NANOMATERIALREGISTRY

An authoritative resource for assessing biological and environmental interactions of nanomaterials

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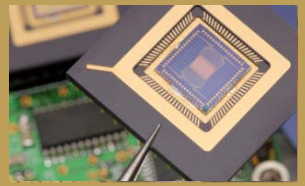
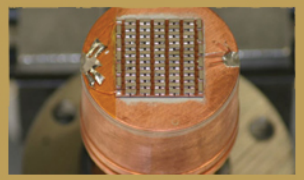
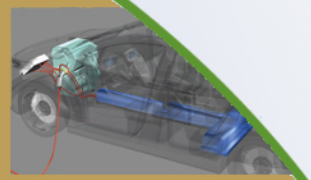
June 21, 2012



NANOMATERIAL REGISTRY

An Overview

- 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

NIBIB

NIEHS

National Cancer Institute

ONAMI
Oregon Nanoscience and Microtechnologies Institute

Intertox

NIST

NIOSH

United States Environmental Protection Agency

Evonik Industries

UMass Amherst

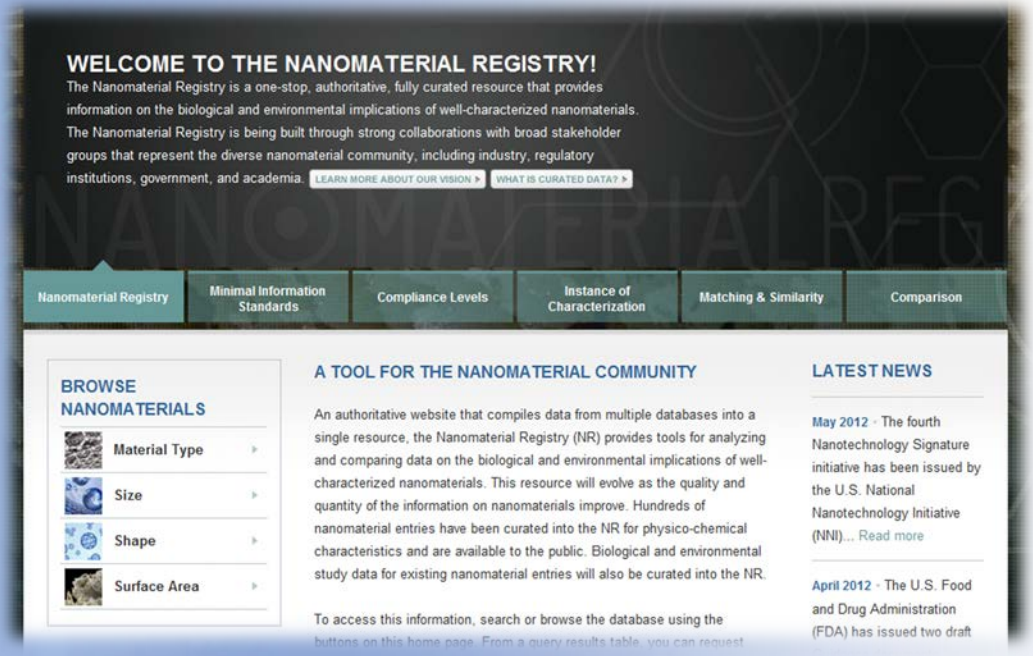
ISO
International Organization for Standardization

RTI International

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



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

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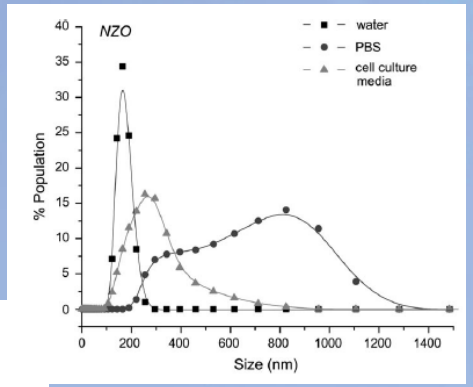
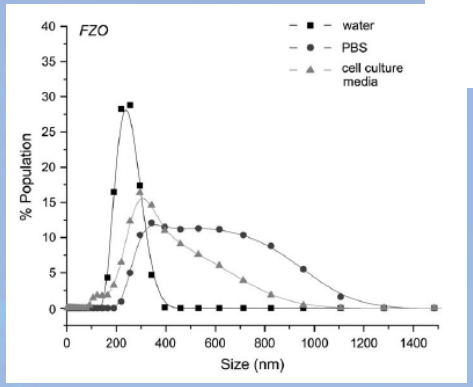
Example: Minimal Information and Protocols

