

# **A Uniform Description System (UDS ) for Materials on the Nanoscale**

**A Draft Framework**

**John Rumble**

**Steve Freiman**

**Clayton Teague**

# Why A Uniform Description System?

## 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

# Who Is Doing This and Why?

## 2011

- International Council of Science (ICSU) approached to help organize multi-disciplinary input to ISO TC229 and other groups
- ICSU asks CODATA to organize workshop to survey issues

## 2012

- CODATA-ICSU Workshop in Paris: consensus that diversity of needs, interested disciplines, and user communities generate need for uniform approach to describing nanomaterials
- CODATA and VAMAS establish joint working group

# Who is Doing This and Why?

## 2013

- Requirements survey done
- CODATA-VAMAS Workshop reviews draft Framework and makes many recommendations (May)
- Revised Framework released for Working Group review and public comments (October)

## 2014

- Three international (regional) conferences to be held
  - Europe (June)
  - Asia (September)
  - North America (December)
- Will discuss next steps at end of talk

# Goals of a Description System

- Develop a systematic approach to describing nanomaterials
- Define a complete set of information categories (descriptors) that can be used by all nanomaterial communities

# Purpose of the Description System

## Uniqueness

- Create a system that has the ability to differentiate one material from every other, and to establish which material is being described

## Equivalency

- Create a system that can establish that two materials are the same such that data sets from each material can be combined

# What makes a nanomaterial different ?

## Challenges in describing nanomaterials

- Surface to volume ratio increase leads to changes from “bulk” properties to surface dominated
- Surface electronic structures different than bulk
- Quantum size effects can occur
- May be dangling surface components
- Small amount of impurities can make a big difference
- Self-assembly of ordered nanostructures

# Framework Background

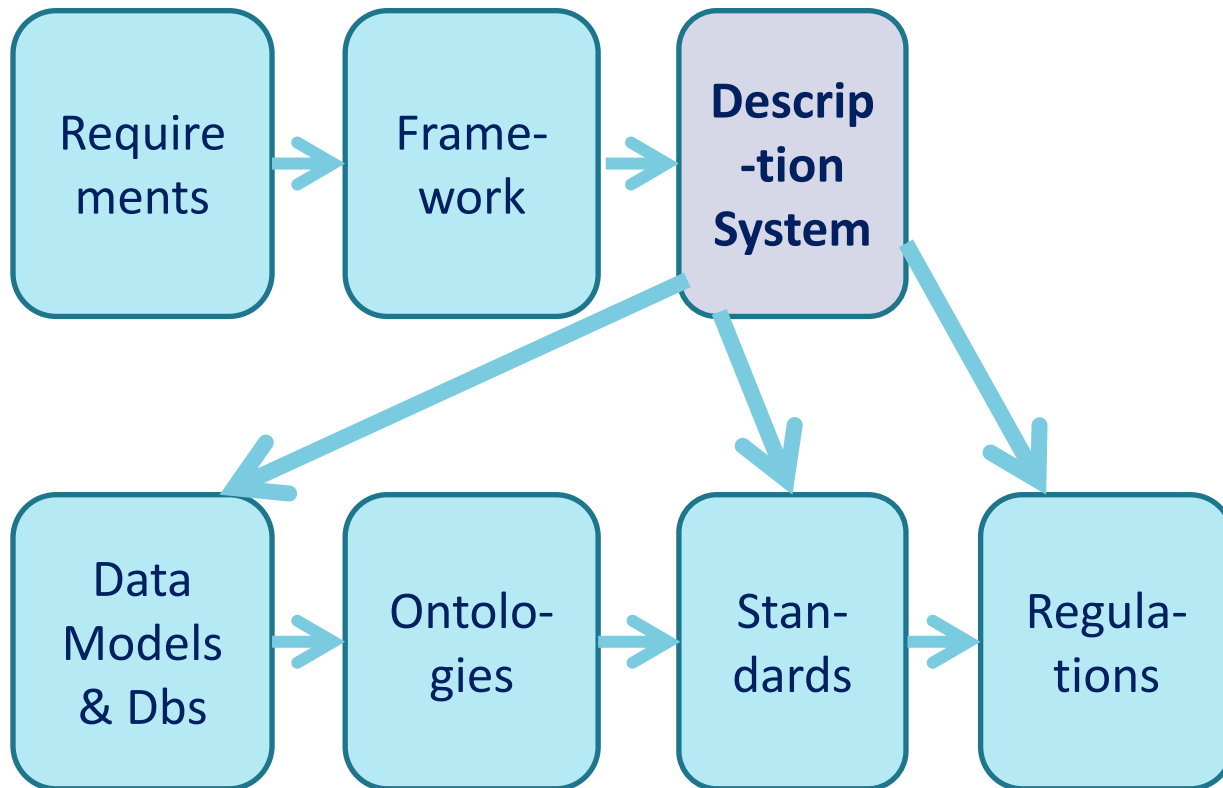
- The Framework relies heavily on that developed by ASTM Committee E49 on the Computerization of Materials Data

