User Policies and Procedures Table of Contents

2DCC-MIP User Policies and Procedures

Overview

The 2DCC-MIP (referred to as 2DCC hereafter) User Policies and Procedures provides a framework for establishing a congenial, collaborative environment where scientifically and culturally diverse researchers can work together in pursuit of the new scientific opportunities presented by this innovative facility.

Access to the 2DCC facility and staff is free to all academic and government researchers that are selected through a proposal review process. Industrial users will be charged for facility use.

User proposals are evaluated by external experts on a user proposal review committee (UPRC) to avoid conflict-of-interest. The 2DCC will identify external reviewers for each proposal. Reviewers are chosen for their scientific and/or technical expertise from the scientific and technical community at large.

A. Safety

The 2DCC is under the auspices of the Materials Research Institute (MRI) at Penn State University, the physical home of the facility. On-site users will follow the established safety and training procedures of the MRI.

For On-site Users

When using the 2DCC facilities, you will either be an:
Internal User (personnel employed by Penn State University), or
External User (personnel not employed by Penn State University)

All on-site users must complete required pre-requisite training in order to gain access to the Millennium Science Complex (MSC), Davey Lab and the labs within.

Required Pre-requisite Online Training
Required in-person Training
Introduction to Safety Classroom Session (on-site every Tuesday 9:00 a.m. MSC N-308A)

For step-by-step instructions to these pre-requisite training course, visit our **Safety Training** page.

Other specific EHS training may be required depending upon the lab to be used. Your 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.

Off-site users are not required to complete training as they will not be using the equipment directly.

B. Proposal Process

Proposers are encouraged to contact an advocate from a 2DCC **user support group** prior to submitting a proposal to help make the submission most effective. Proposal materials are submitted online via the **proposal submission portal**.

Research Project Proposals

Research project proposals are submitted on a rolling basis or in response to topical solicitations.

Required Materials

1. A cover page that will be automatically generated based on information you provide in the submission form fields (PI Information, Project Personnel, and Demographics).
2. An upload of a single PDF containing, in sequential order, a 3-page project description, plus references (no page limit), and an NSF format Biosketch for all senior project investigators such as faculty and postdocs (two pages each). *Biosketches are not required for undergraduate and graduate students*.

Proposals should follow standard NSF GPG format requirements for margins and font size.

Three-Page Project Description Content – The project description section should answer the following questions:

- What is the scientific significance and long-term impact of the project?
- How does your project align with the goals of the 2DCC in chalcogenides for next generation electronics?
- What 2DCC resources and expertise would be used?
- How will the users' expertise contribute to success?
- What work will be performed at your home institution(s) to support the proposed work?
- What are the broader impacts of the proposed work?

You need not provide a highly detailed schedule of facilities use. These are arranged at a later date for successful proposals in coordination with the user support group.

If your proposal is recommended for support by the user proposal review committee, a technical area scientist assigned to your proposal will contact you to develop the details of your experiment. All selected proposals are expected to go through a safety and facilities review prior to the beginning of the experiment.

Sample or Data Request Proposals

Sample request proposals are for standard materials that are routinely synthesized at the 2DCC and can be referenced from the 2DCC list of currently available Thin Films or Bulk Crystals. Data requests can be made for certain experimental data and established ReaxFF 2D potentials.

Required Materials

1. A cover page that will be automatically generated based on information you provide in the submission form fields (PI Information, Project Personnel, and Demographics).
2. An upload of a single PDF containing, in sequential order, a 1-page project description, plus references (no page limit), and NSF-format biosketch for the PI only (two pages).

Proposals should follow standard NSF GPG format requirements for **margins and font size**.

One-Page Project Description Content – The sample request or data request description section of the proposal file should answer the following questions:

- For Sample Requests: What are your material needs and characteristics? Specify details (e.g., material composition, sample size and quantity, doping, etc.)
- For Data Requests: What are your data needs? Specify details (e.g., details of synthesis recipe, characterization or simulation data from in-house research that you are requesting; if data on particular materials systems are needed, please name those chemistries). Consult the currently available samples for Thin Films or Bulk for reference on available materials systems)
- For either request: What is the scientific or technological motivation of your research project?
- How will the samples/data requested from 2DCC enable success of your project?
- What are the broader impacts of your work?

Review

User proposals are evaluated by external experts on a user proposal review committee (UPRC) to avoid conflict-of-interest. The 2DCC will identify external reviewers for each proposal. Reviewers are chosen for their scientific and/or technical expertise from the scientific and technical community at large.
***Confidentiality*:** Reviews will be conducted in strict confidence including content and reviewer identity and will only be shared with 2DCC staff and the UPRC. Dissemination of project summary information (e.g., title, PI name) is limited to NSF reporting and 2DCC user logistics.