- Particle characteristics can change depending upon protocol



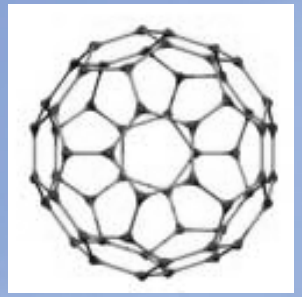


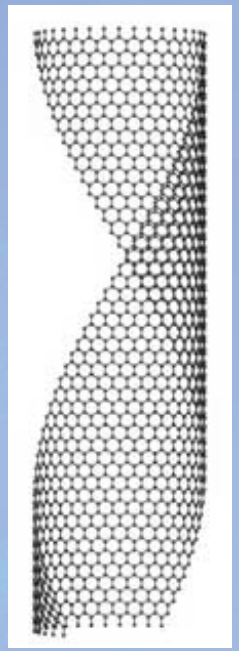
Sample	Solution	Average aggregate size in solution (nm)	% distribution	Surface charge (mV)	Aggregation state
Carbonyl iron	Water	564.5	47.6	–60.52	Mild
	PBS	560.8	80.3	–51.29	Mild
	F-12K media	578.9	86.5	–33.62	Mild
Crystalline silica	Water	534.1	19.8	–61.93	Moderate
	PBS	530.0	66.9	–16	Moderate
	F-12K 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

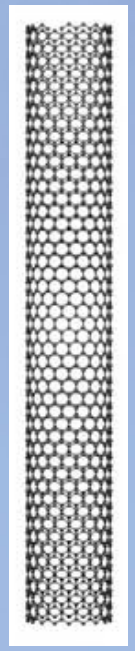
Assessing Toxicity of Fine and Nanoparticles: Comparing *In Vitro* Measurements to *In Vivo* Pulmonary Toxicity Profiles

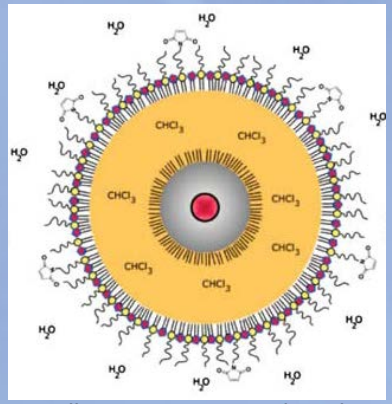
Christie M. Sayes, Kenneth L. Reed, and David B. Warheit[1]