ASTM (1993) ASTM Manual on the Building of Materials Databases, Crystal Newton, Editor, ASTM Manual Series: MNL 19

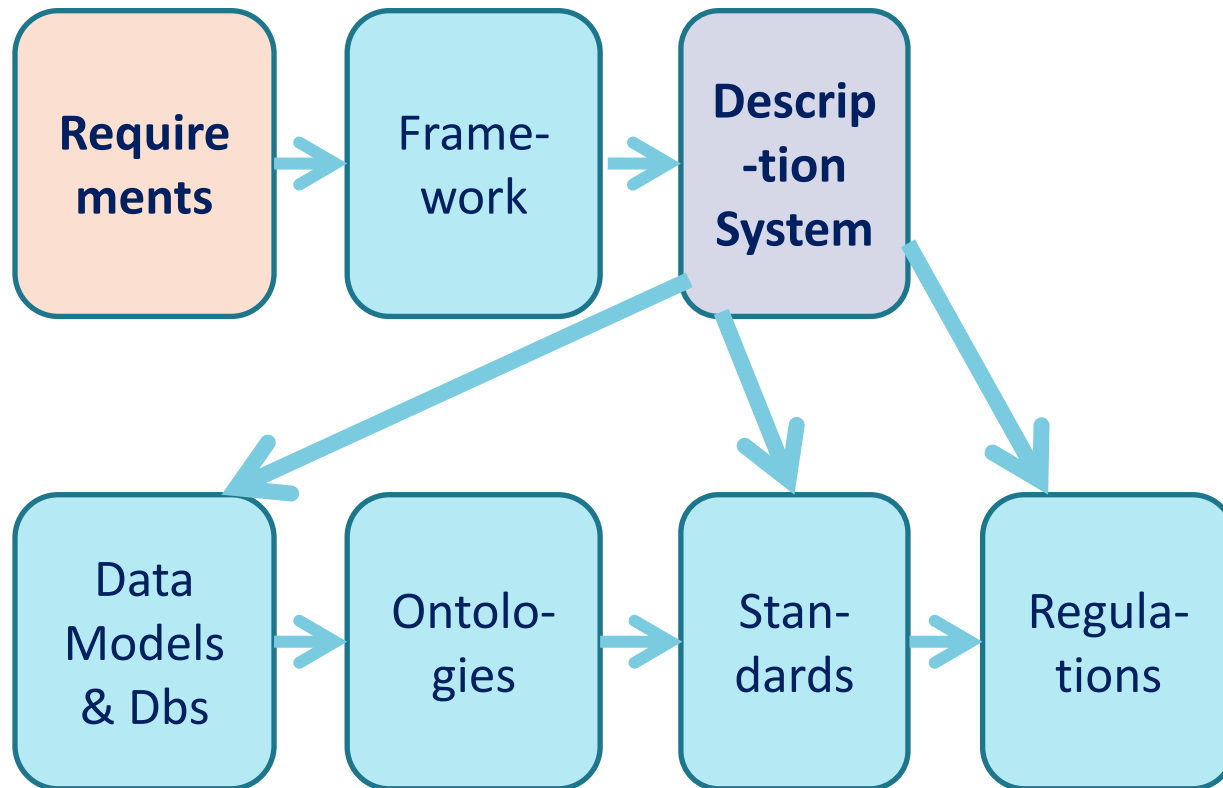
- Used in other materials description standards and approaches (MatML, ISO STEP, EU CEN/SERES)
- Starts with definitions from ISO TC229, OECD, EU, ASTM E-45 and others



