Recent ASTM Meeting & Actions Going Forward

1 December 2016

Fred Klaessig

nanoWG Presentation

Agenda

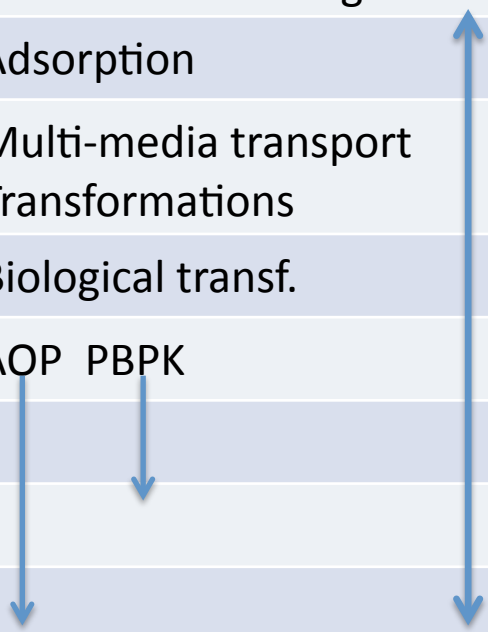
- Mix of review and discussion
- Review of interactions between ASTM and Nanoinformatics Roadmaps
- Status of ASTM ‘minimum ontology’ proposal
- Discussion of best means of identifying a “neutral, core, basic, minimum” ontology that is extendable to NPO, eNanoMapper, etc.
- Likely to involve comparisons among ontologies relative to their purposes

October Rheinfelden Input

- Suggested a map of particle history (life cycle) for orienting roadmap components
- Discussed issues of ‘nanoform’ (nanoscale form in U.S.) and visualizing coatings & layers
- Outlined four pilot projects
  - Dissolution
  - Informatics infrastructure (pertinent to ASTM)
  - Training in informatics
  - Database resources and access
  - AOP’s (added after Rheinfelden)

Particle Journey; Models; & Roles

Models	Stages	EHS
Process & Performance	Particle	Manufacturer/Distributor
Materials Modeling QSAR Cheminfo Modeling ATS	Properties	Performance
Adsorption	Formulation Interactions	Processor/formulator
Multi-media transport Transformations	Fate/Exposure	Inhalation/oral/dermal Air/water/soil
Biological transf.	Test Media Interactions	Protein or Env. corona
AOP PBPK	Receptor	Uptake/biodistribution
	MIE	In organism/cell
	Response	Cellular Mechanism
	Outcome	Whole animal
	Population	



Overlap with ASTM Proposals

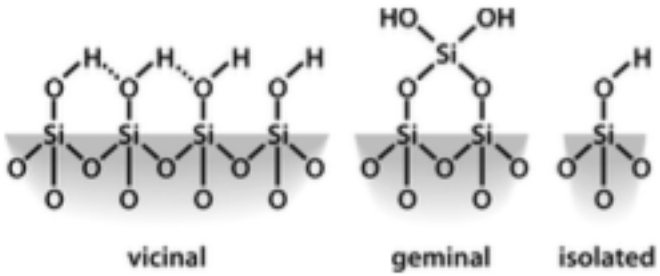
1. Minimum Particle Ontology to provide a simplified base case for ISA-TAB-nano
2. Instances of Characterization to define life cycle stages (location, use, time) where particle property changes may be significant
   - Labels to coordinate across studies/disciplines
   - Provide guidance on appropriate metadata
3. Both related to 2011 Nanoinformatics Road-map (core ontology & minimum information)