Example: Nanomaterial Morphologies

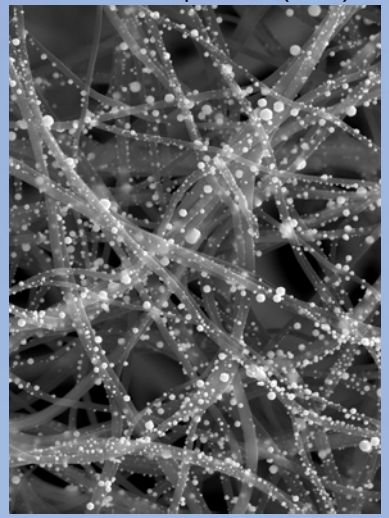


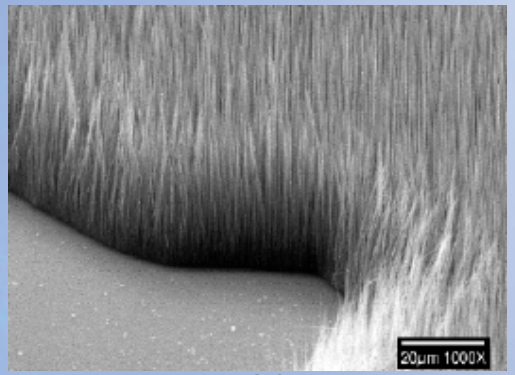




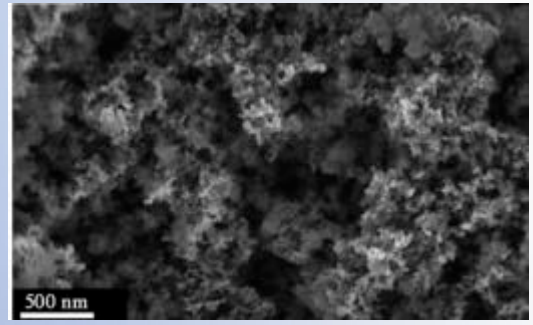


Tomalia, J Nanopart Res (2009) 11

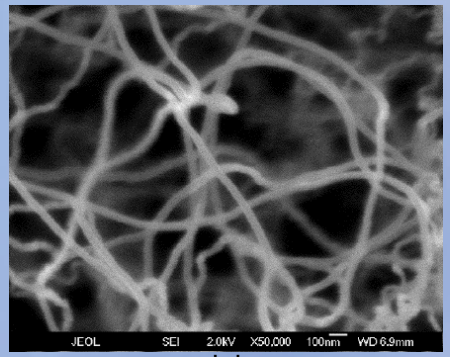




www.nano-lab.com



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



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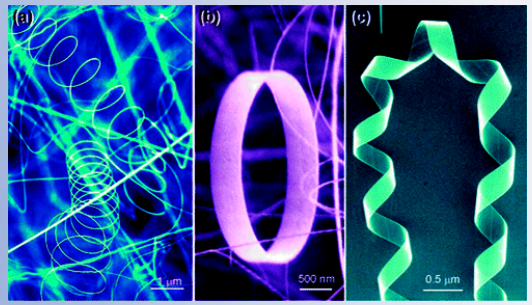
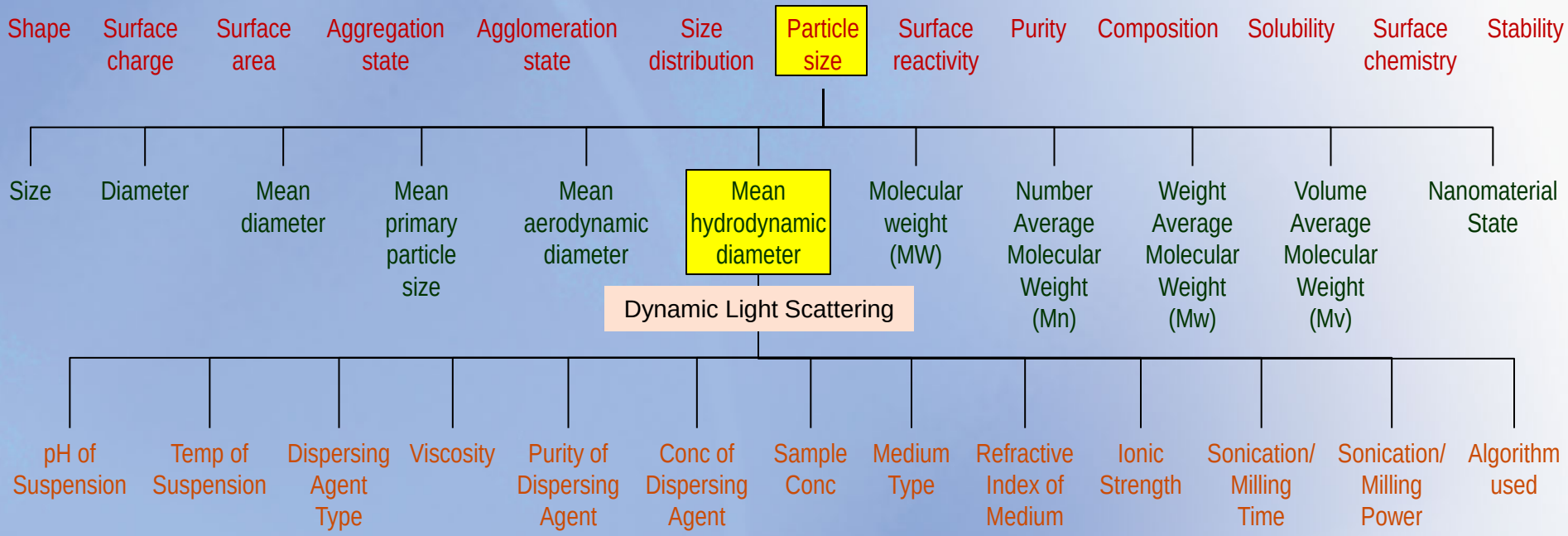


