

Discussion on Curation

Nano WG – June 6, 2013

Karman Mills

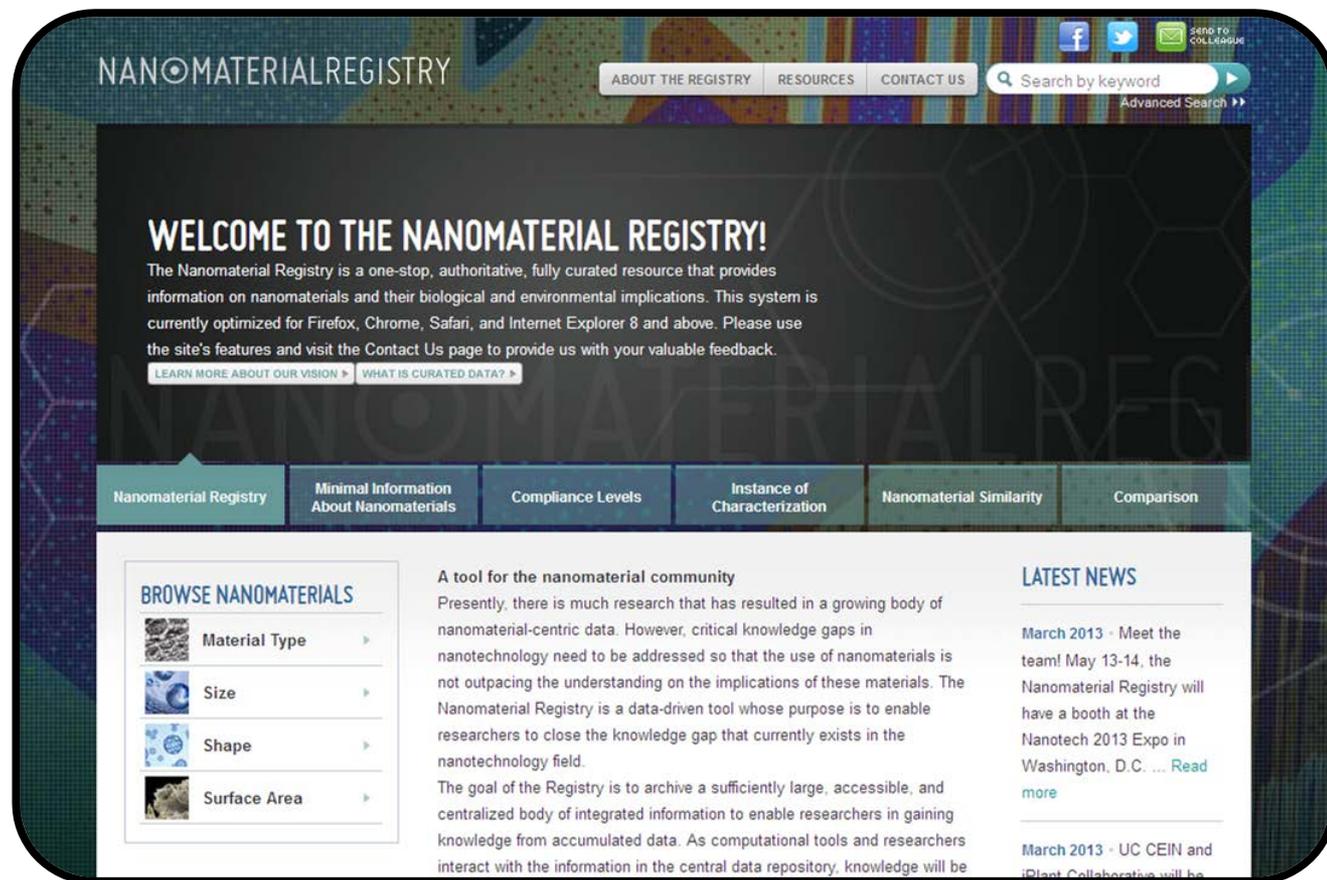
Website, Outreach, & Curation Task
Leader

RTI International

NANOMATERIALREGISTRY



*Comprehensively
curated,
validated data on
a scale suitable
for decision
making*



Web Address:

www.nanomaterialregistry.org

Funded by:



Registry User Goals

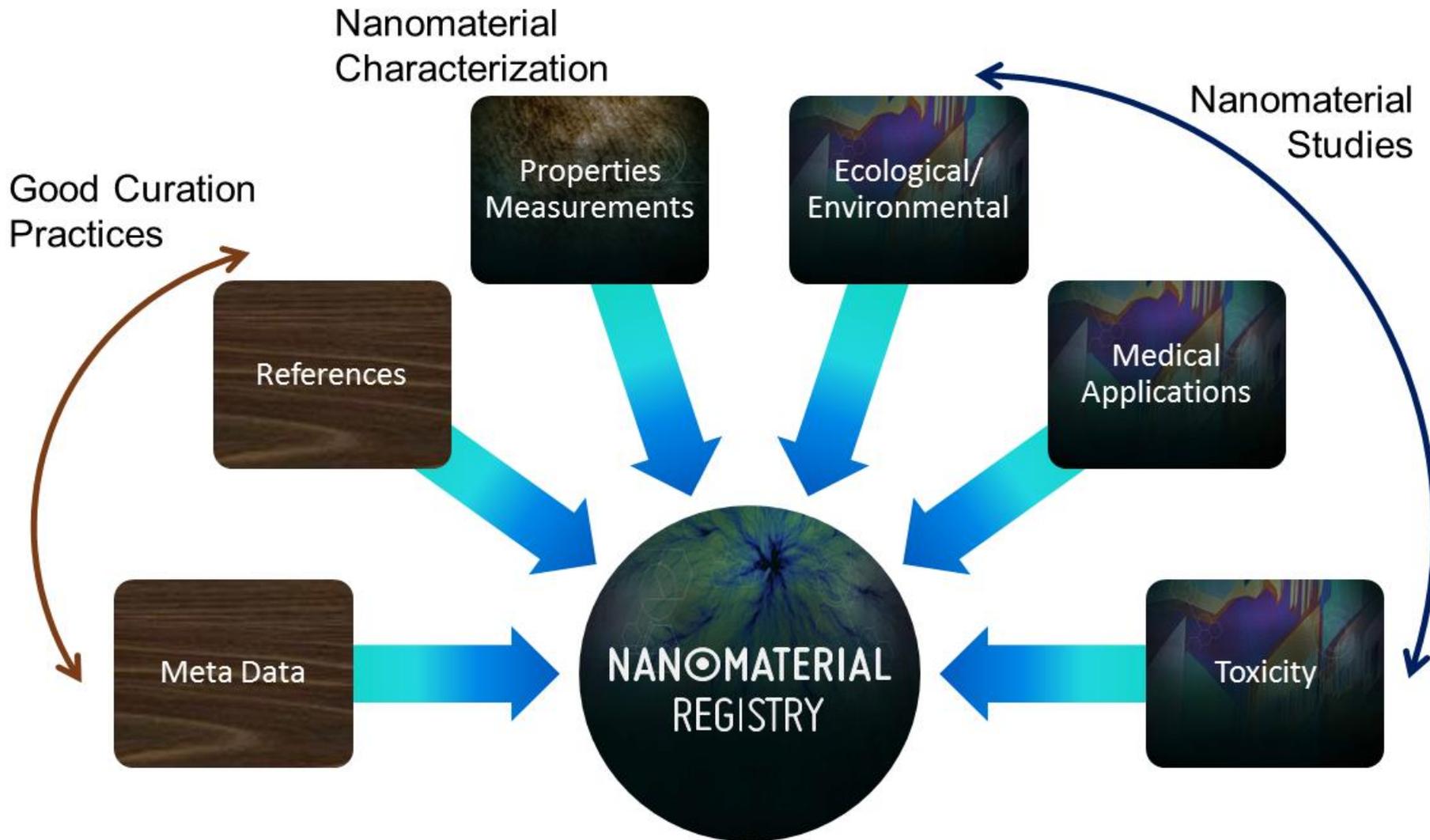
Short Term:

- Easily visualize what been done in the community
 - Instrumentation
 - Assays
 - Chemistries

