

NSTC COMMITTEE ON TECHNOLOGY
SUBCOMMITTEE ON NANOSCALE SCIENCE, ENGINEERING, AND TECHNOLOGY

Nanotechnology Signature Initiative

*Nanotechnology Knowledge Infrastructure:
Enabling National Leadership in Sustainable Design*

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

National Need Addressed

Nanotechnology solves global challenges by generating and applying new multidisciplinary knowledge of nanoscale phenomena and engineered nanoscale materials, structures, and products. The data underlying this new knowledge are vast, disconnected, and challenging to integrate into the broad scientific body of knowledge. The Federal agencies participating in the National Nanotechnology Initiative (NNI)—in conjunction with the broader nanoscale science, engineering, and technology communities—have identified the building of a formal knowledge infrastructure as critical to sustainable progress in nanotechnology [1-4]. This reflects a desire to coordinate existing NNI member agency programmatic efforts that accelerate the vetting of new knowledge and that enable effective data utilization.

Nanoinformatics is the science and practice of developing and implementing effective mechanisms for the nanotechnology community to collect, validate, store, share, mine, analyze, model, and apply nanotechnology information. Nanoinformatics is integrated throughout the entire nanotechnology landscape, impacting all aspects of research, development, and application. An improved nanoinformatics infrastructure will ensure the sustainability of our national nanotechnology proficiency by improving the reproducibility and distribution of experimental data as well as by promoting the development and validation of tools and models to transform data into information and applications. A focused national emphasis on nanoinformatics will provide a strong basis for the rational design of nanomaterials and products, prioritization of research, and assessment of risk throughout product lifecycles and across sectors that include energy; environment, health, and safety (EHS); medicine; electronics; transportation; and national security. In this manner the effort described here will also contribute substantially to the Materials Genome Initiative, a related Federal interagency priority outlined on page 10 [5].

This signature initiative, *Nanotechnology Knowledge Infrastructure: Enabling National Leadership in Sustainable Design*, will provide a community-based, solutions-oriented knowledge infrastructure to accelerate nanotechnology discovery and innovation. This will be accomplished within four major thrust areas that focus member agency efforts on cooperative, interdependent development of:

ⁱ Please note that “collaborating agencies” is meant in the broadest sense and does not necessarily imply that agencies provide additional funds or incur obligations to do so. Agencies are listed in alphabetical order.

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

Through these four thrusts, the Nanotechnology Knowledge Infrastructure (NKI) signature initiative will leverage and extend existing and emerging resources, programs, and technologies to create an architecture for nanoscale science and engineering in the 21st century. Specifically, several NNI agency-supported databases, portals, and resources containing data on nanomaterials will provide the foundation for this infrastructure; these are highlighted in Table 1.

Modern digital technologies such as the life sciences dialogue at WikiGenes [6], the digital physical sciences library ArXiv [7], and the use of Twitter and blogs for scientific debate [8] have already demonstrated their potential to augment and expedite scientific exchange while respecting intellectual property and authorship. These technologies, applications, and systems will be instrumental in working towards establishing a robust modeling and data information infrastructure—including a central access point for existing and emerging modeling, simulation, and data efforts—that will support the research needs identified by the NNI member agencies and relevant stakeholders as outlined in the NNI Strategic Plan [9] and the NNI Environmental, Health, and Safety Research Strategy [10].

The NKI will coordinate the nanoscale science, engineering, and technology communities around the fundamental, interconnected elements of collaborative modeling, a cyber-toolbox, and data infrastructure that will capitalize on American strengths in innovation, shorten the time from research to new product development, and maintain U.S. leadership in sustainable design of engineered nanoscale materials.

Technical Program

As outlined above and shown graphically in Figure 1, the NKI contains four thrusts that synergistically develop a community that will create and harness the tools necessary to aid in advancing nanotechnology. Thrust 1 outlines the important role of the NKI in strengthening and connecting researchers across academia, government, and industry to advance nanoscale science, engineering, and technology. Thrust 1 further focuses on educating and training the next-generation workforce that will develop, maintain, and use the outputs from Thrust 2 (models and data), Thrust 3 (a cyber-toolbox of validated tools), and Thrust 4 (digital data and information infrastructure).

