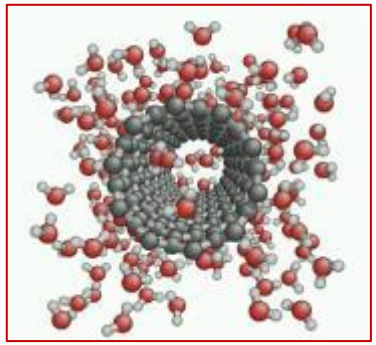
Increasing the Robustness of Nanoinformatics Resources:

The CODATA-VAMAS Uniform Description System (UDS)



John Rumble

Steve Freiman

Clayton Teague

CODATA-VAMAS Working Group on Nanomaterials

Why A Uniform Description System for Nanomaterials?

Many Disciplines

- Physics
- Chemistry
- Materials Science
- **Food Science**
- **Nutrition**
- **Toxicology**
- Ecology
- Environmental Science
- Pharmacology
- Medicine
- Biology

Many Users

- Researchers
- Product Developers
- Regulators
- Physicians
- Pharma
- Legislators
- Purchasers of nanom'tls.
- Sellers of nanomat'ls.
- Many more

Need to be able to communicate accurately about which nanomaterial is under discussion

Who Is Participating

- International Council of Science (ICSU) (funding)
- CODATA - ICSU Committee on Data for Science and Technology
- VAMAS – International materials prestandardization organization organize workshop to survey issues
- 13 international unions participating
  - IUFoST – International Union of Food Science and Technology
  - IUNS - International Union of Nutrition Science
  - IUTOX – International Union of Toxicology
  - IUPAC – International Union of Pure and Applied Chemistry
  - IUCr – International Union of Crystallography
  - 8 others

- **Joint CODATA-VAMAS Working Group on Nanomaterials**

Why an Accurate Description Is Needed

Surface charge of gold nanoparticles mediates mechanism of toxicity: N. M. Schaeublin et al, *Nanoscale,* 2011,**3,** 410

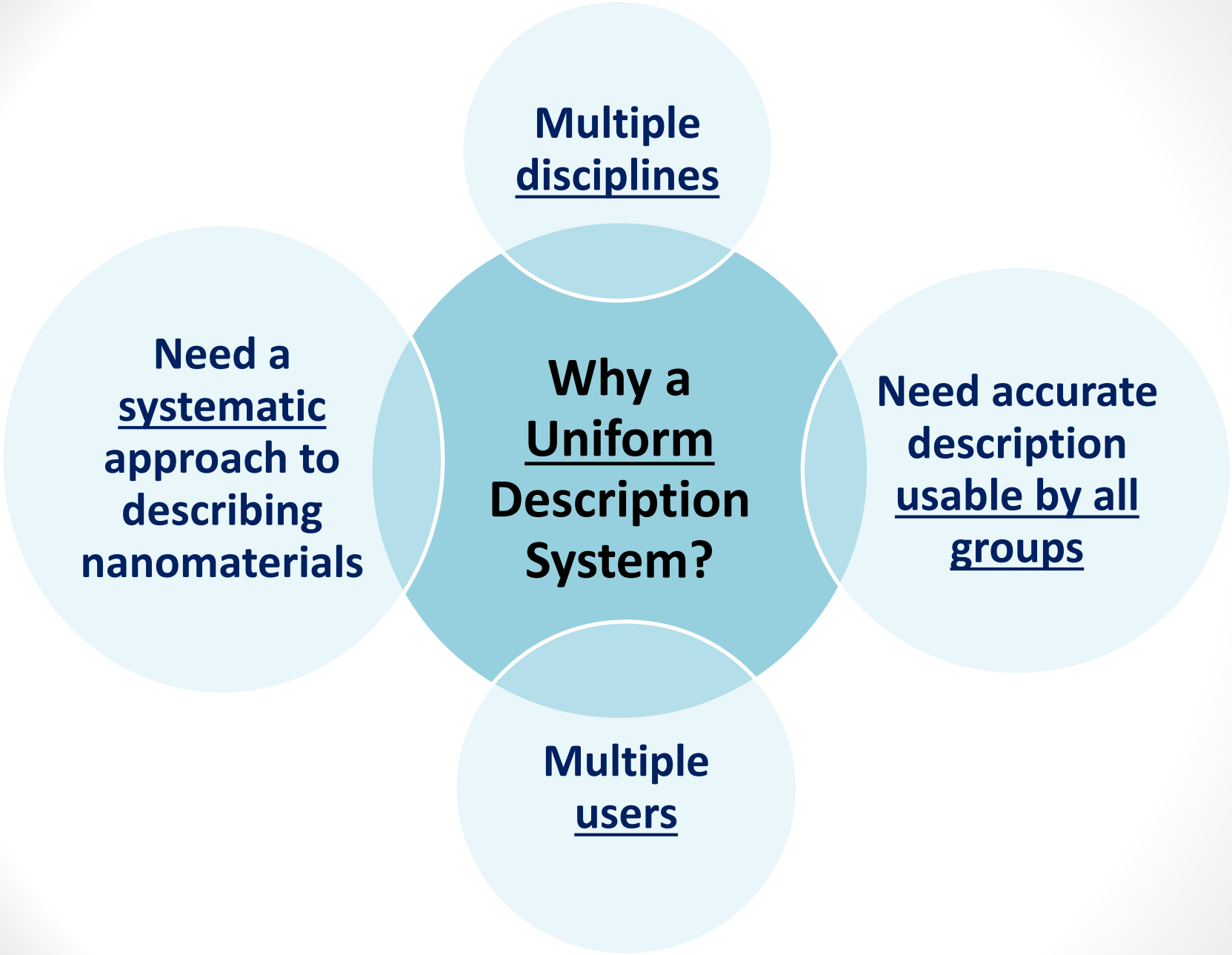
- "surface charge is a major determinant of how Au NPs impact cellular processes"