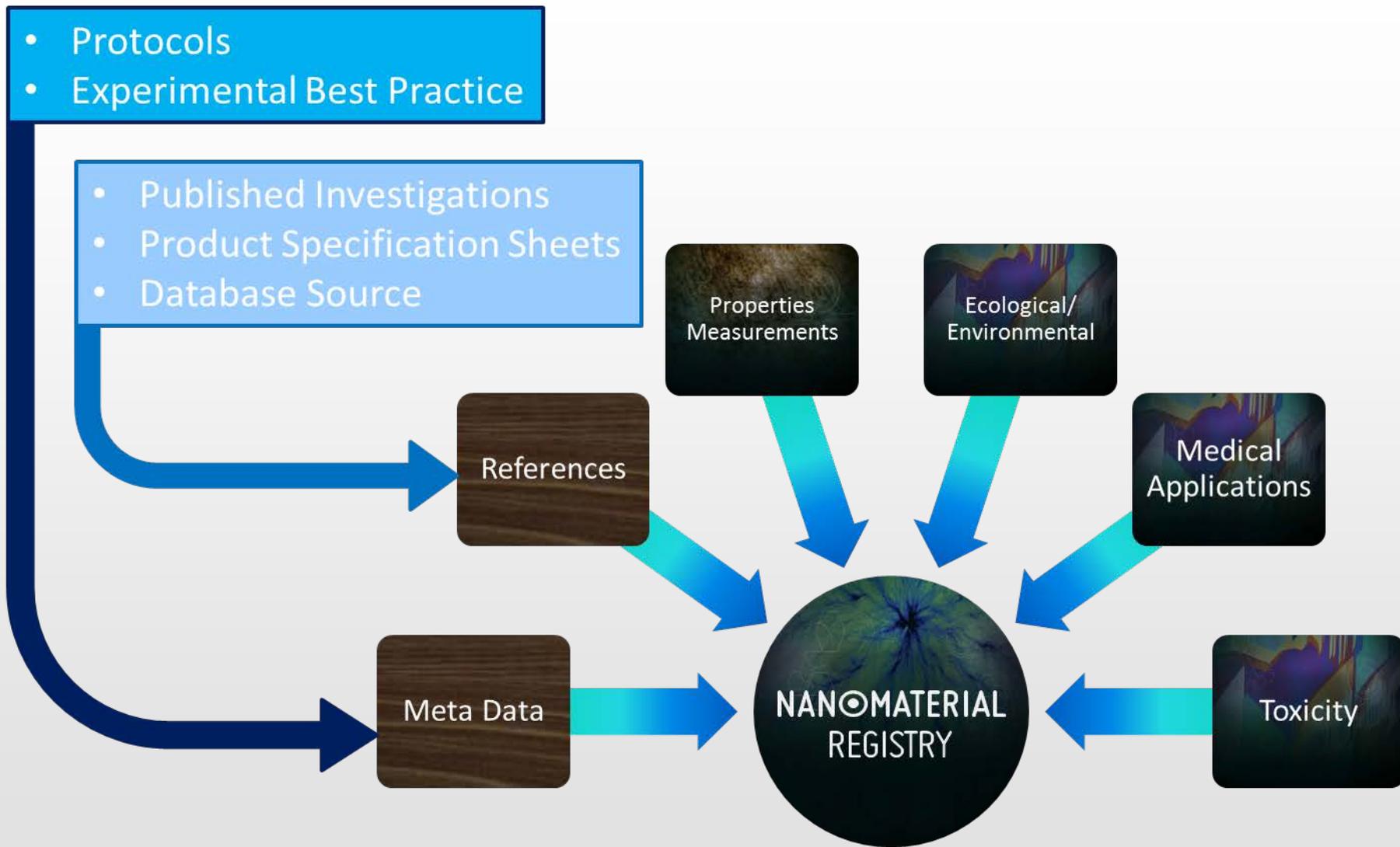
Long Term:

- Use curated data to predict the behavior of new nanomaterials

Current Data Scope 1



Current Data Scope 2





Linking PCCs with Impacts

Capturing Biological and Environmental Impacts

Study Type

Biological (*In Vitro*, *In Vivo*)
Environmental (*Air*, *Soil*, *Water*)

Study Conditions

Media
Media Properties
Subject
Location
Controls
Concentrations
Exposure Summary

Nanomaterial
Physical &
Chemical
Characteristics

Assays

Laboratory
Field

Endpoints

Biodistribution
Cytotoxicity
Mortality
Transformations
Mechanistic
Fate & Transport



Linking Data Example

Analysis of the connections between properties and environmental and biological impacts of nanomaterials

