Nano.gov
U.S. National Nanotechnology Initiative

Nanotechnology Signature Initiative
Nanotechnology Knowledge Infrastructure: Enabling National Leadership in Sustainable Design

December 2, 2013

US-EU Bridging nanoEHS Research Efforts
Arlington, VA

www.Nano.gov

Collaborating Agencies: CPSC, DOD, EPA, FDA, NIH, NIOSH, NIST, NSF, OSHA

NNI Signature Initiatives

The Nanotechnology Signature Initiatives (NSIs) spotlight areas of national significance that can be more rapidly advanced through focused and closely-coordinated inter-agency collaboration.

The NSIs

- **Address R&D gaps** within areas of critical national need
  - Identify research ***thrust areas***
  - Select ***key research targets*** associated with near-and long-term expected outcomes
- ***Leverage*** skills, resources, and capabilities among multiple NNI agencies to maximize scientific and technological progress
- Provide a forum for communication and ***ongoing assessment*** of direction and progress
- ***Catalyze*** communities of practice and public private partnerships to accelerate commercialization

Nanotechnology Signature Initiatives

- Nanotechnology for ***Solar Energy Collection and Conversion***
- ***Sustainable Nanomanufacturing***: Creating the Industries of the Future
- ***Nanoelectronics*** for 2020 and Beyond
- Nanotechnology ***Knowledge Infrastructure***:
  Enabling National Leadership in Sustainable Design
- Nanotechnology for ***Sensors and Sensors for Nanotechnology***: Improving and Protecting Health, Safety, and the Environment
- Related initiative: ***Materials Genome Initiative***

Nanotechnology Knowledge Infrastructure: Enabling National Leadership in Sustainable Design

Agencies involved: CPSC, DOD, EPA, FDA, NASA, NIH, NIOSH, NIST, NSF, OSHA

Goal: Provide a community-based, solutions-oriented knowledge infrastructure to accelerate nanotechnology discovery and innovation.

Thrust Areas:

- A **diverse collaborative community** of scientists, engineers, and technical staff to support research, development, and applications of nanotechnology to meet national challenges
- An **agile modeling network** for multidisciplinary intellectual collaboration that effectively couples experimental basic research, modeling, and applications development
- A **sustainable cyber-toolbox** to enable effective application of models and knowledge to nanomaterials design
- A **robust** digital nanotechnology **data and information infrastructure** to support effective data sharing, collaboration, and innovation across disciplines and applications

NKI is an initiative to accelerate science and engineering *by developing and empowering the community.*

Thrust

Foster an agile ***modeling network*** for multidisciplinary collaboration.

Data
- Many kinds
- Many disciplines

- **Experiment**
- **Theory**

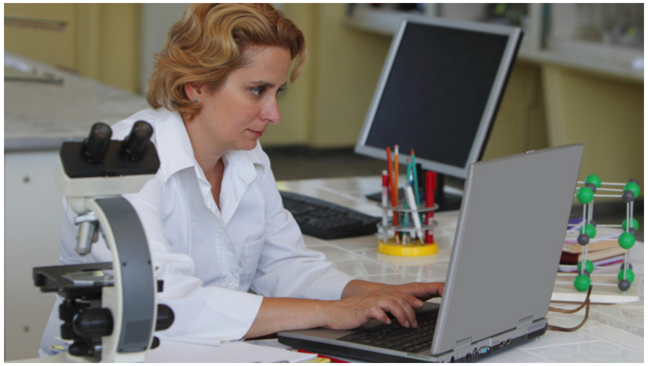
Computation
- 'First Principles'
- 'Models'

Innovative nanoscience and nanotechnology

Our NKI multidisciplinary modeling network will be:

- **Working at the nexus of computation, experiment, and theory**
- **Motivated by specific real-world problems where solutions and discoveries start at the nanoscale**

NKI: A data infrastructure to fuel science and innovation



A *data* infrastructure

- Enables access to *diverse* data of known quality
- Provides a framework to incorporate new data

Thrust

Create a robust digital nanotechnology data and information ***infrastructure***

Our community needs to:

- **Create good practices for data *curation, organization, transfer, and sharing.***
- **Develop *standards and procedures* for data management and use.**
- **Expand data-based *prediction capabilities*.**
- **Engineer responsive mechanisms to assess and meet the needs of scientists for *data and model acquisition, sharing, and archiving*.**

Data Readiness Levels

For Community Discussion

Seven graded definitions (0-6) are defined:

0. **Invalid data**
1. **Raw or unscaled data**
2. **Scaled data**
3. **Scaled data with defined precision or noise level**
4. **Scaled data with defined precision and noise levels, but not related to the larger body of scientific knowledge**
5. **DRL 4 data related to the larger body of scientific knowledge, but with measurement uncertainty too large for data standard**
6. **Standards-quality data of X % measurement uncertainty**

http://www.nano.gov/node/1015

Associated Metadata Classifications

For Community Discussion

Three metadata qualifiers:

Poor Metadata: Failure to include critical information so that the **data cannot be reproduced by others**, or so that there is **ambiguity in interpreting the data**, or so that acceptable measurement **uncertainty estimates cannot be made**; for example, failure to adequately describe the measurement/computational methods used, or failure to provide complete and unambiguous descriptions of data format.

Acceptable Metadata: Inclusion of **all key parameters** so that others **can reproduce the data,** and so that there is **little/no ambiguity** in **interpreting the data**, and so that acceptable measurement **uncertainty estimates can be made**, including adequate descriptions of measurement/computational methods used, boundary and initial conditions, and complete and unambiguous descriptions of data format, curation, and provenance (history).

Excellent Metadata: Inclusion of **all key parameters** so that others **can reproduce the data** and **unambiguously interpret the data**, and so that acceptable measurement **uncertainty estimates can be made**, as well as **other information to judge the data** such as names and pedigree of the data creators; data format, curation, and provenance; and validation of the measurement/computational methods. DRL 6(X), by its nature, can only be data that have excellent metadata.

http://www.nano.gov/node/1015

Tabular Illustration of DRL Attributes

For Community Discussion

Attribute	DRL 0	DRL 1	DRL 2	DRL 3	DRL 4	DRL 5	DRL 6
Units		maybe	yes	yes	yes	yes	yes
Precision and Noise				either	both	both	both
Independent Confirmation				possibly	yes	yes	yes
Related to Larger Body of Scientific Knowledge					no	yes	yes
Measurement Uncertainty					speculative	high	low
Example or use	little to none	unscaled sensor data	scaled sensor data	scaled data; noise levels defined	major scientific advances	coarse validation of theory	theory refinement and methods validation

http://www.nano.gov/node/1015

NKI: Accessible standard computational tools and accepted models

Thrust

Build a sustainable nanotechnology ***cybertoolbox***

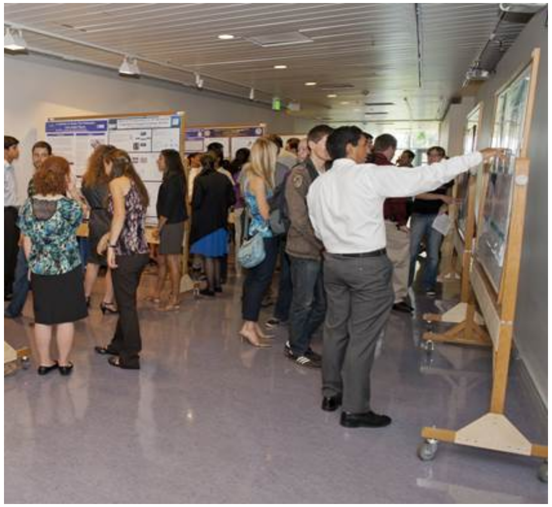
Community Cybertools:

- **We would all use them.**
- ***We would understand them.***
- ***They would always work!***

Our cybertools should include:

- **Theory-based *'first-principles' software* tools**
- ***Models*****,** some ***collaboratively developed ,*** for understanding nanomaterials properties, behavior, and impact on biological and environmental systems,
- ***Theoretical, statistical, and visualization*** tools to facilitate planning, execution, and analysis of experiments.
- ***Education*** support to **the overall** information infrastructure.

