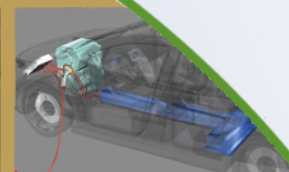
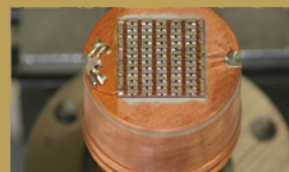
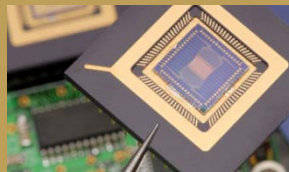


NANOMATERIAL REGISTRY

An authoritative resource for assessing biological and environmental interactions of nanomaterials

Dr. Michele L. Ostraat, Karmann Mills, Damaris Murry, Kimberly Guzan
June 21, 2012



NANOMATERIAL REGISTRY

An Overview



International
Organization for
Standardization

- Authoritative Web-Based Registry
 - Physico-chemical characterization
 - Biological interactions
 - Environmental interactions

- Broad stakeholder involvement
 - Industry, regulatory, government, and academia

- Significant Long-Term Impact
 - Enable development of new models, assays, standards, and manufacturing methods
 - Accelerate the translation of new nanomaterials for biomedical and environmental applications
 - Promote standards and support science-based regulatory decision-making

Registry Priorities

- Minimal information standards
- Curated data
 - Evaluation criteria/Compliance levels
 - Data validation
- Consistent vocabularies
- Ontology
- Interoperability with data sources
- Collaboration across the nanomaterial research community

The Registry leverages existing resources, communities, and best practices

WELCOME TO THE NANOMATERIAL REGISTRY!
 The Nanomaterial Registry is a one-stop, authoritative, fully curated resource that provides information on the biological and environmental implications of well-characterized nanomaterials. The Nanomaterial Registry is being built through strong collaborations with broad stakeholder groups that represent the diverse nanomaterial community, including industry, regulatory institutions, government, and academia. [LEARN MORE ABOUT OUR VISION](#) [WHAT IS CURATED DATA?](#)

NANOMATERIAL REGISTRY

[Nanomaterial Registry](#) [Minimal Information Standards](#) [Compliance Levels](#) [Instance of Characterization](#) [Matching & Similarity](#) [Comparison](#)

BROWSE NANOMATERIALS

- Material Type ▶
- Size ▶
- Shape ▶
- Surface Area ▶

A TOOL FOR THE NANOMATERIAL COMMUNITY

An authoritative website that compiles data from multiple databases into a single resource, the Nanomaterial Registry (NR) provides tools for analyzing and comparing data on the biological and environmental implications of well-characterized nanomaterials. This resource will evolve as the quality and quantity of the information on nanomaterials improve. Hundreds of nanomaterial entries have been curated into the NR for physico-chemical characteristics and are available to the public. Biological and environmental study data for existing nanomaterial entries will also be curated into the NR.

To access this information, search or browse the database using the buttons on this home page. From a query results table, you can request

LATEST NEWS

May 2012 - The fourth Nanotechnology Signature initiative has been issued by the U.S. National Nanotechnology Initiative (NNI)... [Read more](#)

April 2012 - The U.S. Food and Drug Administration (FDA) has issued two draft

Current Focus: Leveraging community efforts

Characteristic	MINChar (2009)	ISO (2009)	OECD (2008)	NIST (2008)	Warheit (2008)	D. Ray (2007)
Aggregation/Agglomeration State	★	★	★	★	★	★
Particle Size/ Size Distribution	★	★	★	★	★	★
Purity	★	★	★	★	★	
Surface Area	★	★	★	★		★
Surface Chemistry	★	★	★	★		★
Composition	★	★	★		★	★
Shape	★	★	★	★		
Solubility		★	★	★		
Stability	★	★	★	★		
Surface Charge	★	★	★			★
Surface Reactivity				★	★	
Synthesis/Preparation				★	★	
Concentration			★	★		
Zeta Potential			★	★		
Crystal Structure/Crystallinity					★	★
Surface/Interfacial Energy				★		
Others?			12 more...			