Study Type

Biological: In Vivo

Environmental: Soil, Water

Study Conditions

Media: Water, Soil

Media Properties 1: Natural soil, 63% sand 10% clay
26% silt

Media Properties 2: Natural water

Subjects: Mosquitofish; Plants

Location: Simulated Field

Exposure Summary: Acute/Chronic;
absorption/dermal inhalation/oral;
0.025 mg/mL; 18 months

Diameter (10nm)
Size Range (30-80nm)
Modality (monomodal)
Aggregation State (aggregated)
Aggregate Size (200 nm)
Coating (PVP)
Impurities (Ag₂O; Ag₂S)

Assays

Laboratory:

graphite furnace AA; ICP-MS;
Acid leaching; Cline method; XAS

Field: YSI probe; sediment coring;
dialysis

Endpoints

Biodistribution:

roots & shoots; body burden

Transformations:

oxidation; sulfidation; sed redox

Mechanistic: organism mobility

SILVER nanomaterial study (data record NR1038)

Data Source: CEINT

<https://www.nanomaterialregistry.org/NanomaterialDetails2.aspx?pid=1038>

Minimal Information about Nanomaterials
Physico-Chemical Characteristics

MIAN PCC

MIAN for Physico-Chemical Characteristics



Composition



Size



Size Distribution



Shape



**Aggregation/
Agglomeration State**



Surface Area



Surface Charge



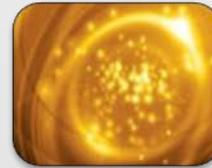
Surface Chemistry



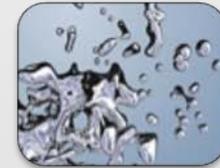
Surface Reactivity



Purity

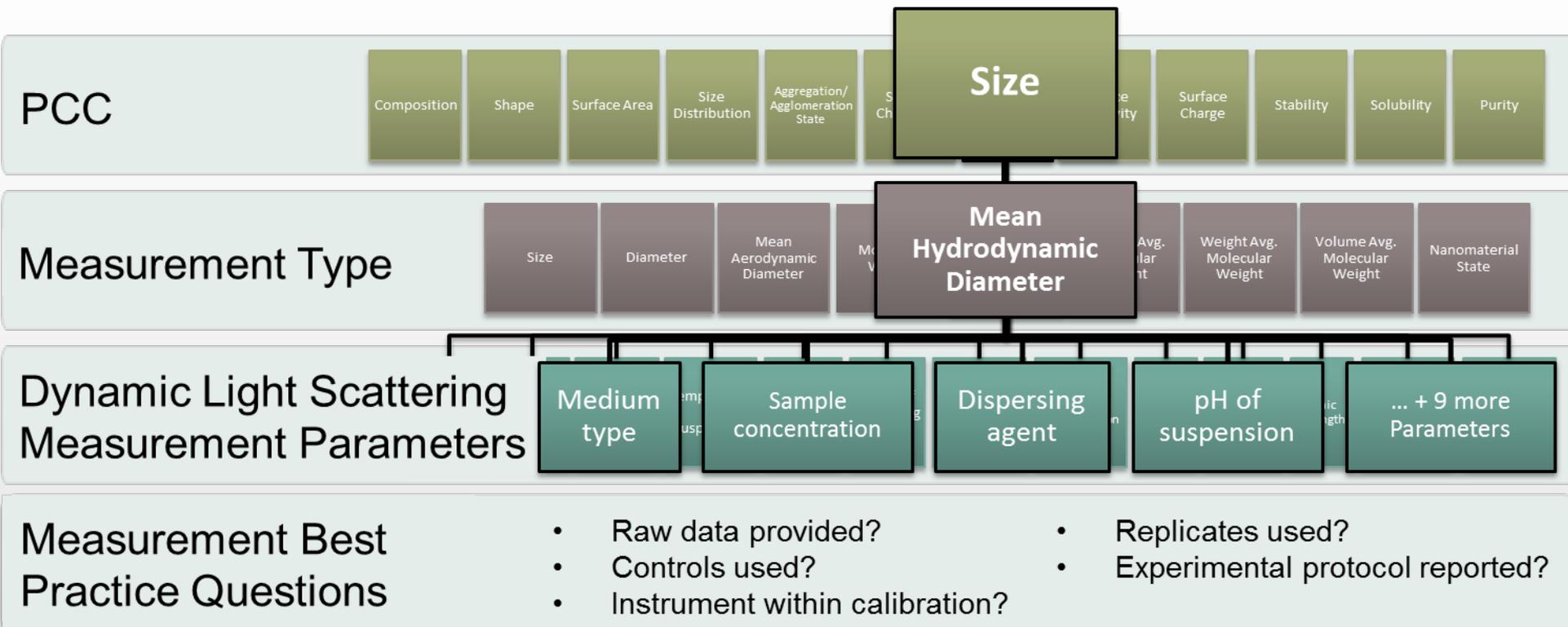


Solubility



Stability

Metadata in the MIAN



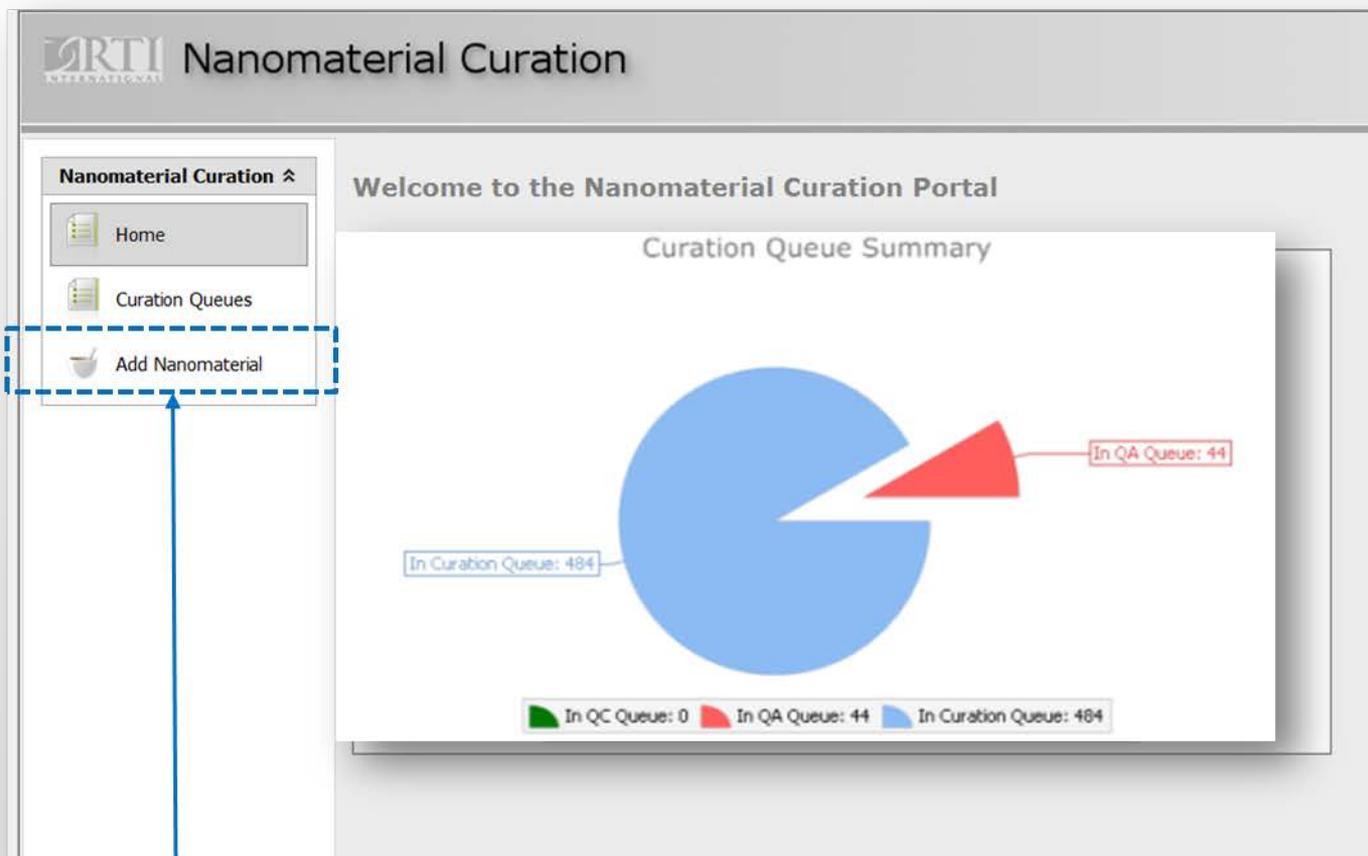
Minimal Information = PCC data + Metadata