Wang, Materials Today 2004

Current Focus: Registry minimal information

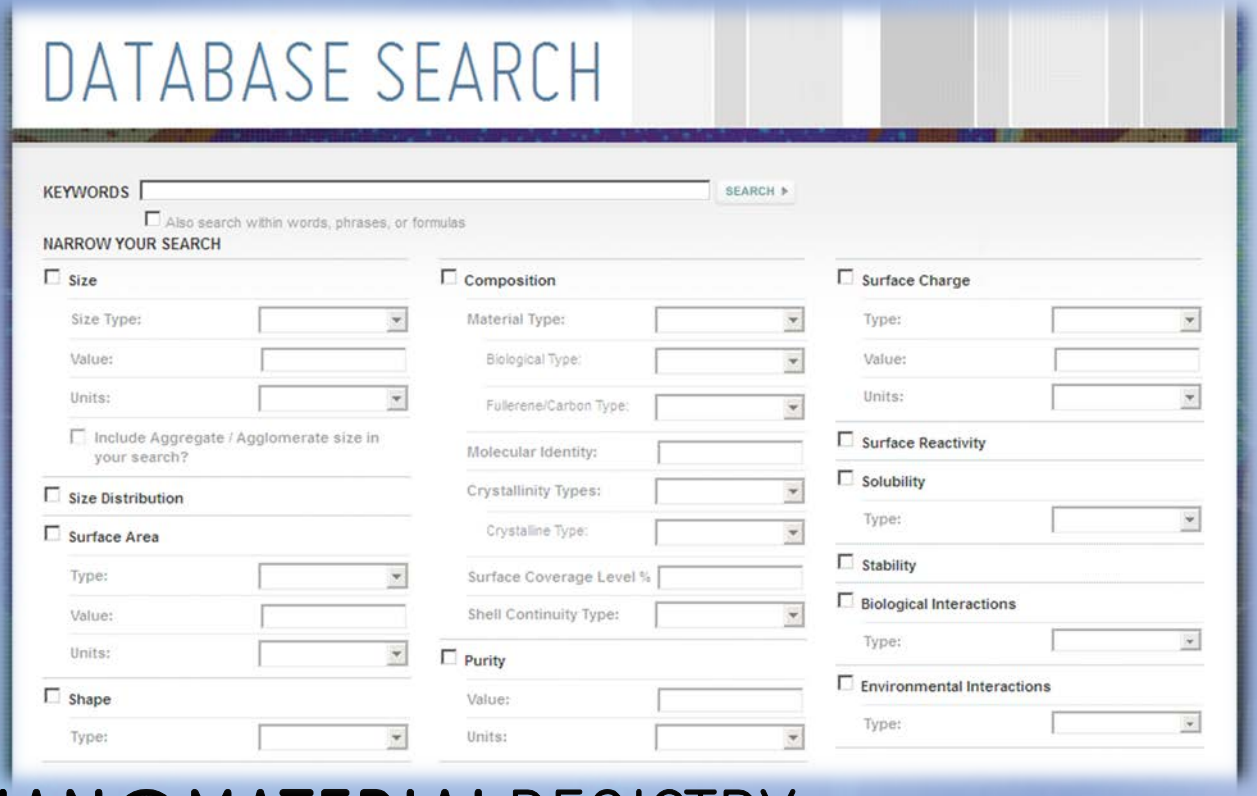


Minimal Information = Physico-Chemical Characteristic + Measurement Type + Protocol Details