NKI: A mechanism to create and sustain a diverse nanotechnology community



A nanoinformatics community that is:

- *Integrated* and highly skilled
- *Capable* of building and sustaining our nanotechnology-enabled U.S. industries
- *Sustained* through *education and training* of the next-generations

Our community needs to:

- ***Enhance communication*** mechanisms through digital networks
- ***Support*** synergistic ***interaction*** of scientists and engineers to ***define the frontiers*** and tackle difficult problems of national importance
- ***Reduce barriers*** to education opportunities
  economic, geographic, …

Thrust

Nurture a ***diverse collaborative community*** to create nanotechnology to meet national challenges

Opportunities

To Enhance and Accelerate Nanotechnology

- **Create rapid and effective ways to share *diverse* data**
  - **Harness data as a discovery tool**
  - **Utilize data as a critical dimension of predictive modeling**
  - **Enhance the *efficiency* of data utilization**

- **Tame the infinite search spaces**
  - **Stimulate conceptual advances**

- **Enable the accessibility of “standard” computational tools**
  - **Empower researchers who are not computationally oriented**
  - **Toward a more quantitative understanding of complex phenomena**
  - **Stimulate design of new models and open new directions**

- **Transform the workforce to engage the challenges of tomorrow**

How do we create the Nanotechnology Knowledge Infrastructure?

What progress have we made to date?

Some existing infrastructure

Greener Nano 2012: Nanoinformatics Tools and Resources Workshop

The goals of the workshop were to establish a better understanding of current applications and clearly define immediate and projected informatics infrastructure needs for the nanotechnology community.

Focus areas were:

- **Data lifecycle**
- **Use of nanoinformatics for predictive modeling**
  - Nanomanufacturing supported by informatics
  - Predicting nanomaterial biodistribution
  - Nanomaterial structure-property relationships
  - Nanomaterial environmental fate modeling
- **Nanoinformatics integration**

http://nanoinformatics.org/2012/overview

ISA-TAB Nano

Facilitating import/export of data on nanomaterials and their characterizations

A standard tab-delimited format for describing data related to

- **Investigations**
- **Nanomaterials**
- **Specimens**
- **Assays**

Leverages and extends the Investigation/Study/Assay (ISA-TAB) format

- **Standard tab-delimited file format**
- **Developed by the European Bioinformatics Institute (EBI)**
- **Represent a variety of assays and technology types**
- **Example: MAGE-TAB**

ISA-TAB Nano supports ontology-based curation

- **Nanomaterials and concepts from the NanoParticle Ontology (NPO) as well as other ontologies**

caNanoLab

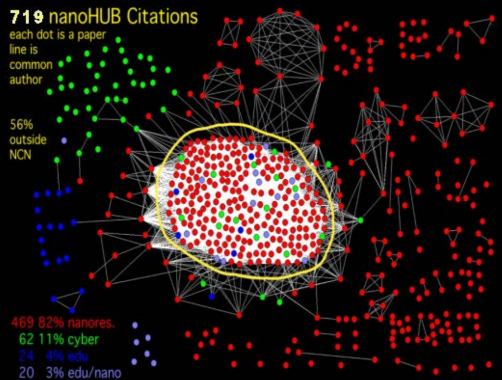
- An open-source portal and database designed to facilitate data sharing to expedite and validate the use of nanomaterials in biomedicine

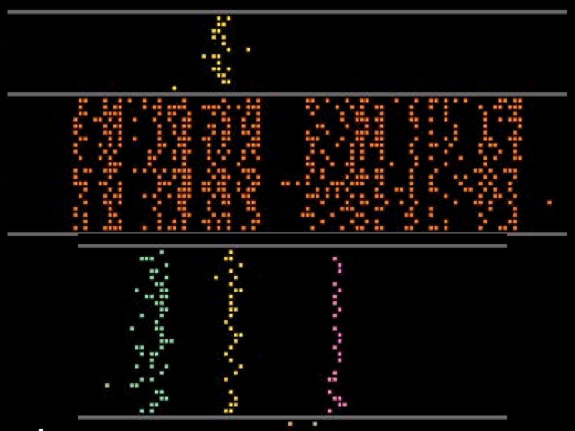
- Provides support for the annotation of nanomaterials with composition information, physico-chemical and *in vitro* characterizations, protocols, and publications

- Leverages and extends concepts from the NCI's Enterprise Vocabulary Services (EVS) and the NanoParticle Ontology (NPO)

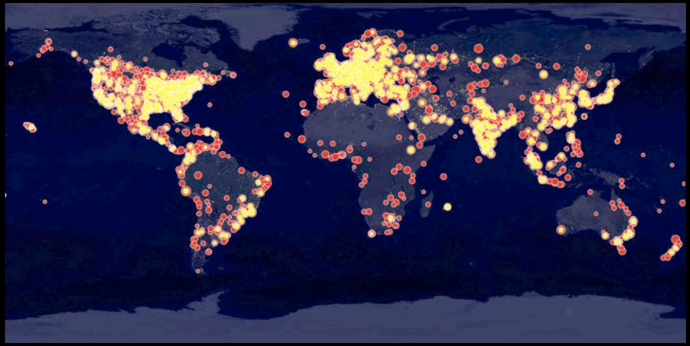
http://cananolab.nci.nih.gov

nanoHUB.org
The World's Largest Nano User Facility
Fully Operational Cloud for End Users