Accelerating the Curation Process
Minimizing Error Propagation

CURATION TOOL

Systematic Data Archiving

A **DATA CURATION TOOL** facilitates the progression of nanomaterial entries through the curation process to the Nanomaterial Registry website



DATA ENTRY

- ✓ identifies, evaluates, and enters data

QUALITY ASSURANCE

- ✓ check for transcription errors

QUALITY CONTROL

- ✓ correct any errors or inconsistencies in the scientific interpretation

★ Curation tool workflow starts with the creation of a nanomaterial record

Systematic Data Archiving: *DATA CURATION TOOL 1*

Data records are promoted through **QUEUES**

Nanomaterials In Curation Queue

Queue: **Curation**

NRID	DB Entry Name	Status	AssignedTo	Date Created	Date Updated			
NR1002	NEU-LWangJNBT2008-01	In Curation Queue	pdurham	1/3/2013	4/17/2013			
NR1036	Muti-Wall CNT	In Curation Queue	jchild	1/31/2013	1/31/2013			
NR1246	NRCWE_UCFV_HC_UC_SST-NJacobsenEMM2008-01	In Curation Queue	jchild	4/29/2013	4/30/2013			
NR1250	JHU_KSU-JGallowayNNBM2012-01	In Curation Queue	pdurham	4/30/2013	4/30/2013			
NR1251	NRCWE_UCFV_HC_UC_SST-NJacobsenEMM2008-02	In Curation Queue	jchild	4/30/2013	4/30/2013			
NR1253	JHU_KSU-JGallowayNNBM2012-03	In Curation Queue	pdurham	4/30/2013	4/30/2013			

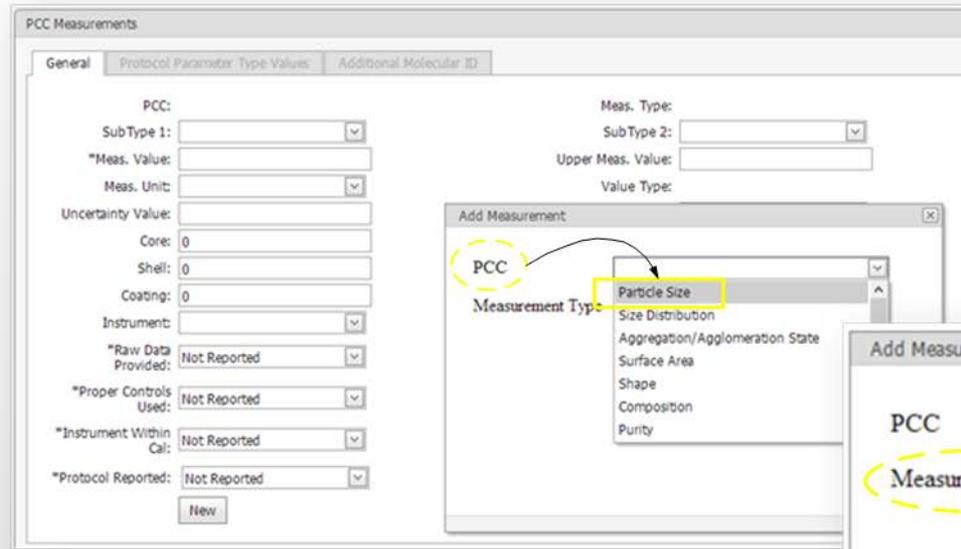
SEARCH and **SORT** options for data in queues

UPDATE information or change the status of a data record

Edit	Assign	Delete

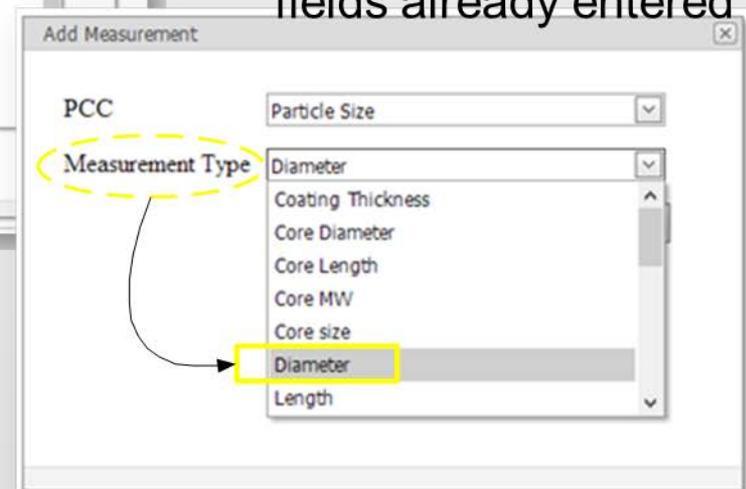
Systematic Data Archiving: *DATA CURATION TOOL 2*