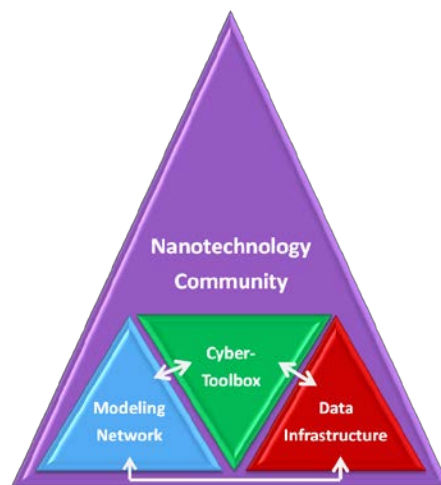


Figure 1. Overview, Nanotechnology Knowledge Infrastructure Signature Initiative

Table 1. Foundational Resources Supporting Thrust Areas Identified in the Nanotechnology Knowledge Infrastructure Signature Initiative

	Description of NNI-Supported Resource
caNanoLab	Cancer Nanotechnology Laboratory portal of NIH/National Cancer Institute; cabig.nci.nih.gov/tools/caNanoLab .
Extreme Science and Engineering Discovery Environment project (XSEDE; follow-on to Teragrid)	NSF-supported advanced digital network of 16 supercomputers and high-end visualization/data analysis resources; www.xsede.org .
InterNano	NSF-supported nanomanufacturing resource run by the National Nanomanufacturing Network; www.internano.org/ .
Nano-Hub	NSF- supported online simulation resources operated by the Network for Computational Nanotechnology; nanohub.org/ .
Nanomaterial-Biological Interactions Knowledgebase	The Nanomaterial-Biological Interactions Knowledgebase, hosted at Oregon State University and supported by EPA, NSF, DOD/Air Force, and NIH; nbi.oregonstate.edu/ .
Nanomaterials Registry	Web-based registry project in development by RTI International and three NIH institutes—NCI, NIEHS, and NIBIB—for biomedical and environmental applications of nanomaterials; www.nanomaterialregistry.org .
Nanoparticle Information Library	A NIOSH tool to help organize and share information on nanotechnology and occupational health; nanoparticlelibrary.net .
Toxcast	EPA program to define and evaluate predictive toxicity signatures of over 10,000 chemicals; www.epa.gov/ncct/toxcast/ .

Thrust 2 seeks to encourage rapid and early modeling collaboration, evaluation, and peer-review through sharing of experimental data, models, and modeling results. This fosters critical relationships between theorists, modelers, and experimentalists through the exchange of data and information that will aid in developing the larger nanotechnology community outlined in Thrust 1. As the new models created in Thrust 2 become validated and verified computational tools, they will become integrated into the cyber-toolbox for broad use throughout the community, as addressed by Thrust 3. The verified data generated in Thrust 3 will further be incorporated into the digital data and information infrastructure addressed in Thrust 4. This overall access to models, validated simulations, and reproducible data will ultimately help ensure that scientific advances are responsibly translated into products through informed design processes.

Described below are the underlying technical details of the NKI thrusts as well as the anticipated outcomes that leverage existing agency efforts. In addition to the NNI agency programs highlighted in Table 1, agency roles and contributions are discussed on page 8.

Thrust 1: *Build a diverse collaborative community of scientists, engineers, and technical staff to support research, development, and applications of nanotechnology to meet national challenges.*

A highly-skilled workforce is essential to U.S. nanotechnology research, development, and applications. Such communities require time to develop purposeful policies and programs. These communities are the backbone of U.S. nanotechnology competitiveness. They consist of (a) experimentalists, computational scientists, and theoreticians to develop and advance the science; (b) engineers and other researchers to apply the science to address national challenges; and (c)

well-trained technicians to execute material synthesis processes, to ensure quality control, to perform advanced tests, to assess risk and benefit, and to employ nanotechnology in practice. The NKI will foster such a community by:

- Enhancing communication mechanisms within the nanoinformatics community by promoting digital networks and network events
- Promoting the development of training tools and courses to efficiently train staff with the required skill levels to accommodate rapid advances in knowledge, methods, and techniques
- Developing an infrastructure to support the synergistic interaction of scientists and engineers to define frontier nanoscale science and engineering problems and to develop strategies to tackle difficult problems of national importance
- Reducing barriers to educational opportunities and careers for economically, geographically, and other disadvantaged or underrepresented communities
- Creating awareness in the community of the relevance and impact of nanotechnology in the United States by promoting educational events aimed at students and the general population

Expected outcomes for Thrust 1 are as follows:

- An integrated and highly skilled nanoinformatics community to build and sustain nanotechnology-enabled U.S. industries
- Education and training of the next-generation modeling network to sustain the intellectual infrastructure for future nanotechnology

Thrust 2: *Foster an agile modeling network for multidisciplinary intellectual collaboration that effectively couples experimental basic research, modeling, and applications development.*

Modeling is the essential mechanism that couples our conceptual understanding of nanomaterials and the empirical knowledge gained from experimentation. For example, reliable computational models will ultimately enable prediction and design of new nanoscale materials with desired properties, inform risk assessment and management of nanomaterials, and likely will have additional applications not yet conceived. Models also play an important role in developing new concepts to expand our understanding of materials, biological systems, and phenomena at the nanoscale. As models and experimental results are shared more rapidly across this network, critical components of the needed intellectual infrastructure will more efficiently connect basic research to applications development. Critical, near-term nanotechnology modeling needs include:

- Models that combine first-principles concepts and link theory, simulations, and experimental results over diverse scales of length and time to expand our knowledge of nanoscale materials and phenomena
- Models motivated by specific real-world problems and validated experimentally in the appropriate biological or physical system
- A dynamic mechanism for sharing, combining, and refining models in accordance with the emergence of new experimental data and new theoretical concepts

By developing an enhanced modeling network for technical collaboration, it will be possible to solve compelling questions across scientific domains; more efficiently bridge the gaps between concept, design, product development, and manufacturing; and identify and take effective measures to maximize the benefit of nanomaterials to humans and the environment while minimizing the risk. This technical collaboration will be intrinsically multidisciplinary and interdisciplinary and will facilitate education of young scientists who will create the next generation of nanoscale models.

Expected outcomes for Thrust 2 are as follows:

- A robust technical network of professionals who will collaboratively develop and work to validate a library of models and simulations to address the spectrum of nanotechnology questions—from grand challenges and problems of national priority to modest problems that fill essential global and social needs
- Improved structural models for nanomaterials on several levels: models to address detailed interactions at the atomic level, molecular level, and particle level; models to address the polydispersity, conformations, and transformations of nanomaterials; and models that link particulate information to simulation of the effects of nanomaterials in models of cellular, tissue, organ, organism, and ecosystem environments
- Broader access to relevant experimental results that are technically sound and important to model, but may not otherwise be considered novel enough for publication
- Shortened development time to achieve similar quality models, due to early and more detailed, frequent, and constructive peer review
- Models with sufficient reliability and validity to design sustainable materials that maximize beneficial properties and minimize potential hazards
- Models that are easily accessible to broader communities and stakeholders, such as communities focusing on other length scales
- A dynamic compendium of “lessons learned” from the modeling activities, including positive and negative results, that will clarify data gaps and inform the design of new experiments and new models

Thrust 3: *Build a sustainable nanotechnology cyber-toolbox to enable application of models and knowledge to nanomaterials design.*

A suite of computational tools that facilitate the analysis of experiments and the understanding of nanomaterials is essential to complete the Nanotechnology Knowledge Infrastructure. Establishing a single access point for available tools will ensure that such a toolbox will have wide-reaching impacts on both the utilization of nanomaterials and the communication of knowledge among the diverse scientific domains of nanotechnology.

