Informatics Framework to Support Integrative Science and Engineering in Nanotechnology

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SNNI  OSU  ONAMI
Need for Rapid Assays and Informatics

Nanomaterial Diversity

[Diagram of compositional diversity]

McNeil SE., 2005
Nanomaterials are Extremely Diverse

Any atom on the periodic table is fair game.
Nanomaterials are Extremely Diverse

“3rd dimension of periodic table”
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Nanomaterial Diversity

Compositional diversity

Synthesis process influences nanoparticle shape

ZnO nanoparticles
Diversity of Zinc Oxide Nanomaterials

Photos: Dr. Z Wang, Georgia Tech
**Nanomaterial Diversity**

Compositional diversity

Relative importance of nanomaterial characteristics are unknown

**Physicochemical properties**
- Chemical Structure
- Core Particle Composition
- Size
- Shape
- Charge
- Surface Chemistry
- Surface Area
- Agglomeration State
- Zeta Potential

**Nanomaterial Complexity**

Synthesis process influences nanoparticle shape

http://www.vincentherr.com/cf/nanomain.html
Which Physicochemical Properties are Important?
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Nanomaterial Diversity

Compositional diversity

Synthesis process influences nanoparticle shape

ZnO nanoparticles

Small changes in nanomaterial can alter conditional behaviors of nanomaterials (performance, exposure, hazard)

Nanomaterial Complexity

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http://www.vincentherr.com/cf/nanomain.html
Data to Consider

- Physical Properties
  - Size
  - Polydisperity
  - Shape
  - Structure
  - Chemical composition
  - Purity
  - Solubility
  - Stability

- Chemical Properties
  - Surface chemistry
  - Surface charge
  - Redox potential
  - Solubility

- Nanomanufacturing
  - Synthesis process
  - Purification process
  - Impurities

- Exposure/Study Scenario
  - Media/matrix
  - Zeta potential
  - Agglomeration state
  - Duration/timing
  - Route
  - Dose/concentration

- Environmental/Ecosystem Response
  - Environmental fate
  - Environmental transport
  - Adsorption
  - Transformation
  - Bioavailability
  - Biomagnification

- Biological Response
  - Whole animal response
  - Cellular response
  - Molecular interactions
  - Beneficial response
  - Toxicity

- Nanomaterial Identifier

EXPOSURE

RESPONSE

STRUCTURE

FUNCTION

SARS
Data and Assay Diversity

Size Distribution Data

Tissue Biodistribution

Anti-tumor Activity

In Vitro Drug Release

Surface Morphology Data

Drug Loading Data

Preparation

Chemical Composition of Nanoparticle Formulation

Integration of Data → Knowledge

- Raw Data → Processed Data → Publication of Findings → Curation of Data → Computational Analysis of Curated Data

- Raw Data → Processed Data → Data Repositories → Computational Analysis of Raw and Processed Data → Re-Informed Data Objectives

- Error Variability → Informed study design

- Inter-laboratory comparisons → Model organism comparisons

- nanoSARs Predictive models
Adapt FRAMES elements from traditional environmental risk assessment to nanomaterial risk assessment

• Identification of sources and transport in the framework of FRAMES for nanomaterial environmental impact analysis
Adapt FRAMES elements from traditional environmental risk assessment to nanomaterial risk assessment

- Identification of food chain and exposure/risk in the framework of FRAMES for nanomaterial environmental impact analysis
Adapt FRAMES elements from traditional environmental risk assessment to nanomaterial risk assessment

- Adapting FRAMES to nanomaterial risk assessment (3)
  - Evaluating models for input and output parameters as well as limitations and assumptions
  - Model components or linkages for nanomaterials

Collaboration of Structural Nanobiology

Complex Nanomaterial Descriptors

Model composition and evaluation tool in FRAMES
Idealized Information-to-Action Continuum

Use risk assessment input to weigh trade-offs in context of alternatives and take action to minimize risks.

Synthesize hazard and exposure research, filter and interpret to arrive at risk forecasts of ENMs.

Draw on emerging and increasingly organized data sources to model potential exposure, transformation, biouptake, and ecological and human health impacts.

Subsume and organize all emerging nanomaterial data and metadata to provide hazard and exposure modelers with rich, integrated data sets.