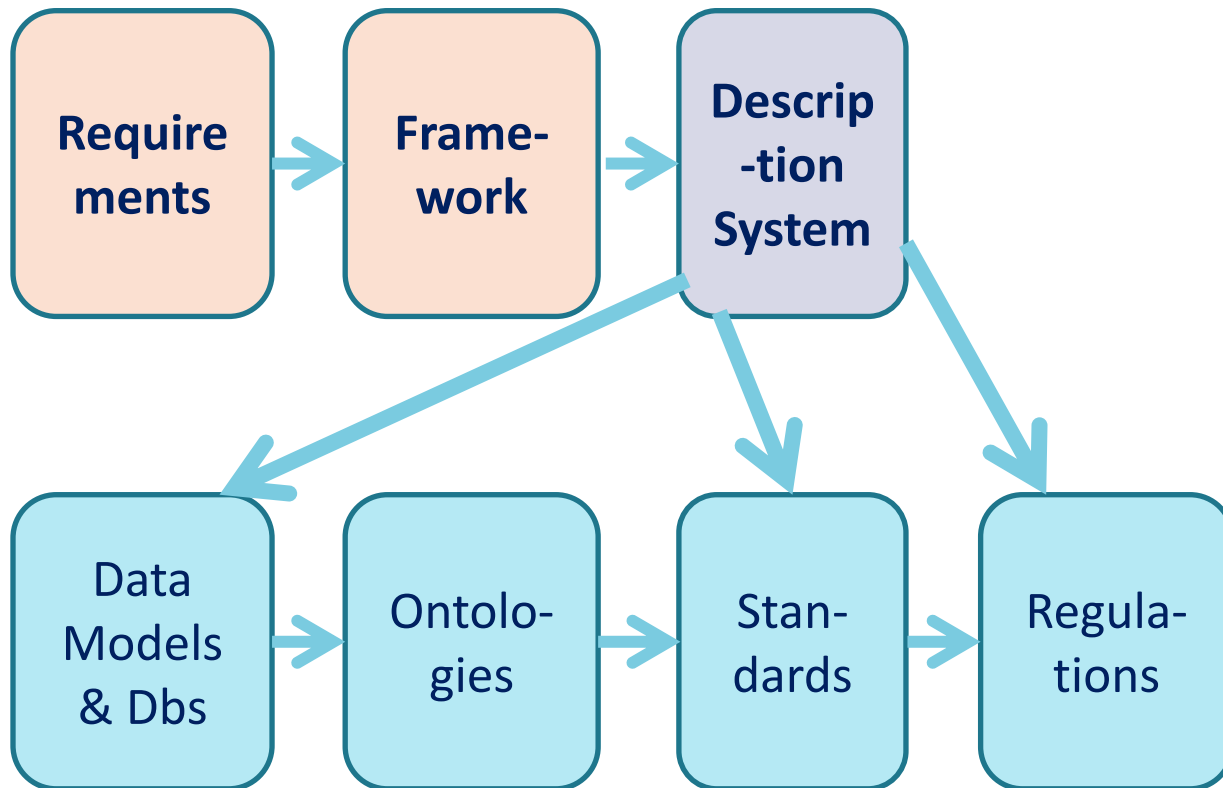
# Path to and from the Description System



# Path to and from the Description System



# Path to and from the Description System



# Some Key Definitions

- **Descriptor** – an item of information about an object (here a nanomaterial) that is measured, calculated, or assigned
- **Information category** – a group of descriptors that explain one aspect of a nanomaterial.
- An information category can be divided into one or more layers of subcategories for clarity or convenience in describing complex information

# Different Types of “Nanomaterials”

**We define three distinct nanomaterials situations:**

- 1. Individual nano-object**
- 2. Collection of nano-objects, which are called nano-products**
- 3. Bulk material that has nano-objects as components**