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



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

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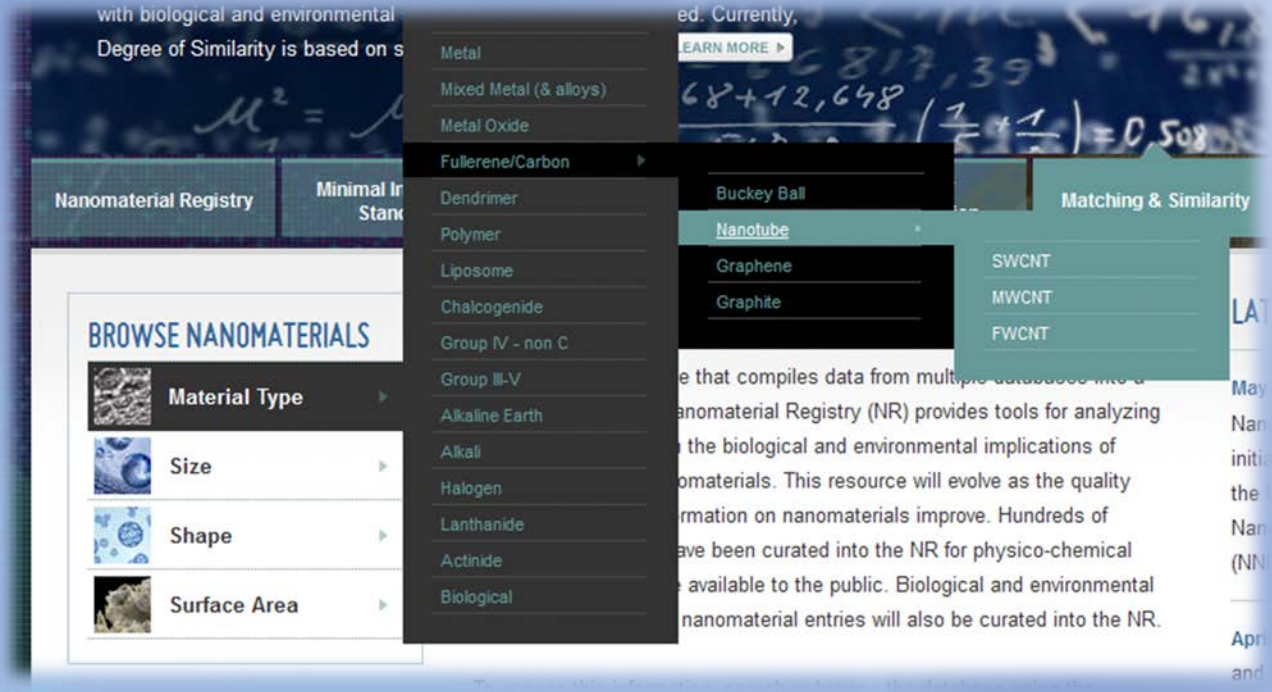
Browse