- No standards in place at this time
- Multiple community efforts
- The Registry has built on these efforts by:
 - Soliciting these communities for additional feedback
 - Expanding concepts to include meta data
 - Building a flexible data model

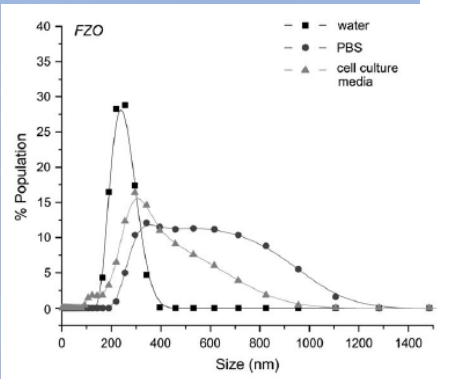
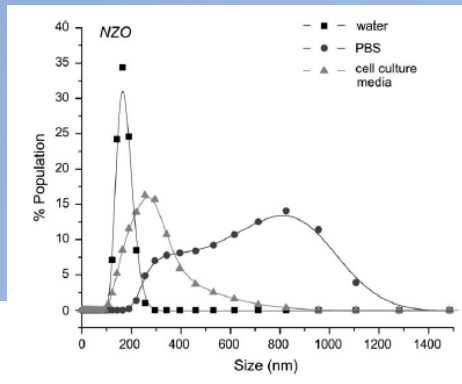
Current Focus: Minimal information standards



- Development of data model for the minimal information about nanomaterials
- Minimal information standards are important
 - Interoperability (data accessibility and usability)
 - Consistency with data and meta-data collection
 - Increased analytical power of datasets
- Challenges
 - The Minimal Information Standard is not simply a listing of physico-chemical characteristics
 - Sufficient information on instrumentation and methodologies used to measure characteristics is required
 - Consistent vocabularies are important

Example: Minimal Information and Protocols

- Particle characteristics can change depending upon protocol

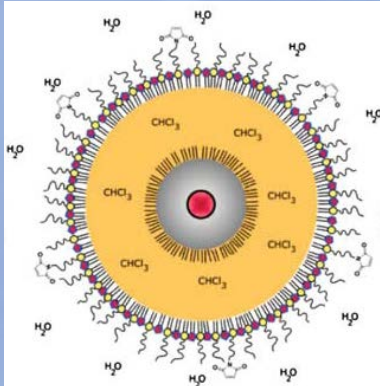
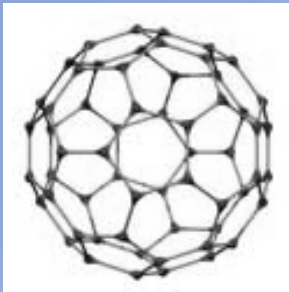


Sample	Solution	Average aggregate size in solution (nm)	% distribution	Surface charge (mV)	Aggregation state
Carbonyl iron	Water	564.5	47.6	-60.52	Mild
	PBS	560.8	80.3	-51.29	Mild
	F-12K media	578.9	86.5	-33.62	Mild
Crystalline silica	Water	534.1	19.8	-61.93	Moderate
	PBS	530.0	66.9	-16	Moderate
	F-12K media	471.5	67.0	-1.1	Moderate
Amorphous silica	Water	213.5	24.4	-48.43	Mild
	PBS	260.7	73.0	-26.96	Mild
	F-12K media	382.2	98.0	-5.26	Moderate
Nano-ZnO	Water	167.5	16.2	-54.51	Moderate
	PBS	313.7	31.3	-28.5	Moderate
	F-12K media	283.0	44.8	-5.7	Severe
Fine-ZnO	Water	242.9	18.8	-55.76	Mild
	PBS	318.6	34.9	-14.9	Moderate
	F-12K media	372.4	45.2	-9.4	Moderate