- ✓ **STEP 1: PCC** “Particle Size” is selected from a list of the 12 MIAN PCCs



An example of SMART CURATION:

- ✓ Drop downs in data entry fields are populated with selection lists that are valid according to the fields already entered



- ✓ **STEP 2: Measurement Type** drop down is populated with options relevant to “Particle Size”

Systematic Data Archiving: *DATA CURATION TOOL 3*

An example of SMART CURATION:

- ✓ **STEP 1: MEASUREMENT**
technique is selected from a list of options relevant to “particle size”
- ✓ **STEP 2: PROTOCOL** tab is populated with options relevant to “Dynamic Light Scattering”

✓ STEP 2

*Protocol	*Value	Unit	#
Temperature of Suspension	20	C	Edit New Delete
Sonication/Milling Time	0	minutes	Edit New Delete

✓ STEP 1

PCC Measurements

General | **Protocol Parameter Type Values** | Additional Molecular ID

PCC: Particle Size

SubType 1:

*Meas. Value:

Meas. Unit:

Uncertainty Value:

Core:

Shell:

Coating:

*Raw Data Provided:

*Proper Controls Used:

*Instrument Within Cal:

Meas. Type: Mean Diameter

SubType 2:

Upper Meas. Value:

Value Type: Free Text

Uncertainty Unit:

ComponentID:

Technique:

Instrument:

*# of Replicates:

*Standard Pub. Citation:

*Modification Desc:

Evaluating the Information

Compliance Level 1

The Nanomaterial Registry's **COMPLIANCE LEVEL FEATURE** provides a **METRIC** on the **QUALITY** of characterization of a nanomaterial entry

Compliance Level	Score	Medal
Gold	76-100	
Silver	51-75	
Bronze	26-50	
Merit	0-25	

COMPLIANCE LEVELS are broken into **MERIT, BRONZE, SILVER, and GOLD** and represent increasing quality of characterization based on our evaluation criteria

$$CL_{IPCC} = \sum_{i=1}^M \frac{W_i}{(M * N)}$$

A COMPLIANCE LEVEL SCORE is a quantitative value calculated by assigning a weight (W) to each value reported in the curated entry (M)

Evaluating the Information

Compliance Level 2

- **COMPLIANCE LEVEL WEIGHTING FACTOR IS HIGHER WHEN:**

- Terms with **greater specificity** are used
- **Well-established techniques** are used
- **Protocols are adequately described**
- **Standard protocols** are used
- Values are measured with **multiple techniques**
- **Good laboratory practices** are reported

Example: Particle Size reported as

- **Diameter**
- **Mean aerodynamic diameter**

$$CL_{IPCC} = \sum_{i=1}^M \frac{W_i}{(M * N)}$$

Example:

- **Instruments within calibration and proper controls were used**
- **replicate measurements were taken**

Evaluating the Information

Compliance Level 3

	 MERIT	 BRONZE	 SILVER	 GOLD
<i>Particle Size</i> 37.5 nm				
<i>Reported as</i> Mean Hydrodynamic Diameter				
<i>Technique</i> Dynamic Light Scattering				
<i>Instrument</i> Malvern Zeta Sizer Nano ZS				
<i>Measurement parameters</i> 11 out of 12 reported				
<i>Protocol</i> ASTM E2490-09				

COMPLIANCE LEVEL
is higher when more
Meta-data about a
characterization are
reported

Evaluating the Information

Compliance Level on the Registry

COMPLIANCE LEVEL for individual characterizations are displayed

	COMPLIANCE LEVELS											ENVIRONMENTAL INTERACTIONS	
	PCC COMPLIANCE	PARTICLE SIZE	SIZE DISTRIBUTION	AGGREGATION / AGGLOMERATION STATE	SURFACE AREA	SHAPE	COMPOSITION	PURITY	SURFACE CHARGE	SURFACE CHEMISTRY	SURFACE REACTIVITY		SOLUBILITY
NR1012 - Au NP	Gold					Gold			Gold				No
NR965 - Au NP	Gold	Gold	Gold	Gold	Gold	Gold	Gold	Gold	Gold	Gold	Gold	Gold	No
NR812 - Au NR	Gold	Gold		Gold		Gold	Gold				Gold		No