- Browse through many key nanomaterial classifications

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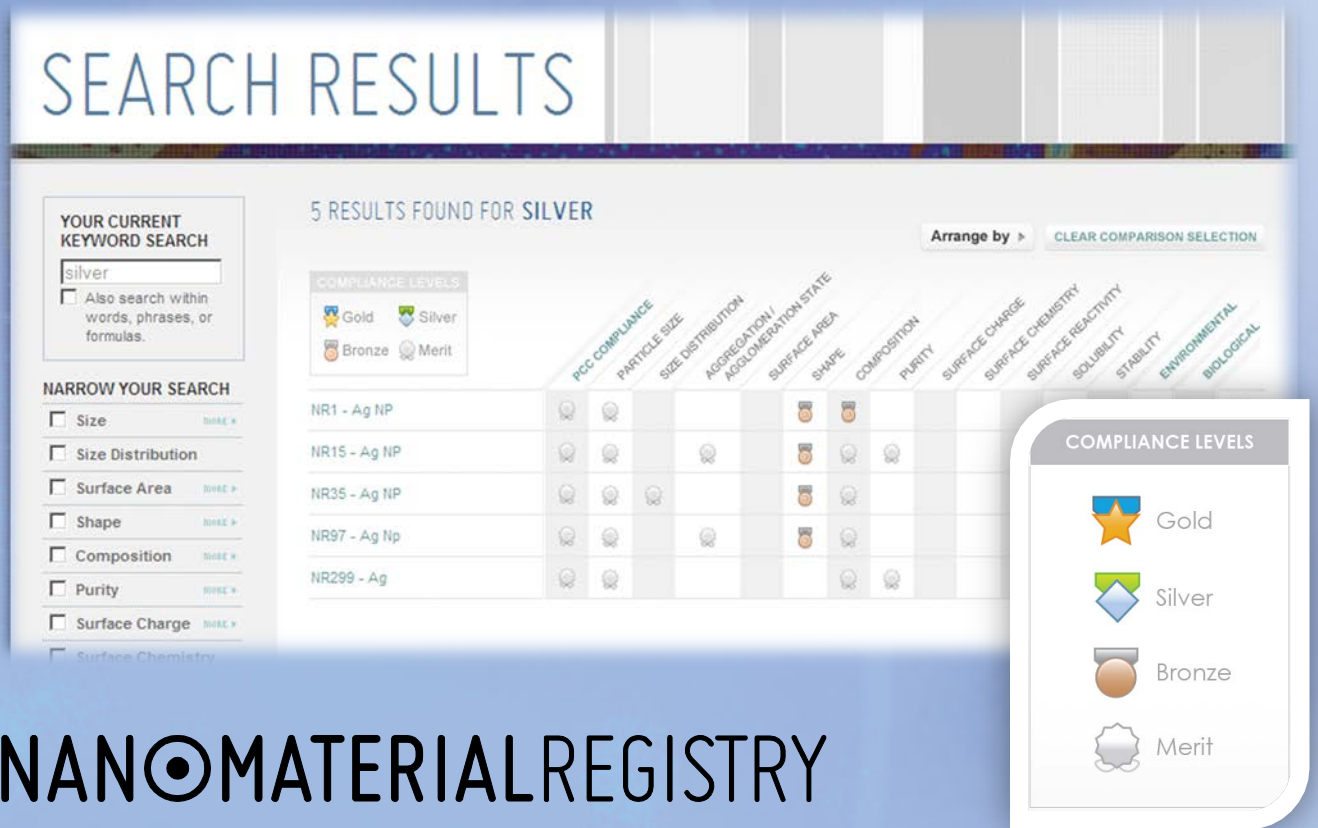
Compliance Levels



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

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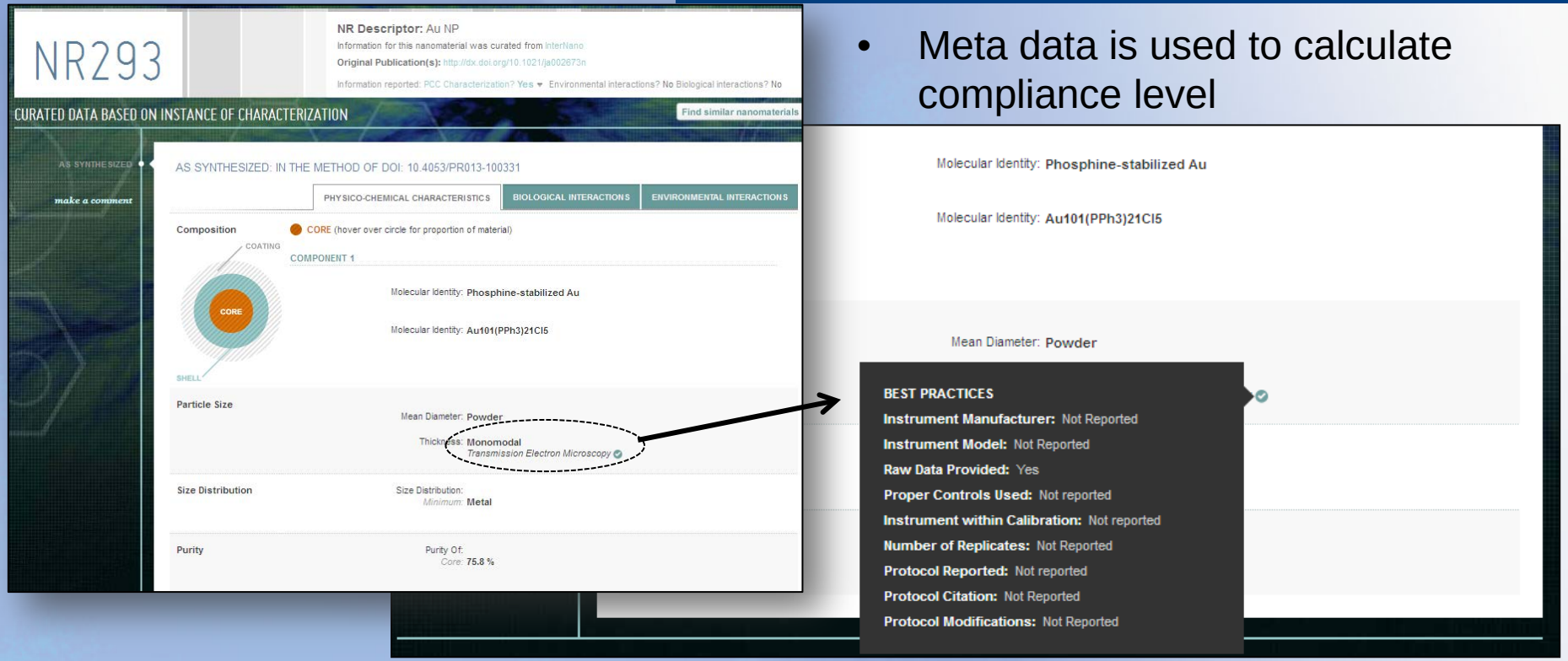
Best Practice Questions