Annually:
240,000 lecture users
830 lecturers
12,000 simulation users
300 sim developers



Quantitative Impact:

- Research use: 966 citations in the literature
- Education use: 14,000 users, 760 courses, 180 institutions
- Collaboration: 350+ tool developers
  260+ simulation tools

OSHA Nanomaterials Health Effects Database

- Focus on existing published data
- Searchable and sortable format
  - Highlight similar effects
  - Develop hazard determination criteria
- Information to be publically available
- Full reference information
  - Biological effects
  - Material characterization – some supplemented with CoA info
- Completing work on Carbon Nanotubes literature

XSEDE: Enhancing Scientific Productivity through Advanced Digital Services

- ✓ A broad array of computational and storage resources from the largest, tightly coupled machines to those designed for high throughput, loosely coupled applications.
- ✓ Direct help to make applications more efficient and/or moving them to new, architectures
- ✓ Receive training in both elementary and advanced computational tools including,
  - Computer languages
  - Supported resources
  - Software and libraries

XSEDE

Extreme Science and Engineering Discovery Environment

NSF

There are more …

… all are only a start!

Community Discussion

Input is needed!

- **Self-Assembly Required!**
  - **Grass roots support will lead to a valuable and usable NKI**
  - **Can we identify good practices that will help create and sustain NKI?**

- **Data in the interdisciplinary field of nanotechnology**
  - **Building blocks that are conducive to data sharing**
    - **How can the 'quality' of data be measured?**
    - **What does 'quality' mean in this context?**
    - **How can data maturity be discussed? (DRLs)**
  - **The important existing community resources**
    - **Can they be improved?**
    - **What is missing?**
    - **How can they work together to form a seamless NKI?**

Community Discussion

Input is needed!

- **Constructing a Cybertoolbox**
  - **Identifying high priority tools that are needed for progress**
    - **What computational tools should be available?**
    - **What *models* are among the most important?**
    - **Are there key models that are not available digitally?**

  - **The important existing community resources for the cybertoolbox**
    - **Can they be improved?**
    - **What is missing?**

- **The NKI workforce**
  - **Nurturing computation and data savy researchers**
    - **How do we weave the use of computational and data tools across research?**
    - **How do we train the next generation?**

We can accelerate discovery,
revolutionize design,
and sustain innovation through a

Knowledge Infrastructure

Thank You!

Questions?

National Nanotechnology Coordination Office

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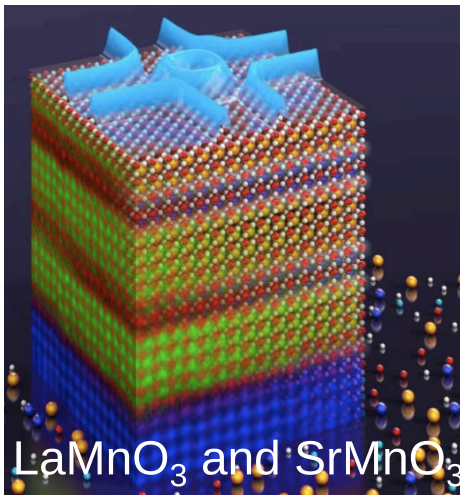
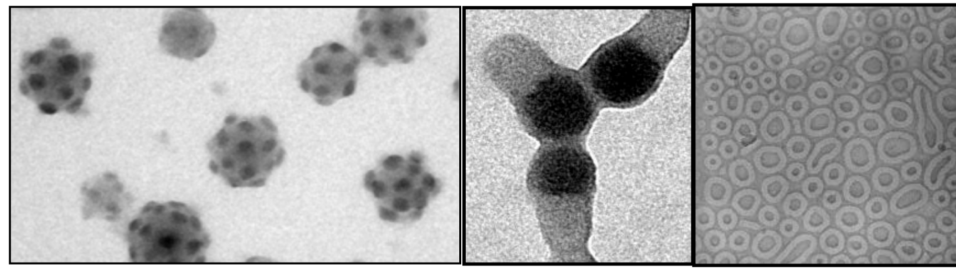
We need to support exciting science that begins on the nanoscale

