2D Layered Materials (beyond graphene) for Structural and Energy Applications

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Nanoscience
The Kavli Prize in Nanoscience is given to Mildred S. Dresselhaus, Massachusetts Institute of Technology, USA, "for her pioneering contributions to the study of phonons, electron-phonon interactions, and thermal transport in nanostructures."

The 2012 Kavli Prize Laureate in Nanoscience: Mildred S. Dresselhaus
Questions / Goals

1. Current state of the field (materials devices, modeling) and how far are we from applications?

2. What is needed in the science infrastructure to transform the promise of this field to an area of US scientific and technological strength?

3. What are the key areas in which knowledge and resources limit the progress of this field which may prevent us from reaching the desired goals?

4. What lessons can we learn from carbon nanotubes that will help speed up R&D of 2D materials and devices?

5. How are other countries positioned to carry out the research in this area and how did they get there?
1. **Current state of the field (materials devices, modeling) and how far are we from Energy / Structural Applications?**

- *Discovery and design phase – many new materials; exploration of characterization and processing techniques, and functionality*

**On substrates / supports**
- Electrodes - Flexible transparent conductive electrodes for macroelectronics - for organic electronics (PV, LED)
- Catalysts – for hydrogen evolution, for industry, photocatalysts - replacing noble metals
- Coatings

**Freestanding**
- Thermal materials – Thermal management, thermofluids, adding thermal conductivity to polymer composites
- Composite Materials – Electrically and thermally conductive, high strength, high toughness
- Energy storage / generation media - Batteries, supercapacitors, fuel cells
- Hydrogen Storage media
- Water purification and desalination
- Thermoelectric materials
- Lubricants
2. What is needed in the science infrastructure to transform the promise of this field to an area of US scientific and technological strength?

1. Stronger connections between basic science explorations, nanomanufacturing initiatives, and industry
   1. Interagency cooperation
   2. Application pull
   3. Science to scalable nanomanufacturing process - (e.g. NSF scalable nanomanufacturing (3-5 investigator projects, 5-6 M$))
   5. Advanced manufacturing – (e.g., inclusion into initiatives in EERE (Manufacturing Demonstration Facilities), NIST (1B$ + 1B$ match, 15 programs for NNI (Nat’l. Network for Manufacturing Innovation), pilot for additive manufacturing),

2. Establishment of standards for material quality, performance
   1. E.g., as in commercial catalysts.

3. For reproducibility of material quality after large scale production methods.
Center for Nanoscale Materials (CNM)  
Argonne National Laboratory

The CNM’s mission includes supporting basic research and the development of advanced instrumentation that generates new scientific insights and creates new materials with novel properties. The CNM, with its array of proximal probes, synthetic and computational capabilities, and scientific staff, enables researchers to extend their reach.

The scientific challenges the CNM tackles involve fabricating and exploring novel nanoscale materials and, ultimately, employing unique synthesis and characterization methods to control and tailor nanoscale phenomena. The unique capabilities of Argonne’s Advanced Photon Source play a key role in that its hard X-rays, harnessed in a nanoscale beamline, provide unprecedented capabilities to characterize extremely small structures.

www.cnm.anl.gov

Center for Functional Nanomaterials (CFN)  
Brookhaven National Laboratory

The CFN provides state-of-the-art capabilities for the fabrication and study of nanoscale materials, with an emphasis on atomic-level tailoring to achieve desired properties and functions. As a premier user facility for conducting interdisciplinary nanoscience research, the CFN serves as a focal point and enabler of advanced materials study in the northeastern United States and beyond. Together with the National Synchrotron Light Source (NSLS) and the proposed NSLS-II, these facilities will complement each other to facilitate the nanoscale revolution. The synergy between these world-class resources, with Brookhaven’s own scientific staff working alongside with university, industrial and government laboratory researchers, offers unique opportunities for breakthroughs in energy research.

www.cfn.bnl.gov

The Molecular Foundry
Lawrence Berkeley National Laboratory

The Molecular Foundry provides users with instruments, techniques, and expertise to enhance their research in the synthesis, characterization, and theory of nanostructures. Its research themes emphasize combinatorial synthesis of nanomaterials, multimodal in situ imaging and spectroscopy, interfaces in nanomaterials, and “single-digit” nanofabrication. The Foundry’s six facilities provide synthesis of novel inorganic, organic and biological nanostructured building blocks, measurement and simulation of their properties, and their integration into complex assemblies. Utilization of these capabilities by users is enhanced through close ties to the other DOE user facilities at LBNL, which include the National Center for Electron Microscopy, the Advanced Light Source, and the National Energy Research Scientific Computing Center.

www.foundry.lbl.gov

Center for Nanophase Materials Sciences (CNMS)  
Oak Ridge National Laboratory

The CNMS integrates nanoscale science with neutron science: synthesis sciences; and theory, modeling, and simulation. Research focuses on understanding, designing, and controlling the dynamics, spatial chemistry, and energetics of functionality of nanoscale systems.

The CNMS’s vision is to become a world leader in nanoscale science by developing the scientific principles that govern the design, performance, and integration of nanoscale materials.