Evaluation Criteria: Research project proposals are reviewed in accordance with NSF primary review criteria for Intellectual Merit and Broader Impact and additional criteria of synergy with the 2DCC-MIP focus.

2DCC-MIP Focus

• Advancing synthesis and characterization of 2D layered chalcogenides and related materials
• Supporting the development of next generation 2D devices
• Accelerating materials discovery through combined theory/simulation/data and experiment
• Promoting knowledge sharing of know-how throughout the 2D community and broadening participation

Scoring

5 - Proposal is of high quality and must be pursued
4 - Proposal is of good quality and access should be granted
3 - Proposal is acceptable, and access should be granted at 2DCC-MIP's discretion
2 - Proposal has minimal merit and access should be low priority; marginal scope; marginal equipment match

1 - Proposal has little merit and access should not be granted; out of scope; not suitable for available resource

Example User Proposal Evaluation Form

Project Priority

The 2DCC will accept as many top-ranked proposals as the capacity of the facility will allow. Capacity can (and will) change based on the portfolio of projects; therefore, the executive leadership team will contribute to decisions on a balanced portfolio of selected projects.
Additional Criteria for decisions on priority may include:

- PI is from a minority serving institution, a predominantly undergraduate institution or is from a group traditionally underrepresented in STEM disciplines
- PI is a first-time user of the 2DCC
- PI has used the facility previously and is in good standing (e.g., engaging 2DCC throughout project; user adherence to data policy for publication and acknowledgement)

Term of Support

Proposals will not be approved for additional support beyond the proposal validity period (sample-only proposals are active for 1 year; research projects are active for up to 2 years). Users must submit subsequent proposals for further use once the project has expired

Costs

The cost structure of 2DCC access and use is governed by the requirements set forth by the National Science Foundation (NSF) in the programmatic terms and conditions of NSF cooperative agreement DMR-2039351.

Access to the 2DCC is free for non-proprietary research of academic and government institutions, for which cost-recovery based expenses (e.g., materials and supplies, personnel time, equipment maintenance) are covered by NSF funds. Industry, international, and any proprietary research projects will be charged for use of the facility.

On-site users are responsible for their own living expenses and travel costs. Limited travel funds may be available for users from minority serving or predominantly undergraduate institutions on a case-by-case basis.

C. Technical Staff

2DCC technical staff split their time between internal research and user support. Internal research is focused on new capabilities that benefit their research as well as advancement of the user community. This synergistic approach to staffing is focused on the community while encouraging professional development of 2DCC staff.

D. Access to Other User Facilities at Penn State University

The 2DCC is under the auspices of the Materials Research Institute (MRI) at Penn State. MRI provides leadership both at Penn State and in the materials community worldwide, coordinating materials-related activities, maintaining core and shared facilities, training students, and fostering collegial exchanges of expertise. The MRI has a common physical location for the

majority of its facilities in the Millennium Science Complex. The 2DCC facility has direct access to three major facilities of interest to users which include the **Materials Characterization Laboratory**, the **Nanofabrication Laboratory** and the **Materials Computation Center**.

Materials Characterization Lab (MCL): Access to the MCL capabilities is part of the user proposal process. For example, the MCL is considered a service facility that may be used to characterize a material that may be created. The MCL is a fully-staffed, open access, analytical research facility charged with enabling research and educating the next generation of highly qualified researchers. For further information contact Dr. Joshua Stapleton (jjs366@psu.edu).

Nanofabrication Lab (Nanofab): Access to the Nanofab capabilities is part of the user proposal process. The Nanofab has world-class capabilities in the areas of deposition, etch, lithography, material modification, and characterization. From the wide variety of available processes, users have the ability to develop and fabricate a wide array of novel devices. For further information contact Dr. Chad Eichfeld (cme133@psu.edu).

Materials Computation Center (MCC): Access to the MCC capabilities is part of the user proposal process. The MCC at Penn State supports computer-based simulations of materials- across the various length and time scales. Computational materials researcher efforts at Penn State are enabled by strong interconnections between the Institute for Computational and Data Sciences (ICDS) and the Materials Research Institute (MRI). For further information, contact Dr. Adri van Duin (acv13@psu.edu).

