2-Dimensional Crystal Consortium - Materials Innovation Platform (2DCC-MIP)

Facility Description:

2DCC Vision

Advance discovery-driven research into the growth, properties and applications of 2D chalcogenide crystals for next-generation electronics through the development of state-of-the-art synthesis and characterization tools within a multidisciplinary user environment to enable expansive national leadership in this important area.

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 minorities underrepresented in science and technology through diverse representation in staffing and research activities.

Key products/services:

The 2DCC platform is defined by three major components: In-house research, user facility, and education/outreach in support of the research mission

Science Drivers (In-house research) -- The 2DCC research priorities are organized by four 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. The science drivers are: Physics of 2D Systems, Epitaxy of 2D Chalcogenides, Next-generation 2D Electronics, and Advanced Characterization and Modeling.

User Facility – The user program focuses on three main facility components:
(1) *Synthesis and In situ Characterization of Thin Films*
(2) *Bulk Crystal Growth*
(3) *Theory/Simulation*

The user program is focused on the synthesis of 2D chalcogenides for next generation electronics 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.

Education/Outreach – 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 STEM. Education/Outreach programs include: 1) an education series that includes executive course, tutorials and hands-on training; 2) a monthly webinar series that is broadcasted live; 3) major sponsorship and participation in the annual Graphene and Beyond workshop; 4) a travel extension program for 2DCC faculty to visit PUIs and MSIs and present the work of the 2DCC and highlight opportunities for involvement; and 5) Opportunities for summer extended stays for users wishing to spend intensive time training at the facility.

Facility CI:
Theory efforts in the 2DCC-MIP aims at accurately modeling the growth of two-dimensional chalcogenides with multiscale methods and simulating a broad range of characterization techniques from first-principles, both in deep collaboration with 2DCC experimentalists. As a user facility focused on synthesis, the 2DCC does not have a dedicated CI; computational work is divided between two facilities, with the majority of the current workload managed by the Penn State Institute for CyberScience Advanced CyberInfrastructure (ICS-ACI), and future works supported by XSEDE research allocation on the Louisiana State University superMIC (420k CPU hours).

The physical infrastructure of ICS-ACI located in the Penn State University Park campus, where about 50% of the facility's power and equipment resources are dedicated to supporting the infrastructure. The ICS-ACI cluster consists of over 1200 nodes on Linux 6, with high-performance Ethernet or Infiniband interconnects. The queueing system supports interactive and batch jobs. In addition, a Guaranteed-Response Time (GReaT) model is offered, guaranteeing queue times of at most one hour to participating subscribers (2DCC users included). In the current phase the 2DCC theory team accesses 60 256-GB nodes and 10 TB shared storage under an allocation of 1000k CPU hours released on a quarterly basis, with expansion planned for the next phase. Software required by the 2DCC team are provided in the ICS-ACI cluster software stack, including highly parallel quantum chemistry and molecular dynamics codes, along with software libraries that allow for custom compilation. The median age of key CI components is less than 1 year.