**Each type requires different set of descriptors**

# 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**

**Major Categories in  
the Framework for  
Uniform Description  
System**

**Nanomaterial  
Description  
Framework**

**General  
Identifiers**

**Characterization**

**Life Cycle  
History**

**Specifications**

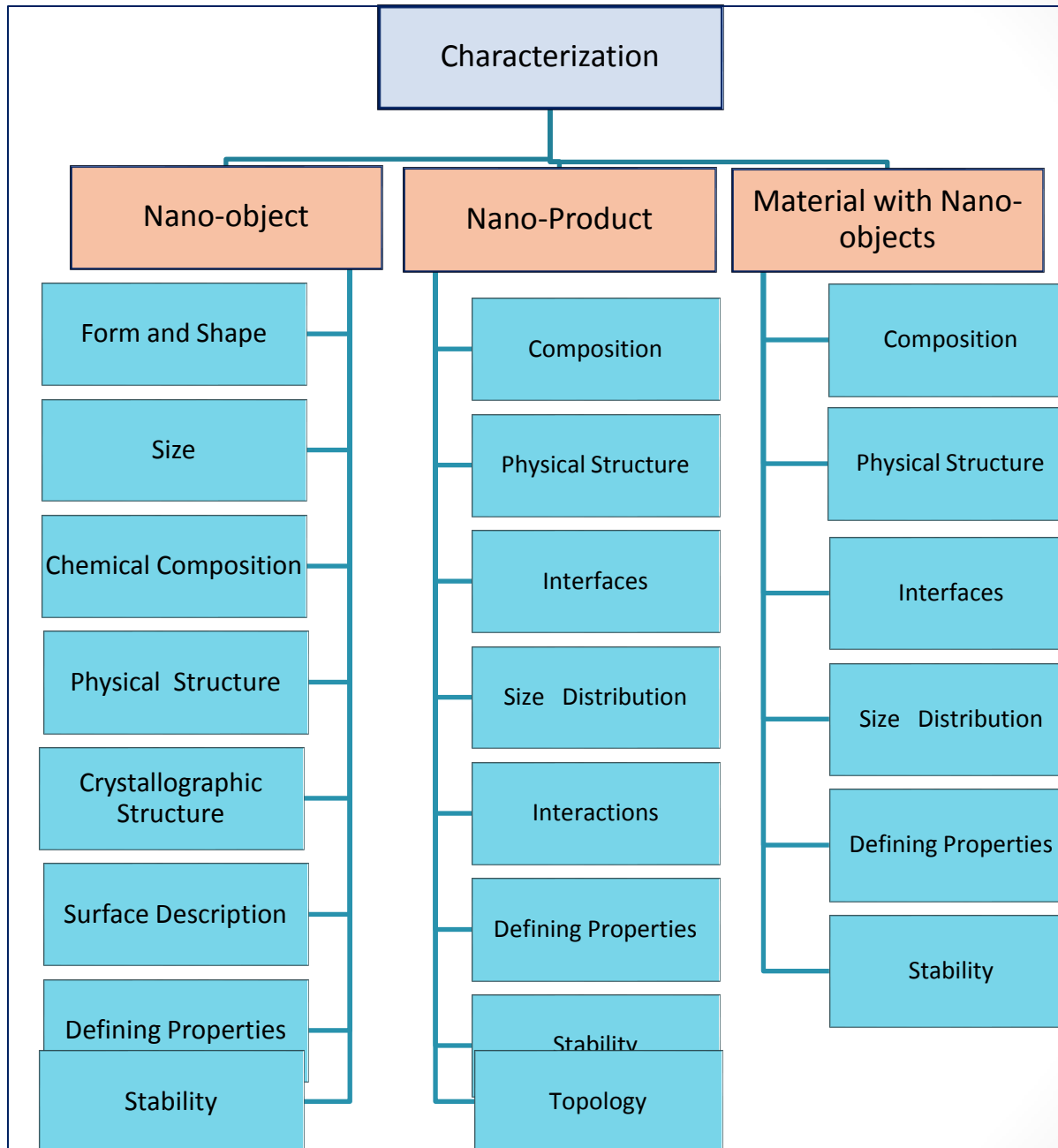
Nano-object

Nano-Product

Material with  
Nano-objects

Initial  
Production

Post- Production  
History





# What is Path Forward?

- Distribution of Framework
  - Now – to Working Group
  - Next week (?) – public distribution, WG Web site
  - [www.codata.org](http://www.codata.org)
- Public comments
  - Next few months
- Three regional conferences
  - Europe (June 2014)
  - Asia (September 2014)
  - North America (November 2014)

# Regional Conferences

- Purpose
- Get additional input
- Discuss how to populate various Framework categories
  - Already some groups have extensive work
  - TC229 for form & more, IUPAC for chemical naming, IUCr for crystallographic structure
  - Many areas have no activity – life cycle history, topology
- Identify areas where UDS needs extension for discipline/use specific reasons
- Intersection of uniform description system and nanoinformatics

# Summary

- **This Framework is the starting point for a more complete uniform description system**
- **Input from broad community is necessary**
- **To join Working Group or comment, contact [udsnano@udsnano.org](mailto:udsnano@udsnano.org)**