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 charged facility use.

"Sample-only" proposals will be evaluated by the 2DCC Executive Leadership Team. "Research Project" proposals will be evaluated by an external panel of subject-matter experts selected for each solicitation.

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

- Cover Page – Automatically generated from information the user provides in the online proposal submission portal
- Proposal – File upload of one PDF arranged in the following order
  - 3 page Project Description including **broader impacts** of the work
  - References (no page limit)
  - 2 page NSF-format Biographical sketch of all project personnel, except students (**Template**)

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 from the **user support group** 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.

Review

Research project proposals will be evaluated by external experts on a user proposal review committee (UPRC) to avoid conflict-of-interest. The 2DCC executive leadership team will identify a minimum of three 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.

Additional Review Criteria for 2DCC User Research Project Proposals:
1) To what extent is the proposed research aligned with 2DCC priorities and to what extent will it make significant scientific or technological advances and produce outcomes for dissemination?
2) Is the project plan feasible for execution at the 2DCC in terms of scope?
3) Is the user properly prepared to make efficient use of the 2DCC?
4) To what extent is the research mutually beneficial to the 2DCC and the user's institution?
5) To what extent are 2DCC's unique capabilities necessary for the project's success?

Scoring
The research project proposal will be scored by the user proposal review committee
Ratings categories: Excellent, Very Good, Good, Fair, and Poor

Sample-only Proposals

Sample-only proposals are for standard materials that are routinely synthesized at the 2DCC.
Current Available Samples

Required Materials

- Cover Page – Automatically generated from information the user provides in the online proposal submission portal
- Proposal – File upload of one PDF arranged in the following order
  - 1 page Project Description including **broader impacts** of the work
  - References (no page limit)
  - 2 page NSF-format Biographical sketch of the PI (**Template**)

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

One-Page Project Description Content – The project description section should answer the following questions:
What are your material needs and characteristics? Specify details (e.g., material composition, sample size and quantity, doping, etc).
What is the scientific or technological motivation of your research project?
How will the samples requested from 2DCC enable success of your project?
What are the broader impacts of your work?

Review

Sample-only proposals are reviewed by the 2DCC user support groups from the appropriate technical areas (synthesis, characterization, and theory), and recommendations for selection are made to the executive leadership team on a rolling basis.

Evaluation Criteria: Sample-only proposals are reviewed in accordance with NSF primary review criteria for *Intellectual Merit* and *Broader Impact*, and *additional criteria*.

Additional Review Criteria for 2DCC Sample-only Proposals:
1) To what extent is the composition and/or proposed analysis of the sample aligned with 2DCC priorities; to what extent will it make significant scientific or technological advances and

produce outcomes for dissemination (e.g., publications)?
2) Is the user properly prepared to make efficient use of the 2DCC sample?
3) How is the sample beneficial to research at the user's institution?
4) Why are 2DCC's unique capabilities necessary for the project's success?

Scoring
Sample-only proposals are reviewed by the 2DCC executive leadership team.
Ratings categories: Excellent, Very Good, Good, Fair, and Poor

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., project reports up to date; 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 2 years) or agreed upon budget. Users must submit subsequent proposals for further use once project funds have been expended or after the proposal validity period, whichever is earlier.

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-1539916.

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 based on cost recovery.

On-site users are responsible for their own living expenses and travel costs. Limited travel funds are available for users from minority serving or predominantly undergraduate institutions.

Once selected to use the facility, the **user support group** advocate will work with the user to estimate the amount of project support, including supplies that are needed to complete the project.

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 developed 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 research 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.

Nanofabrication Lab (Nanofab): Access to the Nanofab capabilities is part of the user research 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.

Materials Computation Center (MCC): Access to the MCC capabilities is part of the user research proposal process. The MCC at Penn State supports computer-based simulations of materials- across the various length and time scales.

E. Project Reporting

Users are required to submit a project report at the midpoint of their award term and a final project report within 30 days of completion of their project. A project report template will be provided and includes metrics such as publications, awards or other research outcomes resulting from 2DCC resources. This information allows us to track the success of our program and will be included in the 2DCC annual report.