- Meta data is used to calculate compliance level



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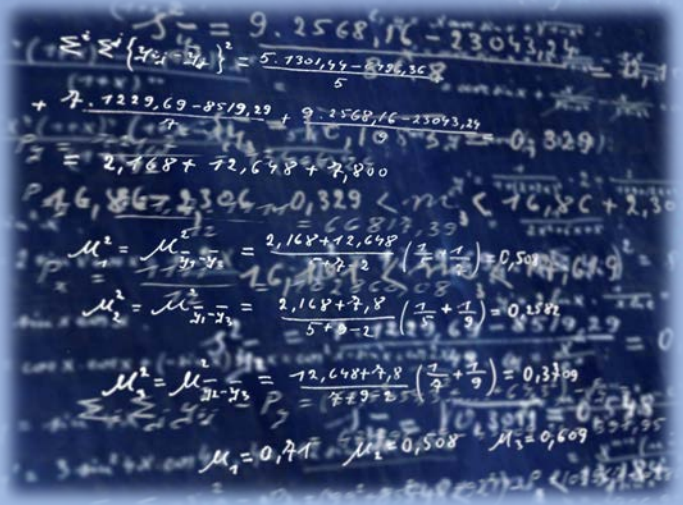

Data Curation

Current Sources: publicly available databases

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

Future Sources:

- Industry
- Academia
- YOU!

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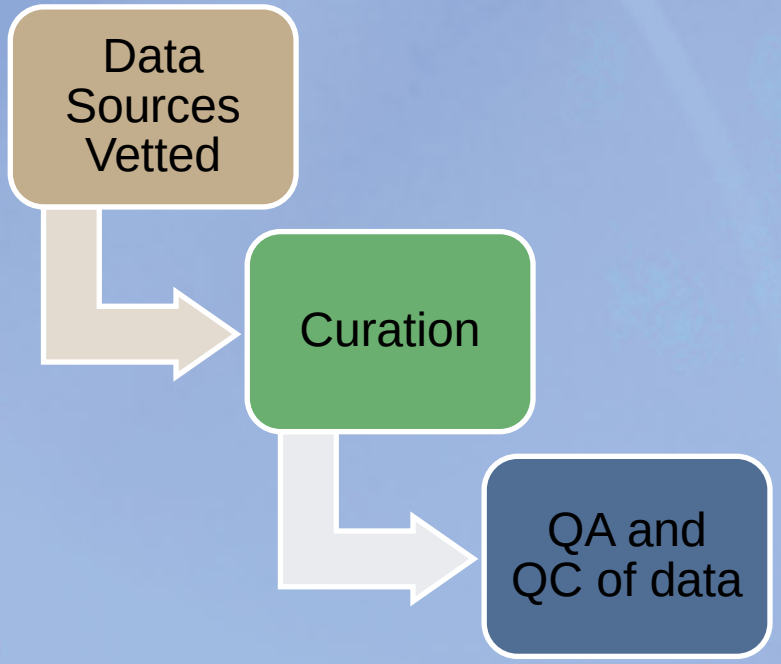
Curation Process



- 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

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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

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