Physics Low Temperature Measurement Laboratory: Access to the low temperature laboratory is part of the user proposal process. The Physics low temperature laboratory has user facilities for low temperature magnetometry and magnetotransport measurements available on a fee-for-use basis. This includes a multimode atomic force microscopy (AFM) / magnetic force microscopy (MFM) / scanning tunneling microscopy (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. For further information, contact Dr. Li-Chun Tung (lpt5154@psu.edu).

E. Project Reporting

2DCC staff will schedule check-ins with users at the midpoint of their award term and within 30 days of completion of their project at a minimum. A user is considered in good standing by participating in check-ins and following the established 2DCC policies and procedures.

F. Publications

Non-proprietary Data: Users are obligated to inform 2DCC of publications based on research involving 2DCC samples, research or its resources which will be included in 2DCC annual reports to NSF. 2DCC policy for its personnel and users is to publish relevant findings expeditiously in the peer-reviewed literature regardless of the data originator or owner.

Proprietary Data: Proprietary data are not expected to be published.

Co-authorship of publications resulting from user projects is governed by accepted scientific practices and may include 2DCC-affiliated faculty or staff scientists when such individuals make substantive contributions towards fundamental discovery, data analysis, or novel samples.

G. Acknowledgement

Users must **acknowledge** NSF award DMR-2039351 in all publications, presentations, websites, press releases, etc, for which use of the 2DCC facility either as samples or a user research project is a part of the content. If any of the samples or research originated from the 2DCC prior to June 1, 2021 please consult with 2DCC faculty at time of publication for proper acknowledgement of the 2DCC support as it may also include DMR-1539916 in addition to DMR-2039351.

H. Data Management Policy

Overview

Operational philosophy: The 2DCC-MIP (hereafter referred to as 2DCC) is a national user facility funded by the National Science Foundation which does not charge fees for non-proprietary use by U.S. academic or government researchers. The 2DCC data mission is to create a *community knowledge base* in synthesis of 2D materials, including detailed, comprehensive synthetic protocols, characterization measurements, and simulation results generated through non-proprietary research in the 2DCC. It is an obligation of all non-proprietary users of the 2DCC to reasonably facilitate this process, consistent with shared norms of scientific conduct.

Data covered by this policy includes that generated directly on 2DCC equipment (thin-film and bulk growth, integrated characterization measurements, 2DCC computational resources) and also that generated at support facilities for characterization (Materials Characterization laboratory), fabrication (Nanofabrication Laboratory) and computation (Materials Computation Center), when 2DCC resources have supported use of those facilities.

NSF best practices and resources for data curation in materials research are evolving. Therefore, the Data Management Policy is a living document that is reviewed regularly by the 2DCC executive leadership team and updated as appropriate to serve the broad interests of the scientific community.

Data Types

2DCC user data cover a broad range, including but not limited to: *simulation data* (e.g., databases of material electronic or structural properties, simulations of kinetic parameters, etc.), *experimental data* (e.g., characterization data from STM, TEM, optical measurements, spectroscopy data, structural information, etc.) and *experimental process information* (e.g. detailed synthetic protocols and processing steps).

In the normal course of research, it is common for much data obtained to be non-archival in quality – a sample may be degraded, instrumental settings incorrect, noise levels too high, or simulation settings improper. Following best practices, it is the intention of the 2DCC to save all data generated, since even low-quality data can be crucial to informing later decisions in process optimization or instrument debugging.

Data is classified into two main categories: (1) Work-in-progress Data – data generated at intermediate stages in an investigation, of uncertain quality and with substantially incomplete contextual information and (2) Archival Data – contextualized data worth saving in a community repository for later reference and reuse. The scientific judgment of the investigators involved, guided by 2DCC policy and goals, will inform what data is deemed archival in quality. In cases where consensus cannot be obtained, the ELT will make this determination.

Data and Metadata Standards

Standards for data vary by the method, equipment, and software used for its generation, and evolve over time. This includes raw data in the native format of an instrument, processed data in standard inter-change formats, and metadata necessary to establish meaning and context for the associated measurement or simulation. The issue of data format is complex and evolving – the philosophy of the 2DCC is to facilitate progress towards data exchange formats and platforms that are accessible, interoperable, and easy to use.

Data Sharing and Access

Data generated at the 2DCC are under the ownership of the user(s). Users, as owners of data, have full control over decisions regarding publication, in accord with shared standards of scientific conduct. Users are responsible for adhering to the policies and procedures of their funding agencies. The user PI grants the 2DCC a non-exclusive license to host non-proprietary data on a community platform as designated by the 2DCC, subject to certain restrictions – designed primarily to protect the users' publication priority – as outlined below.