The distinguishing characteristic of CNMS is its emphasis on exploring the path from scientific discovery to the integration of nanostructures into the micro and macro worlds. This pathway involves the experimental and theoretical exploration of behavior, the development of a wide variety of synthesis and processing approaches, and an understanding of new performance regimes, testing design, and integration of nanoscale materials and structures. Integration itself is key to the exploitation of nanomaterials, and the scientific challenges that it poses are at the heart of CNMS’s mission.

www.cnms.ornl.gov

Center for Integrated Nanotechnologies (CINT)  
Los Alamos and Sandia National Laboratories

CINT’s vision is to become a world leader in nanoscale science by developing the scientific principles that govern the design, performance, and integration of nanoscale materials.

The distinguishing characteristic of CINT is its emphasis on exploring the path from scientific discovery to the integration of nanostructures into the micro and macro worlds. This pathway involves the experimental and theoretical exploration of behavior, the development of a wide variety of synthesis and processing approaches, and an understanding of new performance regimes, testing design, and integration of nanoscale materials and structures. Integration itself is key to the exploitation of nanomaterials, and the scientific challenges that it poses are at the heart of CINT’s mission.

www.cint.lanl.gov
3. What are the key areas in which knowledge and resources limit the progress of this field which may prevent us from reaching the desired goals?

1. **Synthesis and processing challenges.**
   1. Still discovering the types of entirely new 2D materials we can access (e.g. new MXenes, silicene, germanene, oxides,
   2. Role and opportunity of defects very important for new composites
      For chemical functionalization and organic hybrid materials development
   3. Three dimensional constructs of 2D materials must be considered as properties are evaluated for structural/energy applications, surface:volume ratio.
   4. Exfoliation without damage to properties.
   5. Obtaining preferentially single layers in stable suspensions, stable dispersions
   6. Methods of alignment during processing
   7. Fundamental understanding of growth mechanisms – e.g. CVD for large single crystals, rapid growth over large areas,
   8. How to prepare / characterize clean interfaces

2. **Characterization tools needed – multiscale characterization**
   1. Raman selective to particular defects, grain boundaries, but still developing techniques for enhanced selectivity
   2. Scanning probe (multiple) and TEM techniques (in situ, multiple)
   3. In situ techniques for intercalation (e.g. NMR, calorimetry),
3. What are the key areas in which knowledge and resources limit the progress of this field which may prevent us from reaching the desired goals?

3. **Theory / modeling Challenges** –
   1. For general purpose synthesis: ("optimization with constraints")
      Computational design of substrates promoting nucleation into 2D (layer) and preventing nucleation into 3D (bulk).
   2. For electrochemical energy applications
      Energy landscapes assessment for ionic binding and mobility on the 2D substrates and between the layers.
   3. For structural/mechanical and multifunctional:
      Theoretical mechanisms of interface control, with the challenge of sufficiently strong binding yet preserving the structural integrity of 2D-layers.

*2D Materials - A testbed for the Materials Genome Initiative!*
4. What lessons can we learn from carbon nanotubes that will help speed up R&D of 2D materials and devices?

1. Find the killer application
   1. Understanding the unique properties, and what roadblocks in current applications they can overcome – materials by design Materials Genome Initiative
   2. Explore tailoring, testing, optimization of these materials toward particular applications.
   3. Necessary to fund development to cross the valley of death batteries ?, transparent conductive coatings ?

2. New approach: 2D materials allow the versatility of materials choices for particular applications
   1. E.g. – For batteries, choose the 2D layered material with appropriate layer spacing for intercalation of inexpensive, multivalent, large ions. Volumetric vs. gravimetric density an issue.
5. How are other countries positioned to carry out the research in this area and how did they get there?

1. Large scale Nanomanufacturing efforts in Australia, Europe, Japan, proceeding

2. Japan example: Graphene and SWNTs – TASC Project

![TASC Organization Chart]

TASC Organization Chart

- General Meeting
- Board of Directors
- Chairman
- Steering Committee
- President
- CNT Steering Committee
- CNT Innovation Committee
- Assistant to the President
- Intellectual Property Producer (CNT, Graphene)
- CNT Project Team
  - Theme 1: Development of Controlled Growth of CNT
  - Theme 2: Technology Development of Uniform Dispersion of SWCNTs
  - Theme 3: Developing Techniques for Voluntary Safety Management of Nanomaterials
  - Marketing Department
- Graphene Project Team
  - Theme 1: Plasma CVD Technology
  - Theme 2: Roll to Roll Massive Synthesis Method
  - Theme 3: Transparent Film Manufacturing Technology
  - Theme 4: Transparent Conducting Film Efficient Assessment
- Graphene Steering Committee
- Graphene Innovation Committee

![TASC Project Example]

TASC Project Example

- Development of Techniques for Synthesis of High Quality Graphene
- Development of Techniques for Roll-to-Roll Mass Synthesis of Graphene
- Development of Production Technology for Transparent Conductive Films
- Performance Evaluation of Transparent Conductive Films

![CVD by using Microwave Plasma CVD sustained by Surface Wave]

CVD by using Microwave Plasma CVD sustained by Surface Wave

Chemical Vapor Deposition method (CVD) was developed to form a large sheet of graphene, which increased the industrial applicability. However, as this method requires 1000°C to synthesize graphene, it is not practical to achieve continuous production of graphene. TASC has been conducting research and development of the mass production technology of graphene using Microwave Plasma CVD sustained by Surface Wave developed by National Institute of Advanced Industrial Science and Technology (AIST). The plasma-CVD is suitable for low-temperature synthesis. Since this method can synthesize graphene at 300°C, at high speed in a large area, it is suitable for continuous production.