Material Property Database and Environmental Attribute Models for NM Science Research

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Challenges in Understanding “Nano”

- Internet
  - 10,700,000 hits on nanotechnology
  - 199,000 hits on nanotoxicology

- Scientists and regulatory agencies have not yet determined what is most important
  - Assessing hazard
  - Regulating
  - Critical parameters
Goals

1. Provide place “to go” for initial information
2. Basic understanding of what types of information you might need to collect or understand
3. How to interpret information gathered from resources
4. What to expect from R&D community and Regulatory community
Consumer and Product Databases

Woodrow Wilson Center, Consumer product database
http://www.nanotechproject.org/inventories/consumer/

Contains references to research papers, articles, and books on (or related to) potential health and environmental risks of nanomaterials sorted by material or compound, body organ or biological effect studied, or other miscellaneous issues.
http://www.nanoceo.net/nanorisks

U.S. Nano Metro Map - companies, universities, government laboratories, and organizations working in nanotechnology around the United States
UK resource on nanotechnology hazard and risk. Includes a format for nanomaterial specific safety data sheet. www.safenano.org
What Properties are Important?

- Carbon
  - MWCNT, SWCNT, Fullerene, Waste
- Aluminum
  - Explosive, propellant
- Silver
  - Coatings, textiles, polymers
- Titanium dioxide
  - Coatings

*Identified as strategic materials for Army technologies, Shashi Karna, ARL Senior Scientist*
Characterization of Materials

- **Size**
  - Electron microscopy (SEM, TEM)
  - Dynamic light scattering
  - Field Flow Fractionation ICP-MS

- **Surface area**
  - BET (Brunauer, Emmett and Teller)

- **Morphology**
  - Electron microscopy
  - Confocal microscopy
  - Nanoindentor (mechanical properties)

- **Surface Chemistry**
  - Zeta potential
  - Solid-state NMR
  - FTIR / Raman spectroscopy
  - Multispectral fluorometer
  - Auto titrator – zeta potential curves

Field Flow Fractionation, Coupling to ICP-MS/AES allows elemental quantitation as a function of size
Minimum Characterization Standards

- What does the material look like?
  - Particle size/size distribution
  - Agglomeration state/Aggregation
  - Shape

- What is the material made of?
  - Overall composition (including chemical composition and crystal structure)
  - Surface Composition
  - Purity (including levels of impurities)

- What factors affect how a material interacts with its surroundings?
  - Surface Area
  - Surface Chemistry, including reactivity, hydrophobicity
  - Surface Charge
Minimum Characterization Standards

- Overarching considerations to take into account when characterizing engineered nanomaterials in toxicity studies:
  - Stability—how do material properties change with time (dynamic stability), storage, handling, preparation, delivery etc? Include solubility, and the rate of material release through dissolution.
  - Context/Media—how do material properties change in different media; i.e. from the bulk material to dispersions to material in various biological matrices? ("as administered" characterization is considered to be particularly important)
  - Where possible, materials should be characterized sufficiently to interpret the response to the amount of material against a range of potentially relevant dose metrics, including mass, surface-area and number concentration.
Laboratory Safety

NIOSH Nanoparticle Information Database. Online database includes: Nanomaterial composition, Method of production, Particle size, surface area, and morphology, Demonstrated or intended applications of the nanomaterial, Availability for research or commercial applications, Associated or relevant publications. [http://nanoparticlelibrary.net/index.asp](http://nanoparticlelibrary.net/index.asp)

[http://www.cdc.gov/niosh/topics/nanotech/default.html](http://www.cdc.gov/niosh/topics/nanotech/default.html)

How do we integrate this information?

- Information from databases (parameters and endpoints) can be integrated via an ontology
- Specification of logical relationships between concepts
- Also usually includes definitions, synonyms, properties, etc.
- Ontology
  - Standard terminology
  - Logical relationships between concepts
  - Classifiers for computer-aided materials design and modeling
Materials Property Database

- Categories, descriptors, properties based on a common ontology
- Develop inferred relationships
- Used to predict attributes through QSAR, QSPR, mechanistic models
- Applications include materials development

Nanomaterials Hazard Model

- Tool for estimating potential hazards of materials being developed.
- Rely on empirical data when available and modeling approaches for missing/unknown data.

Components:
- Materials database
- Fate calculations
- Toxicity estimates
- Hazard diamonds
- Documentation

Modeling properties
- QSPR/QSAR
- Molecular models

Atomic scale models for prediction based on structure and surface chemistry