Nanomaterial Registry: An authoritative resource for assessing environmental and biological interactions of nanomaterials

M. Ostraat[*], K. Mills[**], D. Murry[***], and K. Guzan[****]

[*]RTI International, 3040 Cornwallis Road, RTP, NC, 27709, USA, mostraat@rti.org
[**]RTI International, 3040 Cornwallis Road, RTP, NC, 27709, USA, kmills@rti.org
[***]RTI International, 3040 Cornwallis Road, RTP, NC, 27709, USA, dmurry@rti.org
[****]RTI International, 3040 Cornwallis Road, RTP, NC, 27709, USA, kguzan@rti.org

ABSTRACT

Assessment of the interactions of nanomaterials with environmental and biological systems is both complex and rapidly evolving. The complexity of these interactions arises from the fact that these interactions are not only a function of the system under consideration, but also of the inherent characteristics of the nanomaterial and the diverse test methods, protocols, and assays used to determine these interactions. At the same time, the quantity of publicly available literature on nanotechnology is staggering. To address these challenges, the Nanomaterial Registry has been developed as an authoritative, web-based tool that systematically organizes and evaluates existing research findings on the impacts of well-characterized nanomaterials from multiple resources. As an authoritative resource, all content is systematically curated prior to inclusion in the Registry. To facilitate development of the Registry, a minimal information standard for nanomaterials has been established which has already been used to develop evaluation criteria and similarity matching criteria for nanomaterials that are included in the Registry. This resource is being built through collaborations with representatives from many stakeholder groups within the nanotechnology community, including industry, regulatory, government, and academia.

Keywords: nanomaterials, registry, nanoinformatics, nanotechnology

1 NANOMATERIAL REGISTRY

1.1 Motivation

The nanomaterial community currently faces many challenges, not the least of which involves building consensus around a minimal information standard for nanomaterial characterization. Also, because the information being gathered across various nanomaterial stakeholder groups is so diverse and complex, nanomaterial interactions with biological and environmental systems are still inconclusive. Nanotechnology takeholder groups also suffer from a lack of standardized protocols and measurement schemes, and debate is still ongoing regarding the utilization and adaptation of current methods and procedures specific to nanomaterials.

1.2 Attributes

Using the defined minimal information standards, the Registry team curates physico-chemical characteristics (PCC) data and study data on nanomaterials in biological and environmental systems. These data are labeled with a unique Registry identification number that may eventually be replaced with a human-readable naming scheme. All of these data are available on the Registry's website via a browse menu as well as through basic and advanced search. From any of these tools, the resulting query will offer a table of relevant nanomaterials, showing the compliance levels of the curated data for PCC and biological and environmental system interaction studies. A user can either view a specific nanomaterial entry or choose as many as three nanomaterials to compare. When a user goes to a specific nanomaterial entry details page, they can also find nanomaterials similar to the chosen nanomaterial, which are dictated by carefully defined matching rules.

2 MINIMAL INFORMATION STANDARDS

The Nanomaterial Registry's minimal information standards have been developed by RTI with the help of an Advisory Board from the nanomaterials community and leveraged from other minimal information working groups, such as the MINChar Initiative [1]. Through the Registry's curation process, data are compared to the defined minimal information standards for PCC, biological interactions and environmental interactions of nanomaterials. If reported data is not within the minimal information standards, it is not included in the Registry. For each PCC, there are three different subsets of information required in the minimal information standards: 1. Measurement values, 2. Analysis technique, instrument, protocol and parameter information, and 3. Scientific method and best practice evaluation. Table 1 gives curated examples of each PCC.

Table 1: Scope of the Minimal Information Standard for Physico-Chemical Characteristics

PCC	Scope of PCC in the Registry	Example of Curated Data
Composition	The qualitative and quantitative makeup of a material as described by its components (ex. core, shell, coating), including shell continuity and crystallinity	• Material Type: **Metal Oxide** • Molecular Identity: **CuO** • Crystallinity: **Crystalline**
Particle Size	The physical magnitude of a particle. For spherical particles, it is their diameter. For irregularly shaped particles it is the diameter of the equivalent sphere which has the same volume as a particle. Also includes physical state of the sample.	• Mean Hydrodynamic Diameter: **8 nm** *Technique: Dynamic Light Scattering* • Nanomaterial State: **Liquid Suspension**
Size Distribution	A list of values or a mathematical function that defines the relative amounts of particles present, sorted according to size – modality, peak magnitude, minimum and maximum are included	• **Monomodal** • Peak 1: **7.37 nm (+/- 27%)** *Technique: Transmission Electron Microscopy* • Peak 1: **5.52 nm (+/- 38%)** *Technique: Atomic Force Microscopy*
Shape	The dimensionality (0D, 1D, 2D) of a nanoparticle along with the rigidity of its spatial arrangement as represented in its external surface	• Dimensions: **0D** *Technique: Transmission Electron Microscopy* • Hard /Soft?: **Soft**
Surface Area	A measurement of the extended two-dimensional outer boundary of a three-dimensional object	• Specific Surface Area: **222.63 m^2/g** *Technique: Brunauer, Emmett and Teller Gas Adsorption Analysis*
Surface Chemistry	The chemical properties of the surface of the sample	• Most outward material: **PEG**
Surface Charge	The electric charge present at the surface of the sample	• Zeta Potential: **-6.05 mV** *Technique: Electrophoretic Light Scattering*
Purity	The degree to which a sample is free from contaminants – includes identity of any contaminants	• Purity of Core: **75.8%** • Purity of Nanomaterial: **99.95%**
Aggregation/Agglomeration State	The extent to which a group of particles, affected by attractive forces, forms groups or clusters	• Aggregated • Size, Volume Weighted: **8000 nm** *Technique: Scanning Electron Microscopy*
Solubility	The categorization of a material as hydrophobic or lipophilic as well as P value and D value	• "W" - Hydrophilic (log D < 0)
Stability	The measure of a system is in its lowest energy state or chemical equilibrium with its environment	
Surface Reactivity	Includes chemical affinities and speeds of reactions	• Excellent affinity toward hydrogen sulfide

