing** and senior personnel **Reinhart** (specializing in data science) and the Operations and User Facilities Director Dressler will work with the research data management specialist and the Executive Leadership Team (ELT) to coordinate data storage, capture, sharing and appropriate cybersecurity protocols through regular meetings of the team. Implementation of plans will occur through the data manager on this project at Penn State University. The ELT is responsible for reviewing data management practices and outcomes throughout the life of the project and ultimate responsibility lies with PI **Redwing**.

Products of the Research: 2DCC-MIP products are expected to cover a broad range, which includes: (1) experimental (e.g. materials descriptions, synthesis recipes and characterization results such as ARPES, STM, TEM, optical measurements, spectroscopy data and structural information), (2) simulation (e.g. simulation results of material electronic properties and growth behavior, software, parameter sets), (3) processed data (e.g. statistical analysis and machine learning data generated from experimental or computational raw data), and (4) evaluation data for program continuous improvement/management.

Data and Metadata Standards: A large portion of the primary data (i.e. experimental and computational) resulting from this project will be in the form of graphical, image and database files, initially stored on the computer dedicated to the device used to acquire the data or perform the computation and in many cases imported by automated workflows into a central database. Where possible common formats usable across a variety of platforms will be used, and these efforts will be coordinated with other MIPs to maximize inter-operability. Both instrument-related proprietary formats and conversions to accessible formats are made available for broadest access and use. 2DCC-MIP uses Javascript Object Notation (JSON), an open standard file and data interchange format, for its broad interoperability and language-independent attributes. Evaluation data will be archived, properly aggregated, password protected and maintained by the research data management specialist. Evaluation data are for internal purposes of program management and sharing with NSF in reporting only and are not for contributions to generalizable knowledge (i.e. research purposes or external publication).

Access to Data, Sharing Practices and Policies: The 2DCC-MIP web site has both a public area for data and information sharing and a private area via a linked, password-controlled Box account for internal project communication and sharing including the link(s) to project data. Project data, including growth protocols, characterization results, and associated computational data, are shared through the Lifetime Sample Tracking (LiST) tool maintained by the Penn State University and 2DCC. LiST is a comprehensive data management and curation software custom designed by the 2DCC to maintain robust and shareable records for synthesis, characterization, simulation testing and design data. Intellectual property and data generated under this project will be disseminated at workshops and conferences with peers and through the 2DCC-MIP web platform, among other venues. Materials generated under the project will be disseminated in accordance with University and NSF policies. Access to databases and associated software tools generated under the project will be available for educational, research and non-profit purposes. Publication of appropriate curated data shall occur during the project if appropriate, or at the end of the project, consistent with normal scientific practices. Research data which documents, supports and validates research findings, will be made available after the main findings from the final research data set have been accepted for publication.

2DCC-MIP policy is to publish relevant findings expeditiously in the peer-reviewed literature. However, research data will not be posted on the public portion of the website prior to publication, because many journals of primary publication (*ACS* journals, *Science*, *Nature* journals, etc.) will not accept papers that contain "already published" data. This embargo does not apply to oral presentations at professional meetings, but it does apply to press releases, which will be made with appropriate care. Following journal publication, data generated in this project is expected to be provided freely to colleagues at other institutions upon request, provided that intellectual property rules do not restrict immediate distribution. Any proprietary or confidential data that is obtained or generated through participation with industry or other external partners will be maintained and secured locally until it is cleared by the partner for release and distribution to other team members or the public. Any non-disclosure/confidentiality (and intellectual property) agreements will be administered through the Penn State Office of Technology Management. Database software in use and planned for use (e.g. ArangoDB for List 2.0) has capabilities for secure access across users, groups, and institutions with defined access rights.