Background Context

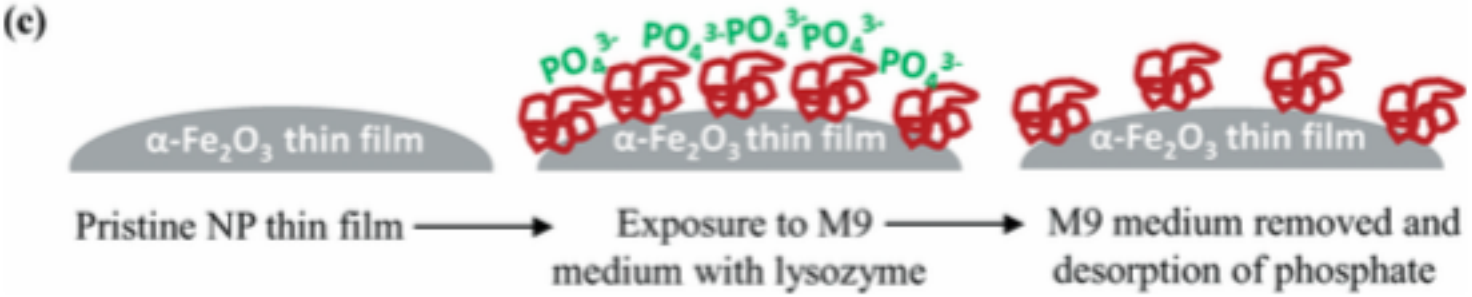
- Europe and US moving towards differentiating particle ‘forms’ based on surface chemistry
- Coatings are durable, surface layer composition may change with journey
- Offer a core ontology readily translatable into NPO, eNanoMapper, etc.
- Plain language directing user to acceptable definitions, metadata requirements etc. in order to meet local requirements

Surface Species

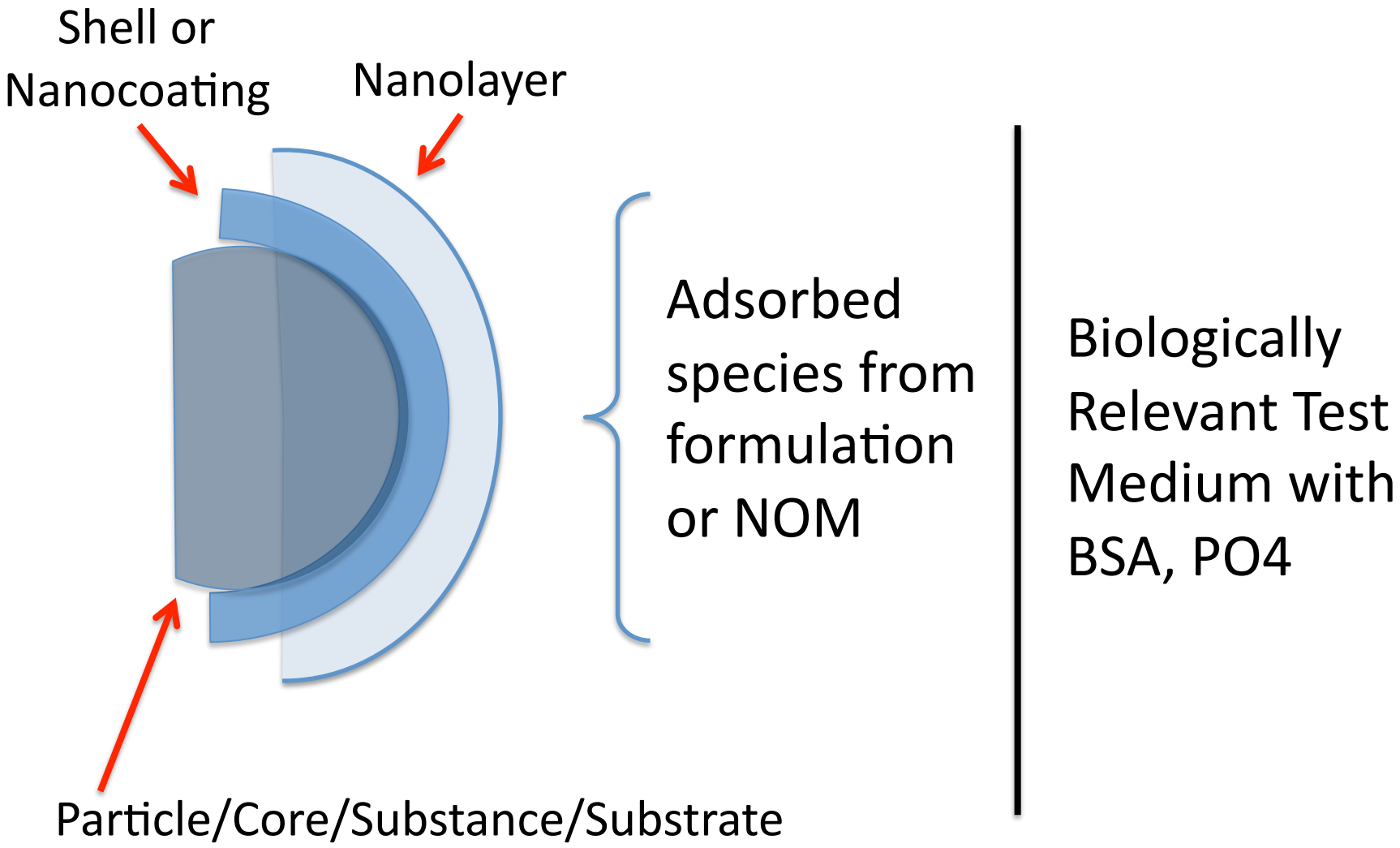
Scheme 2. Types of Silanol Groups That Can Exist on the Amorphous Silica Surface