NSTI-Nanotech 2012, www.nsti.org, ISBN 978-1-4665-6276-9 Vol. 3, 2012

2.1 Time of Measurement

Significant importance is placed upon a so called time of measurement (ToM0 of each nanomaterial. All curated nanomaterial PCC data are associated with a ToM that is descriptive of that nanomaterial's status when characterized. A ToM is assigned to every piece of curated data, and the choices for ToM include:

• As Received from a manufacturer

• As Specified by a manufacturer

• As Reported by a previous researcher

• As Stored by a researcher

• As Synthesized by a researcher

• As Processed by a researcher

By also collecting meta-data surrounding this ToM (e.g. manufacturer, doi of synthesis procedure, etc.), the Registry can track a nanomaterial's pedigree, the importance of this being a better understanding of how similar or dissimilar two originally identical nanomaterials may become in the course of various processing and characterization steps. The Registry aims to aid in the understanding of nanomaterial effects on biological and environmental systems by tracking ToM information. At this time, the Registry uses simple, rule-based, data matching to show the degree of similarity between nanomaterials. As the depth and breadth of data in the Registry increases nanomaterial matching will improve.

2.2 Curated Data, Compliance Levels, and Scores

The Nanomaterial Registry team curates data from existing databases, including Nanomaterial Information Library (NIL) [2], caNanoLab [3], and InterNano [4] databases. Going forward, the Registry will include curated data from other appropriate data sources.

The data in the Registry is available via browse as well as basic and advanced searches. The basic search allows the user to not only search by keyword, but also to find entries where certain PCC have been characterized. The advanced search offers extensive power to find exact data values. All data is curated and rated using the visual representation of compliance levels to help the community understand the minimal information standards on characterization that are being requested and proposed by the Registry.

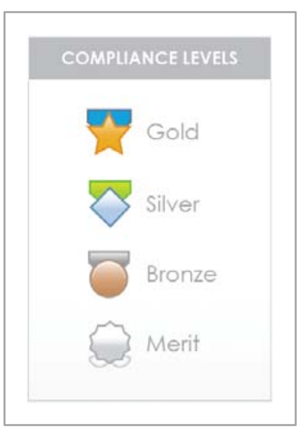

Figure 1. Compliance medals in decreasing order: gold, silver, bronze, merit.

It is recognized that not all nanomaterials have been characterized to the same extent or according to the same prevailing standards. In order to assist in driving these standards, the compliance level feature of the Registry provides a metric on the quality of characterization of a nanomaterial entry. In the many cases where appropriate standards for nanomaterial characterization do not yet exist, the compliance level score serves to identify the data gaps where more emphasis is needed. Figure 1 shows the different compliance levels assigned to particular ranges of compliance scores, with gold being 76-100%, silver being 51-75%, Bronze being 26-50% and Merit being 0-25%.

3 CONCLUSIONS

3.1 Vision of the Nanomaterial Registry

The Registry is intended to be a useful tool for the nanomaterial community that grows organically based on a cyclical relationship with the community it serves (Figure 2) and not a stagnant data repository and website.

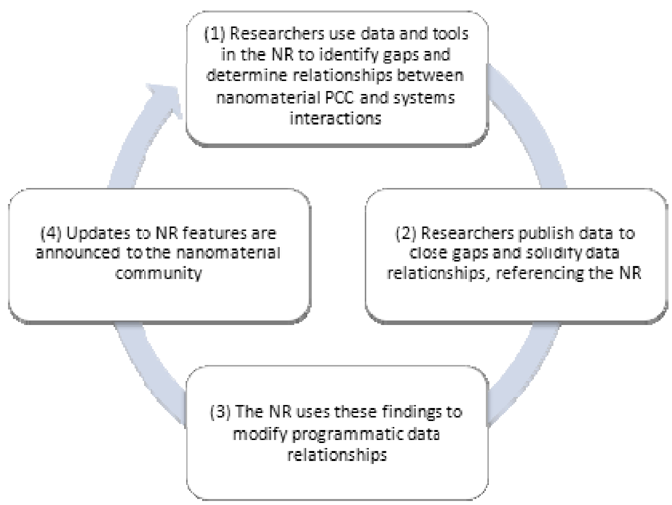

Figure 2. Process by which growth is expected for the Nanomaterial Registry

Over time, we expect the Registry to have tremendous potential for significant long-term impacts, including:

- Aiding in the development of new models, assays, standards, and manufacturing methods
- Accelerating the translation of new nanomaterials for biomedical and environmental applications
- Promoting standards in nanomaterial characterization testing, handling, and disposal and
- Supporting science-based regulatory decision-making

4 ACKNOWLEDGEMENTS

RTI would like to thank the following institutions within the National Institutes of Health for funding this work: NIBIB, NIEHS, NCI. RTI would also like to thank Mellonaid for the design and programming of the Nanomaterial Registry's website.

5 REFERENCES

[1] www.characterizationmatters.org
[2] http://www.nanoparticlelibrary.net/index.asp
[3] https://cananolab.nci.nih.gov/caNanoLab/
[4] http://www.internano.org/