Does **Shape** Matter? Bioeffects of Gold Nanomaterials in a Human Skin Cell Model" N. M. Schaeublin et al, *Langmuir*, 2012, **28**, 3248

- "agglomerates had a smaller fractal dimension (D_f = 1.28 ± 0.08) (i.e., loosely bound) and were found to be cytotoxic to the HaCaT cells"
- "conclude that shape appears to play a key role in mediating the cellular response to AuNMs"

The effect of **particle size** on the cytotoxicity, inflammation, developmental toxicity and genotoxicity of silver nanoparticles**:** M. V.D.Z. Park et al, Biomaterials, 2011, 32, 9810

- potency of silver in the form of nanoparticles to induce cell damage compared to silver ions is cell type and size-dependent


Multiple disciplines
Need a systematic approach to describing nanomaterials
Why a Uniform Description System?
Need accurate description usable by all groups
Multiple users

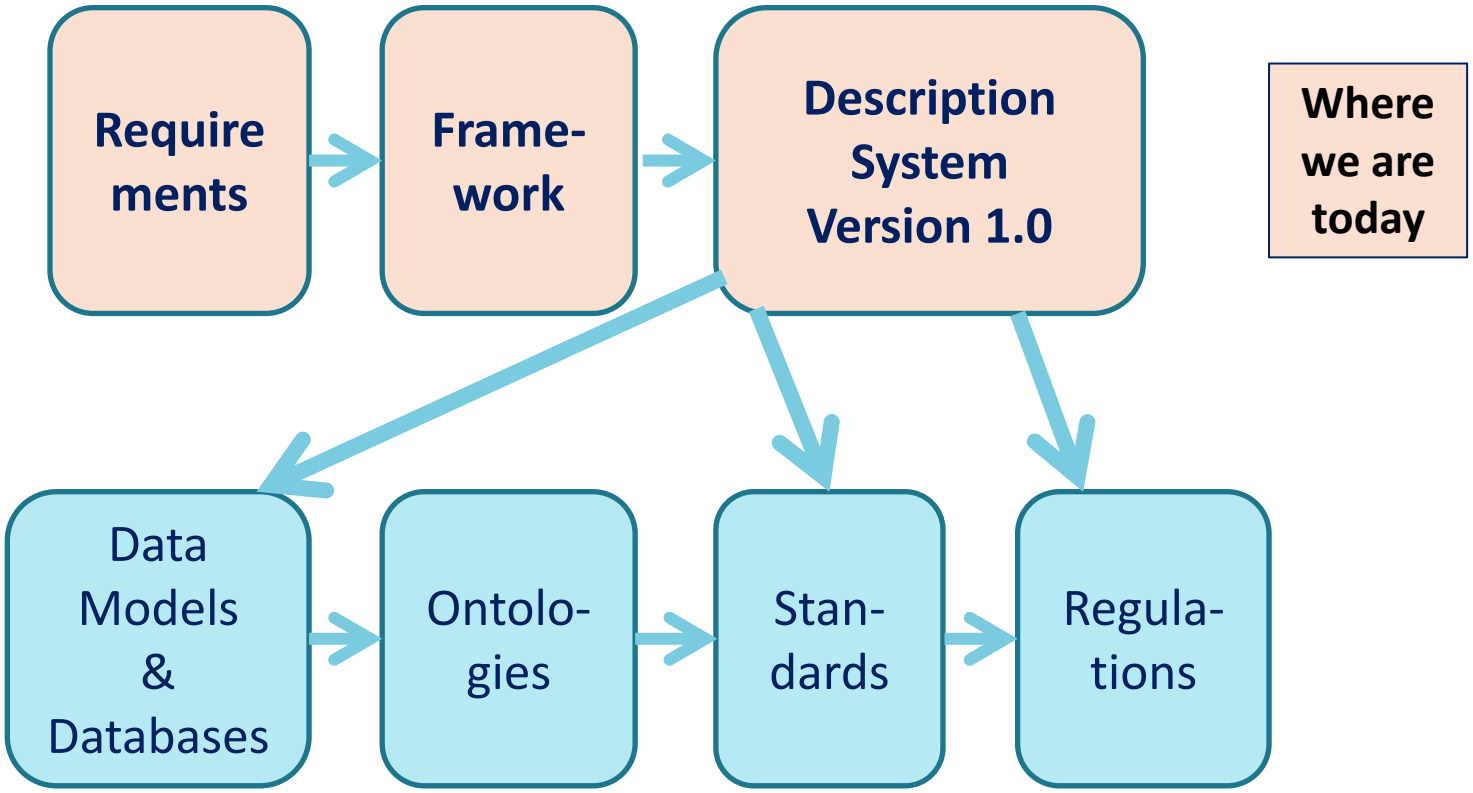
What Types of Nanomaterials

Four types:

- **Individual nano-object**
- **Collection of nano-objects**
  - **Identical components**
  - **Different components**
- **Nano-objects within a bulk material**
  - Bulk material that has nano-scale features

- **Covered in the UDS**

Path to and from the Description System



Initial Framework for a Uniform Description System

The Framework for the Uniform Description System comprises a set of four major information categories

- **General identifiers**
- **Characterization**
- **Life cycle history**
- **Specifications**

Information Categories

Individual Nano-Object	Collection of Nano-objects
Shape	Composition
Size	Physical structure
Chemical composition	Interfaces
Physical Structure	Surface description
Crystallographic structure	Size distribution
Surface description	Stability
	Topology

How Can The UDS Be Used

- Support data preservation
- Facilitate data Reuse
- Assess data quality
- Enable knowledge discovery

Data Preservation

- As measurement techniques mature, saving property data for nanomaterials becomes more important