The central components of this toolbox are computationally efficient software tools to enable reliable and robust simulation of nanomaterial properties and behaviors. Simulation is a process consisting of a set of computer instructions based on well-designed numerical algorithms that utilize models to solve physical, biological, or engineering problems. There is an acute need for the development of new software that is well maintained and broadly accessible to the community to ensure that nanotechnology models will be accurate, predictive, and useful in

accelerating science. Data mining software will enable the discovery of correlations among materials properties and phenomena that are not apparent or are difficult to show in current theoretical frameworks. The software performing simulations and the models underlying them will enable analysis and interpretation of experimental results, prediction of nanoscale phenomena, and sustainable design and control of nanoscale materials and systems. The software must be validated for specific computer architectures because compilation of the source code on different machines could have an impact on its performance. Documentation of the software will include specific information on its range of validity, representative run-time parameters and files, and other associated information necessary to duplicate example results.

Based on multidisciplinary collaborations between theorists and experimentalists, a cyber-toolbox of validated, easily accessible, and well-maintained simulations will inform the design and development of nanomaterials and will enable understanding of nanomaterial behavior from a product lifecycle perspective.

Expected outcomes for Thrust 3 are as follows:

- A nanotechnology cyber-toolbox that will house the collaboratively developed and validated models to enable understanding of nanomaterials' properties, behavior, and impact on biological and environmental systems
- A nanotechnology cyber-toolbox that will include a suite of theoretical, computational, statistical, and visualization tools to facilitate the planning, execution, and analysis of experiments
- A central access point on the NNI website and administered by the National Nanotechnology Coordination Office for linking existing interdisciplinary cyber-toolbox components to improve user accessibilityⁱⁱ
- Educational opportunities that will integrate the cyber-toolbox and the Nanotechnology Knowledge Infrastructure into the intellectual framework of nanoscale science and engineering and aid in developing the next-generation workforce as discussed in Thrust 1

Thrust 4: *Create a robust digital nanotechnology data and information infrastructure to support effective data sharing, collaboration, and innovation across disciplines and applications.*

The nanotechnology community has an immediate need for an overarching digital-data infrastructure that will integrate validated experimental and modeling data and information on nanomaterials design, synthesis, properties, phenomena, and biological and environmental impact from distributed, multidisciplinary databases. Open-source, open-access practices, freely available software, search capabilities, and common formats for data transfer and archiving provide an initial starting point to organize datasets within an overarching infrastructure. While scientists would continue to store and manage access to their own data, this effort will further facilitate collaborations to incorporate consensus-driven improvements in their individual databases and create meaningful connections among databases. Standardized vocabularies and mapped ontologies will be developed through open, online dialogues to provide a shared

ⁱⁱ NNI website; www.nano.gov

terminology for scientific discourse bridging the multiple disciplines encompassed by the nanotechnology research community.

Successful development of this nanotechnology data and information infrastructure will provide a framework to share vetted existing and emerging data and information on nanomaterial design, synthesis, and properties using standardized formats and vocabulary; provide more reliable data and access to the broader research community; and augment and accelerate scientific discourse, discovery, and innovation in all sectors.

Expected outcomes for Thrust 4 are as follows:

- Strategic development of interoperable systems to enable best practices for data capture, curation, organization, evaluation, dissemination, and incorporation into computer models
- Standards and procedures for data management and use to facilitate significantly more efficient utilization of the databases, including lifecycle data management
- Expansion of reliable and efficient data analysis tools, including computer intelligence, data pattern recognition, data visualization, and multivariable structure–property correlation
- Development of robust validation procedures and reference data standards
- Mechanisms for assessing and meeting the evolving needs of scientists for data and model acquisition, sharing, and archiving

Agency Roles and Contributions

A concerted, interagency effort that addresses challenges spanning multiple diverse disciplines, including materials science, chemistry, biology, engineering, and advanced measurement and characterization science, will establish this critically needed Nanotechnology Knowledge Infrastructure. The NKI will leverage Federal agencies' existing and emerging efforts, such as those highlighted in the Big Data Research and Development Initiative [11], to create the infrastructure necessary to accelerate the pace of nanoscale science, engineering, and technology. Databases supported by different agencies and stakeholders will continue to be curated by their respective data experts. However, a central access point on the NNI website will allow data to be stored, administered, annotated, and shared in an easily accessible manner by the broader community.