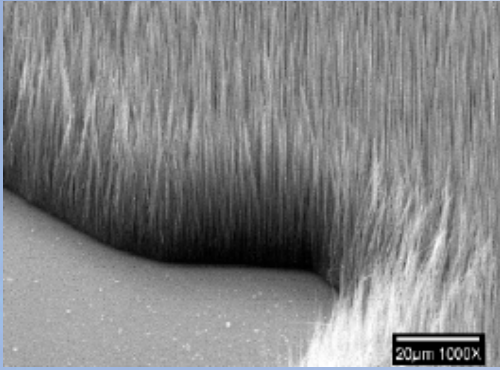
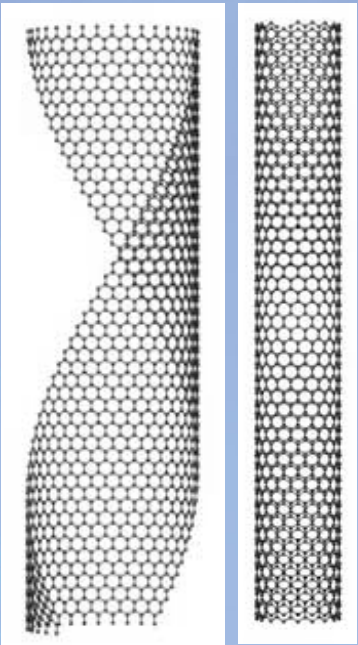
Assessing Toxicity of Fine and Nanoparticles: Comparing *In Vitro* Measurements to *In Vivo* Pulmonary Toxicity Profiles

Christie M. Sayes, Kenneth L. Reed, and David B. Warheit¹

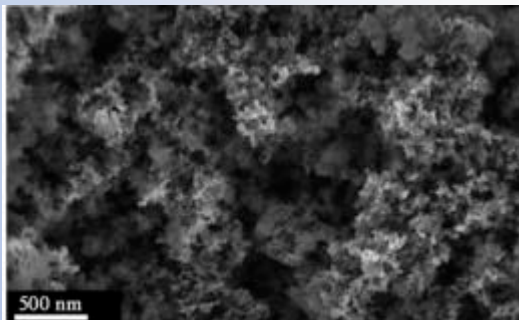
Example: Nanomaterial Morphologies



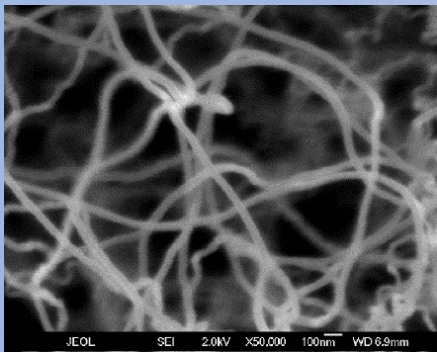
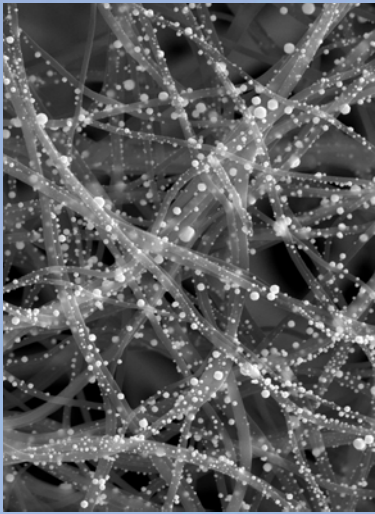
Tomalia, J Nanopart Res (2009) 11