Re-Use, Redistribution, and Production of Derivatives: In general, data will be free for use in scientific research or general education to the maximum extent possible, and no restrictions on re-use or re-distribution will be made for non-commercial use, as long as the original authors/publications are properly acknowledged. 2DCC-MIP encourages publication in journals with flexible copyright policies towards re-use and will respect the copyright policies of all journals in which project results appear, including images and data on websites. Wherever appropriate, data will be redistributed through community data archives determined as beneficial to reach the broadest audience.

Plans for Archiving and Preservation of Access: Data will be maintained on a central repository and archived for a minimum of 5 years after the project ends, with sustainability plans envisioning long-term data curation and maintenance beyond this window within the Materials Computation Center (see Section 12). The Institute for Computational and Data Sciences – Advanced Cyberinfrastructure (ICDS-ACI) provides systems and services that are used for research, teaching and service missions at Penn State. The ICDS-ACI storage infrastructure includes General Parallel, Clustered Network and Common Internet file systems that interconnect across high speed Ethernet, Infiniband, and Fibre Channel network fabrics. The storage architecture contains active storage pools that provide access to Home, Work, Group, and Scratch directories; near-line storage pools that provide a long-term and archive storage repository for files that are not needed real-time to support ongoing research efforts; and data management nodes that enable users to move data between active and near-line storage pools. The high-performance Ethernet network is built on Brocade VCS Fabric Technology and supports connectivity for all processing nodes that are within the ICDS-ACI system boundary. A VCS "fabric" provides a flexible interconnecting network between individual switches, creating a virtual cluster of physical switches. The current ICDS-ACI VCS network fabric includes SonicWall SuperMassive 9400 firewall appliance that provides 20 Gbps, low latency IPsec intrusion prevention; Brocade VDX 8770-8 Enterprise-level switches that are configured with 10/40/100 Gb network link capacity; Brocade VDX 6740 switches that provide 10 Gb link capacity;

and Dell N2024 switches for host integrated remote management over Gb link capacity

Results from Prior MIP Support Regarding Data Management: In years 1–5 the 2DCC-MIP has focused on maintaining robust records for synthesis, characterization and simulation done in the facility as well as developing infrastructure to make that data easily available to users and the broader community guided by FAIR principles. Consequently, the LiST data management tool was developed by professional programmers in collaboration with experimentalists and theorists. LiST is custom-designed to capture "recipes" used for materials synthesis and associated data from *in situ* and post-growth characterization or theory/simulation, including metadata. The LiST user interface has search features that allow visualization of project data for export to statistical analysis software or for aiding in future experimental design. The LiST tool also archives user communications, reports, publications, and other administrative documentation integral to facility operation and reporting. To date, LiST contains data for over 2500 material samples archived in its database.

Appendix D: MRI – MSC Building COVID-19 Supplemental Procedures

Scope: Entry to perform research at MSC during Covid-19 best practices. Subject to change (May 2020)

1) Hazard Assessment

Hazard	Required Engineering Controls and/or PPE
Covid-19 Virus	Hand sanitization stations, 70% Ethanol solution to disinfect high touch work surfaces and social distancing (min 6 ft distance between personnel)
Covid-19 Symptoms including fever, cough or general ill feeling	Stay home and contact your physician!
Typical hazards associated with individual research projects, equipment and chemicals	SOPs, personal protective equipment (PPE) and other engineering controls such as fume hoods and interlocks.