In addition to involving several Federal agencies, the NKI will continue NNI agency engagement of stakeholders in industry, academia, and nonprofit organizations in order to generate an infrastructure that is flexible enough to meet the needs of the greater community. Ongoing activities along these lines exemplify existing interactions and suggest possible approaches and opportunities for further NKI efforts:

- NIOSH collaborates with key NNI agencies and external stakeholders on the development and deployment of the GoodNanoGuide, a wiki-based collection of good risk management practices. In 2013, NIOSH plans to integrate activities in nanoinformatics with the GoodNanoGuide [12].

- NSF established the National Nanotechnology Infrastructure Network, which provides extensive support in nanoscale fabrication, synthesis, characterization, modeling, design, computation, and hands-on training in an open, hands-on environment available to all qualified users [12].
- NIST's expanded nanoscale EHS program is supporting ongoing work in development of standard reference materials, measurement protocols, and predictive models that is coordinated with manufacturers of engineered nanomaterials and engineered nanomaterial-based products; with other NNI agencies, particularly NIOSH, OSHA, CPSC, and EPA; and with major nanoscale EHS university centers [12].

Table 2 illustrates areas of expected agency contributions to each of the key NKI thrust areas and agency overviews outlined below.

Table 2. Expected Agency Contributions by Thrust Area

Thrust Area	CPSC	DOD	DOE	EPA	FDA	NASA	NIH	NIOSH	NIST	NSF	OSHA
1. Diverse Community Development	•	•	•	•	•	•	•	•		•	•
2. Modeling Network	•	•	•			•	•	•	•	•	
3. Validated Cyber-Toolbox		•	•			•	•	•		•	
4. Data and Information Infrastructure	•	•	•	•	•	•	•	•	•	•	•

Specific expertise and perspective that each participating agency will bring to this effort are as follows:

CPSC: CPSC staff will provide support for risk-modeling approaches and expertise in data collection and interpretation of data assessing potential effects from exposure to nanomaterials.

DOD: DOD scientists across many laboratories and fields are actively engaged in research to investigate the novel properties, potential uses, human-health and environmental effects, and other interesting and important aspects of nanomaterials. These investigations include laboratory work to generate data; development and application of modeling tools to fill gaps in that data; and development of databases, publications, and software platforms to use and share these results with the broader scientific population.

DOE: This Signature Initiative will build on DOE's investments in the Computational Materials and Chemical Sciences Network (CMCSN) and Scientific Discovery through Advanced Computing (SciDAC) programs. Progress in many research areas relevant to energy technologies is limited by currently available materials and chemical processes and has the potential to be fundamentally altered by predictive theory and modeling capabilities across multiple length and time scales, including the nanoscale. DOE will support this initiative by leveraging a broad research community that already exists in academia, industry, and at the DOE National Labs, particularly at the five Nanoscale Science Research Centers.

EPA: EPA's efforts will include experimental testing and characterization data for reference and other nanomaterials, standardized relational databases that will support sharing of results, and models linking properties and bioactivity of nanomaterials that will be developed and shared.

FDA: Coordinated databases, portals, and resources containing data on nanomaterials will provide FDA an opportunity to share its published findings on characterization of nanotechnology-based products and models for safety and efficacy assessment as well as to study the behavior of nanomaterials in biological systems and their effects on human health.

NASA: NASA is supporting R&D efforts, both in-house and with industry and academia, to develop, mature, and demonstrate high-impact nanotechnologies for use in future planetary exploration and earth and space science missions, and in the development of next-generation, environmentally responsible aircraft. These efforts include a combination of experimental activities and data collection, modeling, and simulation to develop new materials and devices for these applications. NASA will support the Nanotechnology Knowledge Infrastructure Signature Initiative through collaborations to develop multiscale modeling and database tools and provide experimental data to support these activities and validate computational tools.