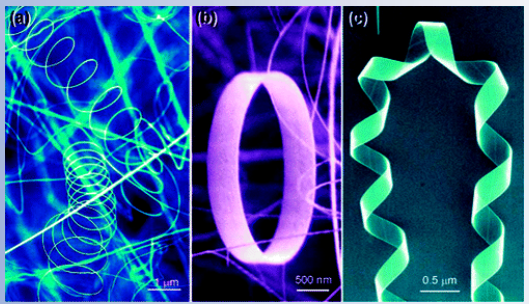
www.nano-lab.com



Zhang, J Coll Int Sci, 2(15) 2009

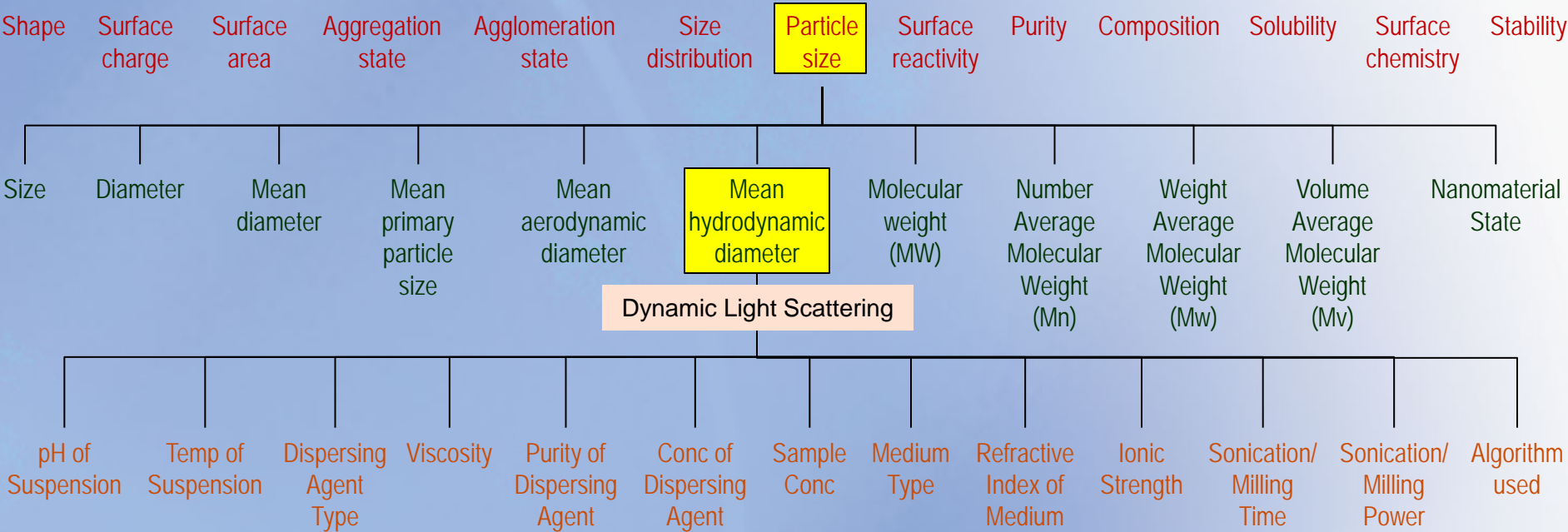


www.nano-lab.com



Wang, Materials Today 2004

Current Focus: Registry minimal information



Minimal Information = Physico-Chemical Characteristic + Measurement Type + Protocol Details

Current Focus: Infrastructure Development

- **Flexible data model**
 - Built on minimal information standards
 - Easily expandable to include new developments
 - Use case for adaption of standardized data formats
 - Hosted in an enhanced security network to ensure data integrity
- **Publically available website**
 - Search
 - Browse
 - Side-by-Side Comparison
 - Matching
 - Detailed view of nanomaterial records
 - Compliance levels for characterization data



Advanced Search

DATABASE SEARCH

KEYWORDS

Also search within words, phrases, or formulas

NARROW YOUR SEARCH

<input type="checkbox"/> Size Size Type: <input type="text"/> Value: <input type="text"/> Units: <input type="text"/> <input type="checkbox"/> Include Aggregate / Agglomerate size in your search?	<input type="checkbox"/> Composition Material Type: <input type="text"/> Biological Type: <input type="text"/> Fullerene/Carbon Type: <input type="text"/> Molecular Identity: <input type="text"/> Crystallinity Types: <input type="text"/> Crystalline Type: <input type="text"/> Surface Coverage Level %: <input type="text"/> Shell Continuity Type: <input type="text"/>	<input type="checkbox"/> Surface Charge Type: <input type="text"/> Value: <input type="text"/> Units: <input type="text"/>
<input type="checkbox"/> Size Distribution	<input type="checkbox"/> Purity Value: <input type="text"/> Units: <input type="text"/>	<input type="checkbox"/> Surface Reactivity
<input type="checkbox"/> Surface Area Type: <input type="text"/> Value: <input type="text"/> Units: <input type="text"/>		<input type="checkbox"/> Solubility Type: <input type="text"/>
<input type="checkbox"/> Shape Type: <input type="text"/>		<input type="checkbox"/> Stability
		<input type="checkbox"/> Biological Interactions Type: <input type="text"/>
		<input type="checkbox"/> Environmental Interactions Type: <input type="text"/>