- Data repositories, databases, data supplements to journal articles

- **Need complete documentation about nanomaterial measured, including its production information**
- UDS provide detailed descriptors that need to be reported when depositing data for preservation

- Hopefully preservation resources adopt same standards

Data Reuse

- No one resource will have all available data on nanomaterials
  - Too expensive, conflicting mandates, public vs private data resources, etc.
- Users will need to access and combine data from multiple resources as well as data generated at different times and by different groups

- **UDS provides a mechanism for ensuring data fields are consistent and comparable across data resources**
- If that is the case, users will have confidence that data sets can be meaningfully combined

Assessment of Data Quality

- Reference property data are possible when measurement technology has progressed to show all relevant independent variables are identified and controlled
- Data quality assessment is evaluation of how close that condition is met

- **UDS provides a framework for enumerating all relevant variables and evaluating whether a measurement has actually controlled them**
  - This process can take years.

Knowledge Discovery

- Discovering the relationship between one or more independent variables and some measurement result
- Can lead to new nanomaterials, or better properties, or both

- **UDS provides a mechanism for ensuring independent variables are defined and reported correctly**
  - Especially important when doing knowledge discovery across different data resources

Where We Are

- Review of Framework (2013) Three regional conferences
  - North America (April 2014)
  - Europe (April 2014)
  - Asia (September 2014)
- Version 1.0 of Description System released January 2015
- Period for public comments
  - Document freely available
  - www.codata.org/nanomaterials
  - Comments, suggestions, extensions welcomed