✓ On the SEARCH RESULTS page

✓ On the DETAILS PAGE

NR965

NR Descriptor: Au NP
 Information for this nanomaterial was curated from [National Institute of Standards and Technology](#)
Original Publication(s): Not reported
 Information reported: PCC Characterization? Yes ▲ Environmental interactions? No Biological interactions? No

Overall PCC Compliance Level: Gold

Particle Size	Gold	Size Distribution	Gold	Aggregation/Agglomeration State	Gold	Surface Area	
Shape	Gold	Composition	Gold	Purity		Surface Chemistry	
Surface Charge	Gold	Surface Reactivity		Solubility		Stability	Gold

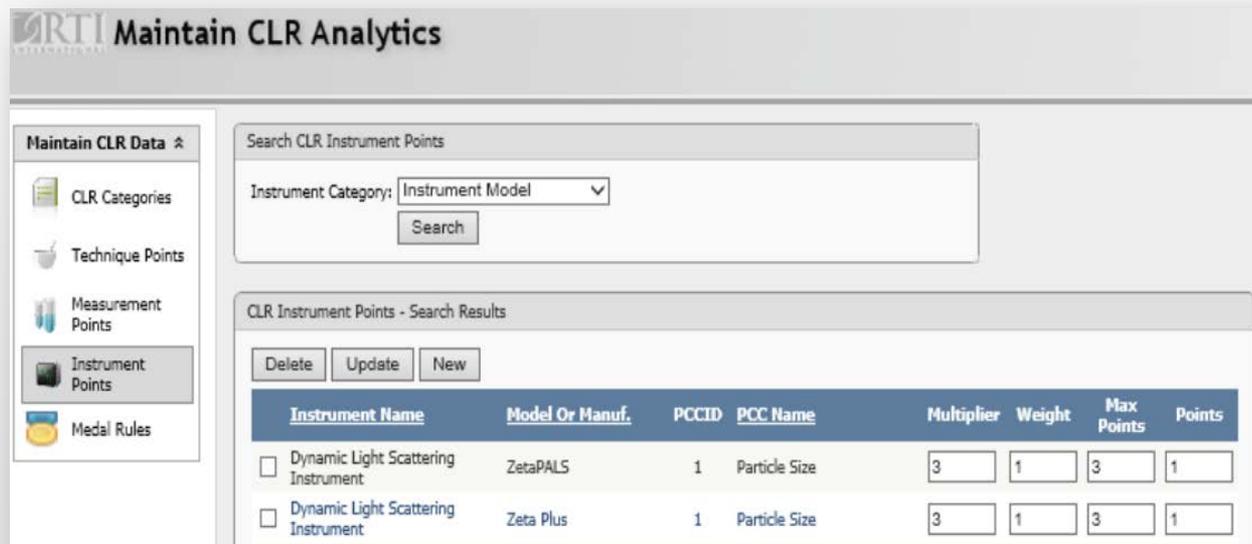
Evaluating the Information

Compliance Level - work is ongoing

The **COMPLIANCE LEVEL** was designed as a **FLEXIBLE** tool

Implementation of new algorithms can be tested on actual data sets

As terminology, standards, and techniques become relevant and/or obsolete, the terms and weighting factors behind the *compliance level score can be updated.*



Maintain CLR Analytics

Search CLR Instrument Points

Instrument Category: Instrument Model

Search

CLR Instrument Points - Search Results

Delete Update New

Instrument Name	Model Or Manuf.	PCCID	PCC Name	Multiplier	Weight	Max Points	Points
<input type="checkbox"/> Dynamic Light Scattering Instrument	ZetaPALS	1	Particle Size	<input type="text" value="3"/>	<input type="text" value="1"/>	<input type="text" value="3"/>	<input type="text" value="1"/>
<input type="checkbox"/> Dynamic Light Scattering Instrument	Zeta Plus	1	Particle Size	<input type="text" value="3"/>	<input type="text" value="1"/>	<input type="text" value="3"/>	<input type="text" value="1"/>