- Search by keyword(s) and specific characteristic(s)

Browse

The screenshot displays the Nanomaterial Registry website interface. On the left, there is a sidebar with the heading "BROWSE NANOMATERIALS" and four filter categories: "Material Type", "Size", "Shape", and "Surface Area". A central navigation menu is open, listing various material classes such as Metal, Mixed Metal (& alloys), Metal Oxide, Fullerene/Carbon, Dendrimer, Polymer, Liposome, Chalcogenide, Group IV - non C, Group III-V, Alkaline Earth, Alkali, Halogen, Lanthanide, Actinide, and Biological. A sub-menu for "Fullerene/Carbon" is also visible, listing Buckey Ball, Nanotube, Graphene, and Graphite. Further sub-menu items for Nanotube include SWCNT, MWCNT, and FWCNT. The background shows a blurred view of the website's main content area, including a "Matching & Similarity" section and a "Minimal In" section.

- Browse through many key nanomaterial classifications

Compliance Levels

SEARCH RESULTS

5 RESULTS FOUND FOR SILVER

Arrange by > CLEAR COMPARISON SELECTION

YOUR CURRENT KEYWORD SEARCH
silver
 Also search within words, phrases, or formulas.

NARROW YOUR SEARCH
 Size VIEW >
 Size Distribution VIEW >
 Surface Area VIEW >
 Shape VIEW >
 Composition VIEW >
 Purity VIEW >
 Surface Charge VIEW >
 Surface Chemistry VIEW >

COMPLIANCE LEVELS
 Gold Silver
 Bronze Merit

	PCC COMPLIANCE	PARTICLE SIZE	SIZE DISTRIBUTION	AGGREGATION / AGGLOMERATION STATE	SURFACE AREA	SHAPE	COMPOSITION	PURITY	SURFACE CHARGE	SURFACE CHEMISTRY	SURFACE REACTIVITY	SOLUBILITY	STABILITY	ENVIRONMENTAL	BIOLOGICAL
NR1 - Ag NP															
NR15 - Ag NP															
NR35 - Ag NP															
NR97 - Ag NP															
NR299 - Ag															

- Data validation
- Algorithm uses minimal information to score nanomaterial data
 - Quality
 - Completeness

COMPLIANCE LEVELS

Gold

Silver

Bronze

Merit

Best Practice Questions

- Meta data is used to calculate compliance level

NR293

NR Descriptor: Au NP
 Information for this nanomaterial was curated from InterNano.
 Original Publication(s): <http://dx.doi.org/10.1021/ja002673n>
 Information reported: PCC Characterization? Yes Environmental interactions? No Biological interactions? No

CURATED DATA BASED ON INSTANCE OF CHARACTERIZATION Find similar nanomaterials

AS SYNTHESIZED: IN THE METHOD OF DOI: 10.4053/PR013-100331

PHYSICO-CHEMICAL CHARACTERISTICS BIOLOGICAL INTERACTIONS ENVIRONMENTAL INTERACTIONS

Composition ● CORE (hover over circle for proportion of material)

COATING
 COMPONENT 1
 Molecular Identity: Phosphine-stabilized Au
 Molecular Identity: Au101(PPh3)21Cl5

SHELL

Particle Size
 Mean Diameter: Powder
 Thickness: Monomodal Transmission Electron Microscopy