1. Surface area, not stoichiometry
2. Not the molecular identity
3. Reversible-to-Irreversible
4. Inner sphere to outer sphere
5. Coating or layer or both



Particle Surface Regions



Minimum Ontology

1. **Nanoparticle Ontology is well suited to drug delivery; less so to 'industrial' particles, e.g. silica.**

2. **ASTM standard on ISA-TAB-nano leaves ontology choice open**

3. **UDS ontology for nano-object would serve as a base version compatible with the NPO**

4. **Would modify surface description to reflect emerging definition of nanoform (Europe) and nanoscale form (US-EPA)**

5. **UDS would be one source of parameters for the categories**

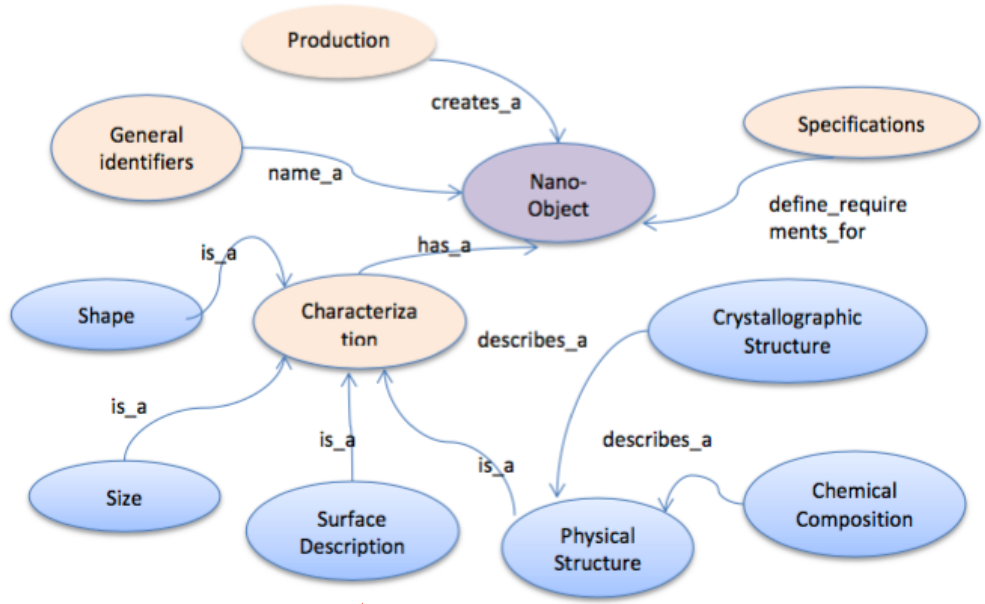
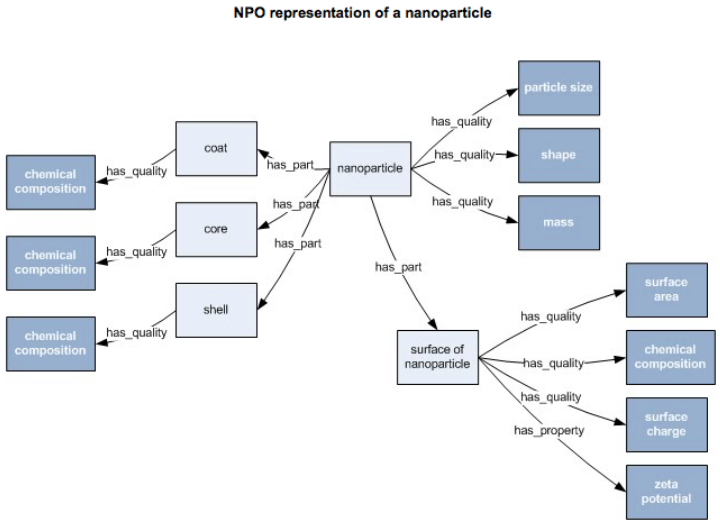


