

Nanotechnology Signature Initiative*

Nanotechnology Knowledge Infrastructure (NKI): Enabling National Leadership in Sustainable Design

Overview

Nanotechnology has a vital role in providing solutions to global challenges by generating and applying new multidisciplinary knowledge of nanoscale phenomena and engineered nanomaterials (ENMs), structures, and nanotechnology-enabled products (NEPs). The data underlying this new knowledge base are vast, disconnected, and challenging to integrate into the broad scientific body of knowledge. 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 is critical to the sustainability of our national nanotechnology proficiency by improving the reproducibility and distribution of experimental data and 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 ENMs and NEPs, prioritization of research, and assessment of risk throughout NEP life cycles and across sectors that include energy; environment, health, and safety (EHS); medicine; electronics; transportation; and national security.

Goal

To provide a community-based, solutions-oriented knowledge infrastructure to accelerate nanotechnology discovery and innovation.

Thrust Areas

To focus efforts on cooperative interdependent development of

- A diverse collaborative community
- 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 the design of engineered nanomaterials
- A robust digital nanotechnology data and information infrastructure to support effective data sharing, collaboration, and innovation across disciplines and applications

Agencies Involved

Consumer Product Safety Commission, Department of Commerce (National Institute of Standards and Technology), Department of Defense, Department of Health and Human Services (Food and Drug Administration, National Institutes of Health, National Institute for Occupational Safety and Health), Department of Labor (Occupational Safety and Health Administration), Environmental Protection Agency, National Aeronautics and Space Administration, and National Science Foundation.

Opportunities to Enhance and Accelerate Nanotechnology

- Create rapid and effective ways to share diverse data
- Tame the infinite search spaces
- Enable the accessibility of 'standard' computational tools
- Transform the workforce to engage the challenges of tomorrow

Resources that Support the Goal of the NKI:

Working toward the Cyber Toolbox

nanoHUB.org

NANOPARTICLE
INFORMATION
LIBRARY

NanoParticle
Ontology (NPO)

GoodNanoGuide

ClinicalTrials.gov

caNanoLab

NCI Wiki

National Cancer Institute
Nanotechnology Working Group

ORGANISATION
FOR ECONOMIC
CO-OPERATION
AND DEVELOPMENT
OECD
Database on Research into Safety
of Manufactured Nanomaterials

International Clinical Trials
Registry Platform
Search Portal

InterNano
Resources for Nanomanufacturing

ToxCast™

MATERIALS
PROJECT

NBI
KNOWLEDGEBASE

XSEDE

Extreme Science and Engineering
Discovery Environment

Data Readiness Levels

Concept for Expressing Data Maturity for Community Discussion

DRL:	Data Readiness Level	Description
0	Invalid data	Data that have been assessed and found to be invalid or so inaccurate or inadequately documented as to be of little practical value.
1	Raw or unscaled data	Data from sensors or calculations not converted to final (appropriate) physical units. An example is a recording of the electrical output from a speedometer not scaled to units of distance per unit time, or archived unscaled output from a numerical simulation.
2	Scaled data	Data converted to the intended final physical units. Noise levels are undefined. Data precision is undefined. Duplicate measurements are not cited or are not available. Data uncertainty estimates are not cited, or are not accepted. Example are speedometer data appropriately scaled to units of miles/hour or km/hour, but without adequate information on calibration and background noise.
3	Scaled data with defined precision or noise level	Data precision or data noise levels defined by accepted duplicate measurements or accepted noise measurements. Data not confirmed by independent observations. Models fit to data are not yet related to the larger body of accepted scientific knowledge. Data uncertainty estimates are not cited, or are not accepted. Examples are scaled speedometer data, adjoined by data defining the noise levels of the instrument and recording system or adjoined by multiple speed measurements of the same event.
4	Scaled data with defined precision and noise levels, but not related to the larger body of scientific knowledge	Data precision and data noise levels defined by accepted duplicate measurements and accepted noise measurements. Data confirmed by independent observers using similar methods. Models fit to data are not yet related to the larger body of accepted scientific knowledge but are speculative and inspire scientific debate. Data uncertainty estimates are speculative. DRL 4 data often lead to fundamental scientific advances. An example is the 1887 Michelson-Morley data of the speed of light before Einstein's development of the Theory of Special Relativity, or the 1965 Penzias and Wilson radio telescope data before incorporation into the Big Bang Theory.
5	DRL 4 data related to the larger body of scientific knowledge, but with measurement uncertainty too large for data standards	Data precision and data noise levels defined by accepted duplicate measurements and accepted noise measurements. Data confirmed by independent observers using similar methods. Models fit to data relate to the larger body of accepted scientific knowledge and can be used for coarse validation of existing models or development of refined models. Data uncertainty is larger than current standards for like data. An example is the Michelson-Morley data after the development and acceptance of the Theory of Special Relativity.
6(X)	Standards-quality data of X % measurement uncertainty	Data precision and data noise levels defined by accepted multiple duplicate measurements and accepted noise measurements. Data confirmed by independent observers using independent methods. Data uncertainties are accepted by the scientific community to be X % or less. Models fit to data relate to the larger body of accepted scientific knowledge and can be used to validate existing models to X % accuracy, or to advance higher-fidelity scientific hypotheses. Data are used as a standard to validate other data, providing the bases for data traceability. An example is the light travel time interval specified by U.S. NIST to define the meter.



* Nanotechnology Signature Initiatives (NSIs) are topical areas identified by the National Nanotechnology Initiative and its agencies as benefiting greatly from close and targeted interagency interactions. The NSIs spotlight key areas of national priority and provide a mechanism for enhanced collaboration to leverage research and development programs across multiple agencies.