Size Distribution
 Size Distribution:
 Minimum: Metal

Purity
 Purity Of:
 Core: 75.8 %

Molecular Identity: Phosphine-stabilized Au

Molecular Identity: Au101(PPh3)21Cl5

Mean Diameter: Powder

BEST PRACTICES

Instrument Manufacturer: Not Reported

Instrument Model: Not Reported

Raw Data Provided: Yes

Proper Controls Used: Not reported

Instrument within Calibration: Not reported

Number of Replicates: Not Reported

Protocol Reported: Not reported

Protocol Citation: Not Reported

Protocol Modifications: Not Reported

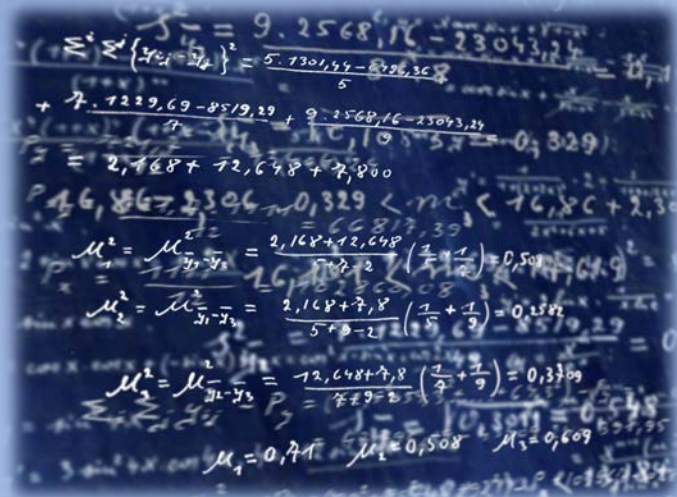
Data Curation

Current Sources: publicly available databases

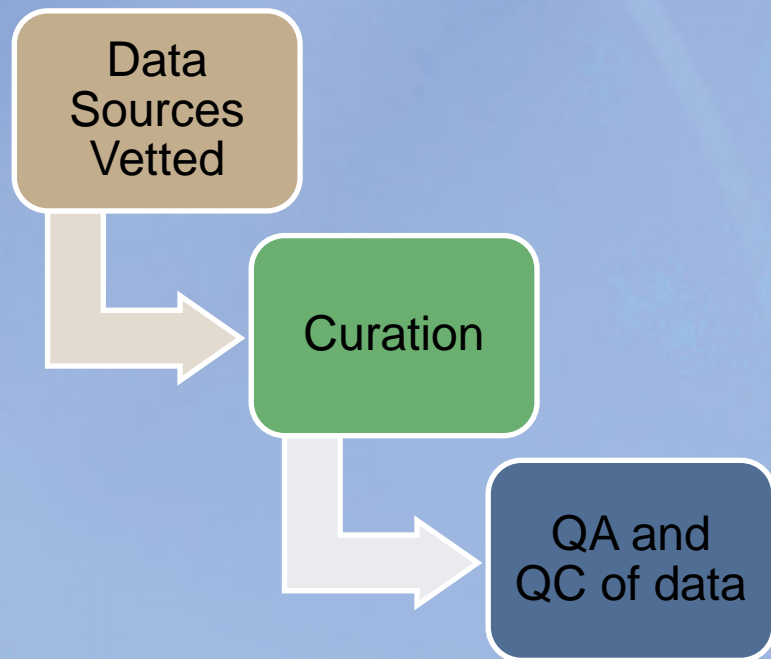
- CaNanoLab (cancer research)
- NIL (Nanomaterial Information Library)
- InterNano (manufacturing)

Future Sources:

- Industry
- Academia
- YOU!



Curation Process



- Data sources vetted by SME
- Minimal information curated by experienced nanomaterial researchers via web-based tool
- QC of curated records for proper scientific interpretation by SME

Current and Future Efforts

- Nanomaterial entry enhancement
 - Implementing Biological and Environmental Implications information
 - Increasing the number of nanomaterial entries
 - Vetting new data sources – databases, peer-reviewed data
- Refinement – The Registry has been designed to be evergreen
 - Updating minimal information, compliance level and matching algorithms
 - New findings from external resources or from the Registry itself
 - Ontology
 - Understanding the scope and granularity needed for Registry users
 - Leveraging community-based tools, best practices
 - Developing ontology for additional information presented in the Registry
- Interoperability
 - Currently looking at ISA-TAB-Nano and vetting other standard ways to capture nanomaterial data
 - Working with data sources and enabling early adapters of data format standardization

Thank You



- Next Nanomaterial Registry release:
 - August 2012
 - Redesigned pages for improved usability
 - Curated biological and environmental interaction data
- Please visit www.nanomaterialregistry.com
- Contact us at **NANOREGISTRY@RTI.ORG** to become a part of the nanoinformatics effort