Proposals submitted by former users who have not submitted their annual or final project reports will be rejected without review.

F. Publications

Non-proprietary Data: Users are obligated to inform 2DCC of publications or theses based on research involving 2DCC samples, research or its resources. During the project period these may be included in the annual report or at the project end and will be accompanied by the supporting data and metadata of those publications. If a publication has resulted from 2DCC samples, data, or resources *after the project period*, you may provide the publication at the time of acceptance. Acknowledgement of 2DCC in these publications is required as shown in Section G of this guide this document, below.

Generally, 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. However, research data will not be posted on the public portion of the 2DCC 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 should be made with appropriate care.

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-1539916 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.

Material Samples-only: "[Your specific sample(s)] for this publication was provided by The Pennsylvania State University Two-Dimensional Crystal Consortium – Materials Innovation Platform (2DCC-MIP) which is supported by NSF cooperative agreement DMR-1539916".
User Research Projects: "This study is based upon research conducted at The Pennsylvania State University Two-Dimensional Crystal Consortium – Materials Innovation Platform (2DCC-MIP) which is supported by NSF cooperative agreement DMR-1539916".

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 covered the user fees at 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 will be classified into two main categories:
1) Work-in-progress Data – data generated at intermediate stages in an investigation, of uncertain quality and with incomplete contextual information which limits its usability
2) Archival Data – high-quality 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. As a general guide, data of sufficient quality to publish is archival. User input is crucial for deciding when data is archival; but 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 by the user after publication. It is the current intention of the 2DCC to act as liaison for ensuring community access to data and facility personnel will work with users to make every effort to do so.

Data Re-use or Redistribution

User data will not be shared publicly by the 2DCC prior to publication 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 monitors 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

Physical samples produced at the 2DCC under auspices of an approved user proposal may be transferred to the user after implementation of a **materials transfer agreement** with their institution, administered by the Penn State **Office of Technology Management**.
The user will have access to generate a copy of their data for their own local storage.

The 2DCC will maintain non-archival user data for a period of at least five years following the close of the user project. The 2DCC intends to maintain archival user data indefinitely, likely 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-Only Projects

2DCC sample-only projects (physical samples) are covered by a materials transfer agreement. These agreements are between the user's institution and Penn State University and form the contractual basis for use of the physical sample.

Research Projects

2DCC research projects are covered by a 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. Below is an executive summary of how IP is handled and does not represent the entire agreement.

Research Collaboration

Research collaborations are covered by a standard research agreement.

Research IP Summary

- If research (not research services) is conducted at the 2DCC-MIP:
  - If research is conducted solely by Penn State researchers, then any resulting IP will be owned by Penn State.

- If research is conducted solely by non-Penn State researchers, then any resulting IP will not be owned by Penn State.
- If research is conducted jointly by Penn State researchers and non-Penn State researchers, then any resulting IP will be owned on the basis of inventorship as determine by United States patent law.

- If Penn State and a non-Penn State entity cannot agree on inventorship, then a neutral third party patent attorney with appropriate technical expertise and mutually acceptable to Penn State and the non-Penn State entity will determine inventorship. Penn State and the non-Penn State entity will equally share the expense of the inventorship determination.

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 by filling out an online user survey or by sending email to the Director of User Programs (Joshua Robinson; jar403@psu.edu).

Regardless of providing comments during the project, users will receive an email invitation to take part in an online user survey after their project ends. Although the 2DCC cannot require users to fill out the survey it is highly encouraged as the user experience is central to this national facility.

K. Users Committee

Members of 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.

L. External Advisory Committee

The external advisory committee (EAC) consists of five members representing both academic and non-academic interests across the research and user facility aspects, including 1) experiment and theory, 2) education and broader impact, and 3) technology transfer. The EAC will provide critical feedback on the portfolio of user projects, facility level goals, strategic plans and outcomes such as the diversity of users, tool and instrument development and commercialization opportunities, and assessment of knowledge transfer and education activities.