Figure 4. Information categories for describing an individual nano-object

Surface description should align with nanoform definition and instances of characterization

Comparability Needed



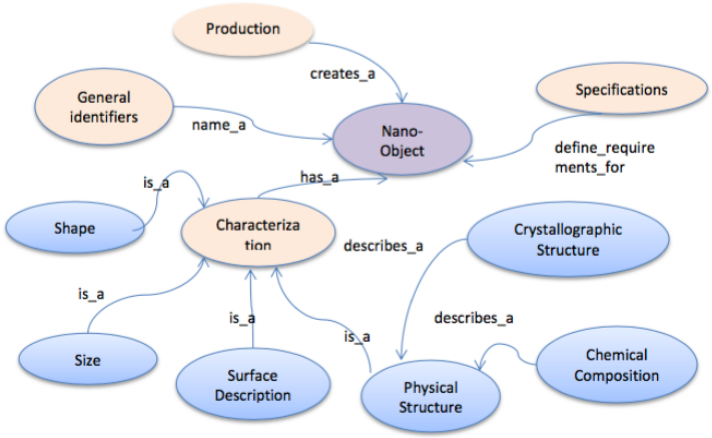
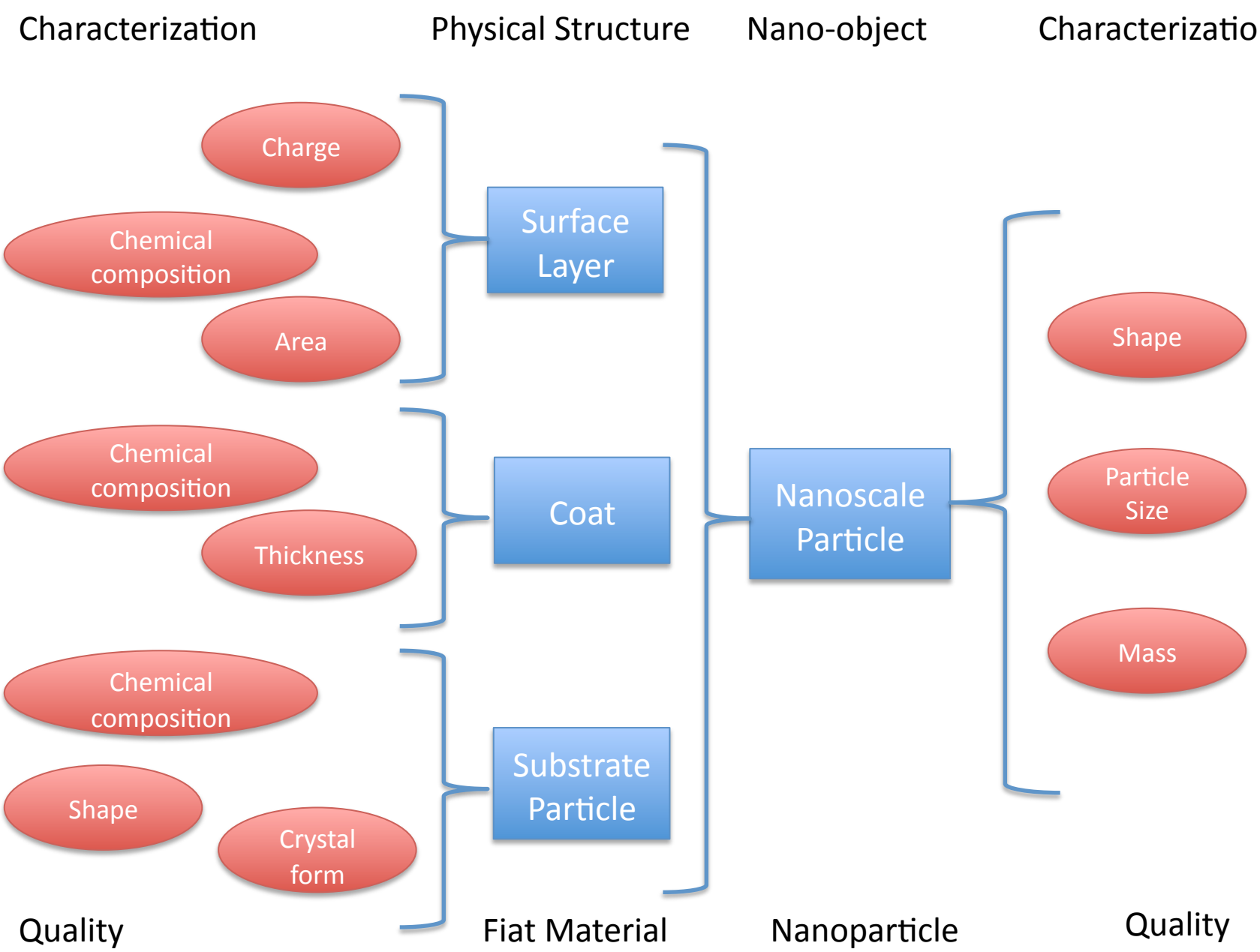