Procedures

1. *Entering the Millennium Science Complex for Research*
   a. If you feel ill, have traveled recently or have roommates who have traveled outside the area recently please stay home and self-quarantine for 14 days.
   b. Travel into MSC following all CDC and Pennsylvania state guidelines for travel.
   c. You must be wearing a mask to enter the facility.
   d. Enter the MSC building using the front doors. Only bring essential items into the building with you.
   e. Immediately upon entering the building wash your hands with soap and water for (>20s) or use one of the sanitizing stations such as the one in the MSC Lobby.
   f. Use the most direct route to your desk and the laboratory where work will be performed. Use caution to open doors by minimizing touching high touch surfaces such as door handles if possible.
2. *Preparing and performing laboratory work safely*
   a. Each faculty must have a plan in place for safely carrying out research including plans to minimize individual interaction, maintain strict sanitation and hygiene. This must be communicated to the essential personnel carrying out that research.
   b. Reserve the lab and time you will be working using the MRI calendar system to facilitate social distancing.
      (1) Maintain a density of no more than one person per lab room, unless the room exceeds 400 ft^2, then two people may be acceptable.
      (2) If the tool(s) that will be used require a RIMS reservation, please also reserve this with standard RIMS procedures in addition to signing up on the MRI Lab Calendar.
   c. If performing work alone in the lab, please follow the MRI Ebuddy SOP to ensure you have a virtual buddy to ensure your safety while working in the lab.
   d. Drop off what you do not need in the lab at your desk or if working in MCL/Nanofab use the lockers provided. Bring only what you need to the lab and do not bring other items into the laboratory.
      (1) If using the lockers, wipe down surfaces with 70% Ethanol
   e. Always wear the mask you have been provided unless the research procedures dictate different PPE. When not wearing the safety PPE required for your laboratory work, reapply your mask. Be sure to always wash hands before and after handling ANY face covering.

f. Prior to starting any work disinfect any work surface or high touch area in the lab with 70% Ethanol that was provided in each lab. Follow the SOP to disinfect the area by spraying the 70% Ethanol and waiting 5-6 minutes before beginning work
g. Minimize shared items (pens, notebooks etc.) as much as possible.
h. Once work is completed, disinfect work surface and any shared equipment again prior to leaving lab.
i. Remove any lab PPE such as lab coats and gloves upon leaving lab.
j. Proceed out of the lab making sure to bring anything you brought in with you.
k. Immediately wash your hands at one of the sanitizing stations on each floor or in the bathroom with soap/water (>20s).
l. Added Note 6-3-2020 If you need to enter a lab to retrieve a sample or end an experiment and will be in the lab less than 5 minutes, you do not need to reserve the space. If the lab is occupied, please maintain safe social distancing and retrieve your sample and exit immediately.

3. *Masks*
   a. Employees approved to return to work should at minimum follow the CDC and PA state guidelines and wear a cloth mask.
      (1) If you do not have a face mask use a bandanna or cloth in compliance with the Pennsylvania Governors recommendations.
      (2) If uncomfortable with recommended masks please talk to your PI about other mask options for work.
4. *Creating safe space*
   a. Maintain a minimum 6 ft distance at all times.
   b. Wash hands frequently with soap and water before entering and after leaving the lab. Wash them after touching shared accessory devices such as phones.
   c. Basic lab PPE such as lab coats and safety glasses should not be shared. Everyone should have their own.
   d. Shared PPE should be disinfected before and after use such as face shields, aprons etc.
5. *Common/shared spaces and samples*
   a. Transfer of samples should be arranged by leaving them in a designated location as opposed to handing them over in person when possible.
   b. Use of shared facilities and labs must be pre-arranged through the calendaring system to avoid accidental contact. Be sure all users know lab sign-in procedures.
   c. Use precautions when entering a restroom. Use a disposable towel to touch door handles and be sure to wash your hands upon entering and leaving.
   d. Kitchen areas are restricted to one person at a time. You must disinfect the space before and after using with the provided cleaning products.
   e. Wash hands after using a break room.
   f. The commons area will remain open, however, seating will be removed to better assist with social distancing. Please use provided disinfectant to sanitize tables/chairs before and after using.
   g. Please minimize unnecessary travel between the Huck and MRI side of the building unless needed.
   h. There should be only one student per graduate student area at a time in order to minimize close contact. If you do not have laboratory work to perform do not stay around longer than necessary to perform your experiments.
6. *Heading Home*
   a. Wash your hands with soap and water (>20s)
   b. Pick up anything brought with you to the building.

c. Proceed directly out of building via most direct route.
d. Proceed home and immediately wash or sanitize your hands upon return home.