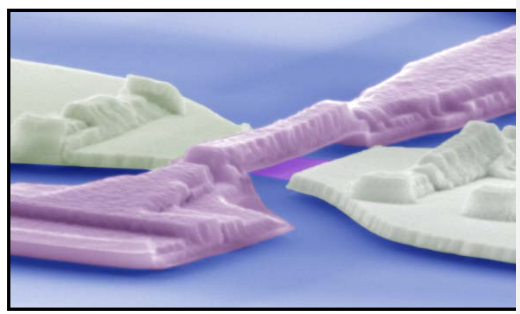
Controlling and Imaging Electron Motions in Atomic-Scale Sandwiches, Cornell **MRSEC**



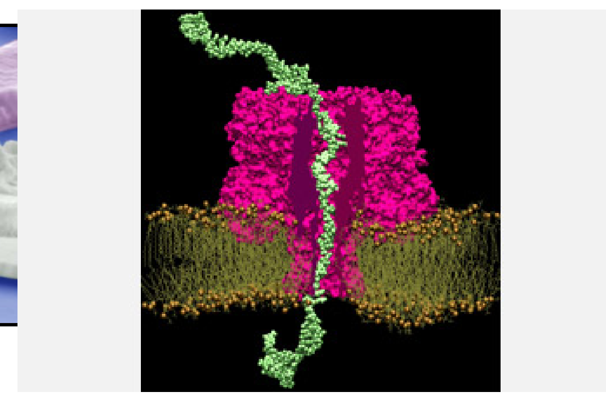
E. J. Monkman, C. Adamo, *et al.* ***Nature Materials***



Pochan and Wooley – controlled synthesis of polymer structures



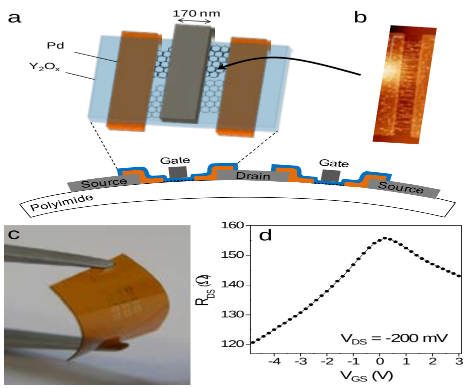
Bilayer graphene device to study Dirac matter.



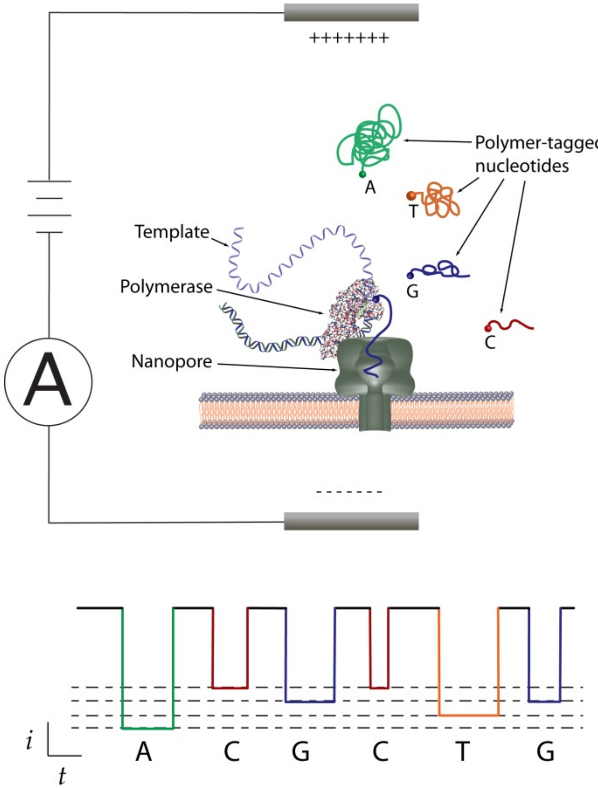
Aksimentiev – simulation of polymer translocation

Talented scientists and engineers making discoveries that drive new technologies …

Emerging nanotechnologies require more effective informatics



Flexible transistors based on DGU graphene operate at frequencies that are 1000x faster than competing flexible organic electronic materials. Hersam, Northwestern, EPM



Schematic of NIST-Columbia inexpensive DNA sequencer.

There are many more with potential to revolutionize how we live …