Non-proprietary data including databases, software and metadata that were produced using NSF funds are expected to be shared publicly after publication. Data that is not indicated by the user PI as intended for publication may be shared publicly by 2DCC no sooner than one year following the end date of the User Project under which it was generated. It is the intention of the 2DCC to provide a central data repository for ensuring community access to non-proprietary data generated under support from 2DCC resources. In cases where publication is intended to take place more than one year after the end date of the project, Users may request a delay of data sharing, subject to approval by the ELT.

Data Re-use or Redistribution

User data will not be shared publicly by the 2DCC prior to publication – or one year following the end date of the associated User Project, as indicated above – without the permission of the user PI. Public sharing includes cases where data reported to NSF becomes part of the public record. Data may be shared internally with NSF program officers as part of NSF oversight, with notice given to the user. Users are free to redistribute their data, following NSF policies, given that **acknowledgement** of the 2DCC in providing resources for generation of those data is made.

Users performing non-proprietary projects at the 2DCC are expected to analyze and submit their results for publication on a reasonable timescale, with proper **acknowledgement** of the facility.

Storage and Archive

The 2DCC will maintain non-archival user data and sample storage for a period of at least five years following the close of the user project. The 2DCC intends to maintain archival user data indefinitely through a central data repository managed by 2DCC or in partnership with external entities that adopt the mission of long-term data curation for the materials research community.

Proprietary or confidential data that is obtained or generated through participation with users will be maintained and secured locally as a copy of that shared with the user and is subject to a non-disclosure/confidentiality (and intellectual property) agreement administered by the Penn State Office of Technology Management between the user institution and Penn State University.

I. User Agreements

Sample Request Projects

For requests that involve standard samples from the 2DCC currently available samples in Thin Films or Bulk Crystals, there is a simplified online agreement in the proposal portal that the submitting PI agrees to at the time of proposal submission.

For requests of more experimental samples that the 2DCC is making in the in-house research program but are not currently listed as available samples in the standard sample catalog the following applies:

If Penn State non-standard samples are being sent to a user at an external institution/company, then execution of Penn State's Materials Transfer Agreement (MTA) is required. The 2DCC team will contact the Penn State Office of Technology Management (OTM) with the necessary information for preparing the MTA. OTM will prepare and forward the agreement to the user's institution/company for signature and notify 2DCC personnel when the agreement is fully executed so arrangements can be made by 2DCC staff to send the subject materials to user at their institution/company.

Research Projects

2DCC research projects are covered by a non-financial user agreement with Penn State University. This agreement, between the user's institution and Penn State University forms the contractual basis for use of the 2DCC facility and is administered by the Penn State Office of Sponsored Programs.

J. User Feedback

The user experience can only be improved by user feedback. All users are strongly encouraged to contribute to improvement of user experience at any time during the project. At the annual users meeting, users are given an online user survey for anonymous feedback as well as encouraged to participate in a private session with the User Committee chairs at the meeting. If any users cannot attend the annual users meeting and would like to provide feedback they will be provided with the same user survey by sending an email to the Director of User Programs (Joshua Robinson; **jar403@psu.edu**).

Although the 2DCC cannot require users to fill out a survey it is highly encouraged as the user experience is central to this national facility.

K. Users Committee

The Users Committee will be *external users* of the 2DCC facilities and knowledgeable in their development and operation. These members will not come from *internal users* defined as

being employed by Penn State University. The User Committee will meet at least annually to provide advice to the 2DCC Director on policies relating to the use and development of the facilities, safety concerns, access to products, and the curation and full use of data-related products of the facility. Facility products include, but are not limited to, samples, code, and data. The User Committee will prepare at least one written report to the 2DCC Director annually, which will be included in the annual report to NSF.

The 2DCC's User Committee consists of two experienced external user co-chairs as well as volunteer users of the 2DCC facilities who are knowledgeable in their development and operation. The User Committee provides advice to the 2DCC Director annually concerning the use and development of 2DCC facilities, safety concerns, and access to 2DCC products. Facility products include, but are not limited to, samples, code, and data. The committee conducts an annual meeting in May of each year which is paired with the annual users meeting and prepares a written report to the 2DCC Director annually that is included in the annual report to NSF.

L. External Advisory Committee

The external advisory committee (EAC) consists of members from academia, industry and national user facilities. The EAC meets annually to assess the overall performance, safety, policies, objectives and mission of the MIP, recommends changes and reviews new directions as appropriate. Annual reports of the EAC are included in the 2DCC-MIP annual report to NSF. The current membership may be referenced here.