NIH: NIH will guide the nanotechnology field with a set of minimal information about nanomaterials (MIAN), ontology, and standards developed through a community effort with broad representation, that will serve as the foundation for sharing the nanomaterial data, building the modeling infrastructure, validating models against experimental data, and developing modeling tools.

NIH will also contribute to building databases and registries to store and index information on nanomaterials and protocols needed for their characterization, defining standards for nanomedicine data sharing and exchange, and providing vocabulary and semantic support to the nanotechnology community.

NIH will also support the development of experimentally-validated multiscale models that allow predictions across scales of space, biological organization, and time as well as data and predictive models on the toxicological implications of exposure to engineered nanomaterials.

NIOSH: NIOSH's contribution will include the Nanoparticle Information Library, nanoinformatics tools, and real-life data on current and emerging nanotechnology practice in the workplace; data on workplace exposures; experimental evidence and modeling of toxic effects from exposures to categories of nanomaterials; knowledge and data on efficacy of controls; recommended exposure limits; and tools and guidance to support sustainable nanotechnology.

NIST: NIST's contributions to this signature initiative will leverage its long-standing expertise in metrology and data information science. Activities at NIST in support of this NSI include the Advanced Materials for Industry program, which is focused on the development of reference data standards and data management infrastructures that will enable reliable computer modeling and simulation for materials discovery and optimization. This activity will be coordinated with other agencies' efforts on software and experimental tool design, including at DOE and NSF.

NSF: This Nanotechnology Signature Initiative will build on NSF's investments in Cyber-enabled Discovery and Innovation and on efforts within its Cyberinfrastructure Framework for the 21st Century program such as Software Infrastructure for Sustained Innovation. These NSF programs will also contribute to the foundations of the NKI through specific databases for

nanoscale materials and processes; transformative thinking about models for linkage of properties and behaviors at different scales; extension of computational and statistical techniques to support development and use of the nanotechnology cyber-toolbox to accelerate nanomaterials discovery and manufacturing; advances in fundamental theory and modeling; software optimized for specific computer architectures that includes documentation, representative run-time parameters and files, and other associated information necessary to duplicate example results; techniques across the scales from first principles to coarse-graining to phase-field modeling; and education to integrate the cyber-toolbox into the fabric of next-generation science and to train the next-generation modeling community.

OSHA: OSHA will provide expertise and support in the area of data collection and interpretation of the biological and toxicological effects of exposure to various categories of nanomaterials.

Coordination with the Materials Genome Initiative

The Materials Genome Initiative (MGI) [12] is a multistakeholder effort to accelerate domestic advanced materials discovery and deployment. Synergistic areas for the NKI and the MGI exist in all four thrust areas of the NKI and in particular include community-building, protocols and best practices for data. Engagement with, and connection to, the MGI will bring mutual and reciprocal benefits to the NKI. Thus, the NKI activity described here is a Nanotechnology Signature Initiative that contributes directly to both the NNI and the MGI, making it a first-of-its-kind effort in linking, impacting, and implementing multiple related Federal interagency initiatives.

The NKI is intended to advance the development and curation of modeling, simulation tools, and databases that enable the prediction of specific phenomena on the nanometer length scale and in the sub-microsecond regime. The MGI scope more broadly covers materials information over a range of length scales and timeframes, including those at the nanoscale as well as the inherent properties of bulk materials. Activities of the NKI that effectively bridge the spatial and temporal spectrum are expanded upon in other MGI-related efforts including standardization of data formatting, linking experimentalists to theorists to accelerate the production of “materials by design,” and fostering communication between multidisciplinary stakeholders to develop a community that pushes technologies forward. Similarly, approaches, protocols, and standards developed through other MGI activities may be initially explored, tested, or evaluated specifically for nanoscale materials under NKI efforts. This cross-fertilization between the NNI and MGI will yield broader knowledge dissemination and can be facilitated by the proposed NKI effort. Through continual dialogue, the integrated, easily accessible infrastructural elements generated by interagency coordination under these initiatives will support materials development across length and time scales and across the innovation pipeline to ensure U.S. competitiveness.

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