Figure 4. Information categories for describing an individual nano-object


Characterization
Physical Structure
Nano-object
Characterization
Charge
Chemical composition
Area
Surface Layer
Chemical composition
Thickness
Coat
Chemical composition
Shape
Crystal form
Substrate Particle
Nanoscale Particle
Shape
Particle Size
Mass
Quality
Fiat Material
Nanoparticle
Quality

NPO Drill Down

	Entity					
Entity	Continuant	Entity				
Continuant	Dependent Continuant	Continuant				Entity
Dependent Continuant	Specifically dependent continuant	Dependent Continuant				**Continuant**
Specifically dependent continuant	**Quality**	Specifically dependent continuant	Entity	Entity		Independent Continuant
Quality	Individual Quality	**Quality**	Continuant	Continuant	Entity	**Material entity**
Individual Quality	General Indiv. Quality	Individual Quality	Independent Continuant	Independent Continuant	Continuant	**Chemical entity**
General Indiv. Quality	Ind. Gen. Individ. Quality	General Indiv. Quality	Material entity	Material entity	Independent Continuant	particle
Ind. Gen. Individ. Quality	Physical State	Ind. Gen. Individ. Quality	**Fiat Material Part**	**Fiat Material part**	**Material Boundary**	Primary particle
Shape	Crystalline State	Chemical Composition (coat, surface, core)	Core	Coat	Surface of Nanoparticle	Nanoparticle
Shape	Crystal form	Chemical Composition	Particle substrate	Coat	Surface Layer	Nanoscale particle

eNanoMapper Drill Down

						Entity
						Material entity
	Entity	Entity	Entity	Entity		**Molecular entity**
Entity	**Quality**	**Quality**	Material entity	Material entity		particle
Quality	Chemical Substance Quality	Molecular entity quality	**Fiat material part**	**Fiat material par**t		Primary particle
Shape	Crystalline State	Composition (coat, surface, core)	Core	Coat		Nanoparticle
Shape	Crystal form	Chemical Composition	Particle substrate	Coat	Surface Layer	Nanoscale particle

Comparability

- An independent **continuant** that is spatially extended whose identity is independent of that of other entities and can be maintained through time. (eNano)
- Any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer etc., identifiable as a separately distinguishable entity. (eNano)
- A material entity which can be identified as an atom, ion, isotope, molecule/compound **or particle**. (NPO)
- A molecular entity is any molecule, ion, ion pair, radical ion, complex, conformer,etc., identifiable as a separately distinguishable entity. (separate category in NPO)

1. Continuant is in NPO; absent in eNanoMapper, but it appears in material entity
2. Material entity differs between the two, but particles are not molecules and both ontologies mix the two.
3. Overlapping of shell, core, coat, surface, surface treatment, etc.
4. Entity has as many meanings as structure

Proposed Actions

- John Rumble & I have had exchanges, which combine UDS, ISO, ASTM & nanoWG experience
- nanoWG to be a sounding board discussing a neutral ontology and translation key to others
- Use ~5 particle examples for comparison
- Merge ‘product’ into ASTM workspace discussions
- ‘Comparability’ with ASTM, ISO and ISA-TAB-nano terminology concepts

Particle Examples

- Suggest
  - NANoREG/OECD/Commercial
  - Done in NPO → map to eNanoMapper
  - Done in eNanoMapper → map to NPO
- Commercial examples:
  - Silica has Si-OH silanol groups on surface
  - Hydrophobic silica has Si-OH and methyl
  - Pigment grade is $Ti_{0.996}Al_{0.04}$ dioxide with Al_2O_3 coating