

# A Uniform Description System for Nanomaterials

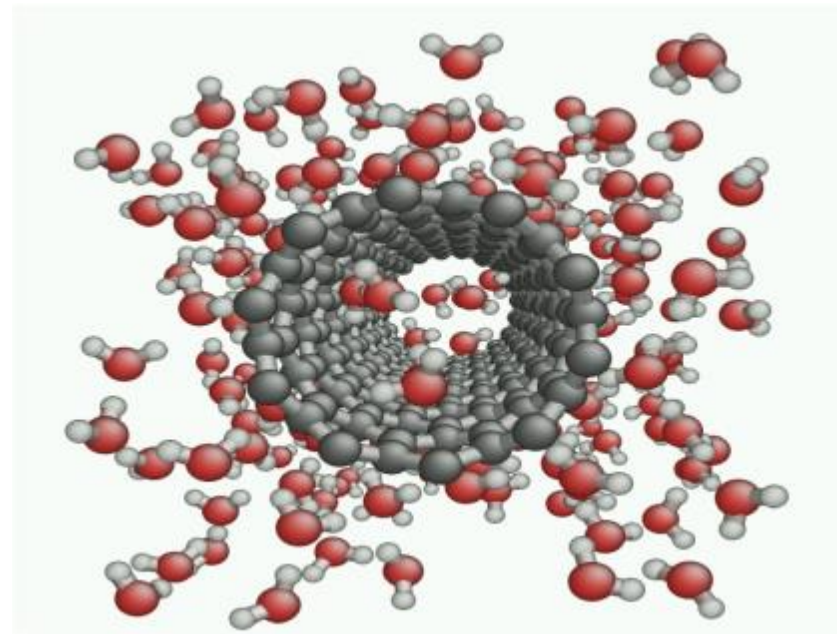
**CODATA-VAMAS Working  
Group on the Description of  
Nanomaterials**

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**Gaithersburg, MD**

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# CODATA

## Committee on Data for Science and Technology

**An interdisciplinary scientific committee of the International Council for Science (ICSU)**

### Mission

**To improve the quality, reliability, management and accessibility of data of importance in all fields of science and technology**

# VAMAS

- **Supports trade in products using advanced materials through pre-standards research**
- **16 Current Members: Australia, Brazil, Canada, China, Chinese Taipei, France, Germany, India, Italy, Japan, Korea, Mexico, South Africa, UK, USA, and the EC**

# Why a Description System for Nanomaterials?

## Motivation

- Chemical nomenclature is not enough
- Bulk materials descriptions cannot handle quantum and size effects
- Why care?

## Need method to

- Specify a specific nanomaterial (uniqueness)
- Correlate accurately a functionality (F) or property to a specific feature(s)
- $F = f(x_1, x_2, \dots, x_n)$
- If F is toxicity, critical to know which  $x_i$ s are important and describe them accurately

# Purpose of the Uniform Description System (UDS)

- **To describe nanomaterials accurately and effectively on an international, multi-disciplinary basis**
  - **To bridge the gap between chemistry (individual molecules) and bulk materials ( $10^{23}$  atoms)**
  - **Capture unique features of nanomaterials**
- **Build on work of ISO, OECD, IUPAC, IUCr, ASTM, others**
- **Prestandardization effort to be extended by SDOs and other groups**
- **Make it available widely available; put it in the public domain**

# UDS Works with both Nanomaterials Definitions

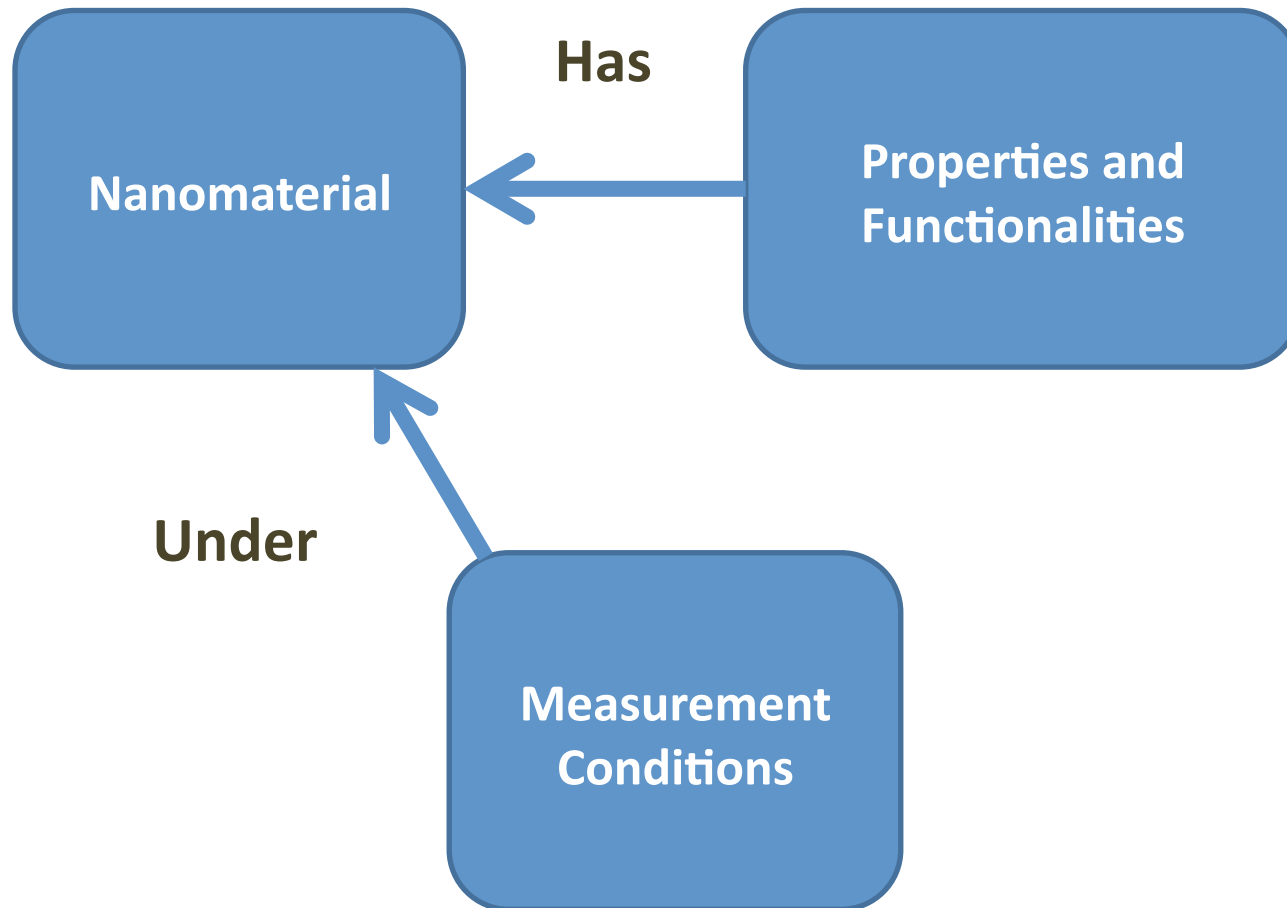
## **ISO TC229 definition of a *nanomaterial* :**

- ***“A Nanomaterial is a material with any external dimension in the nanoscale [approximately 1 nm to 100 nm] and or having internal structure or surface structure in the nanoscale.”***

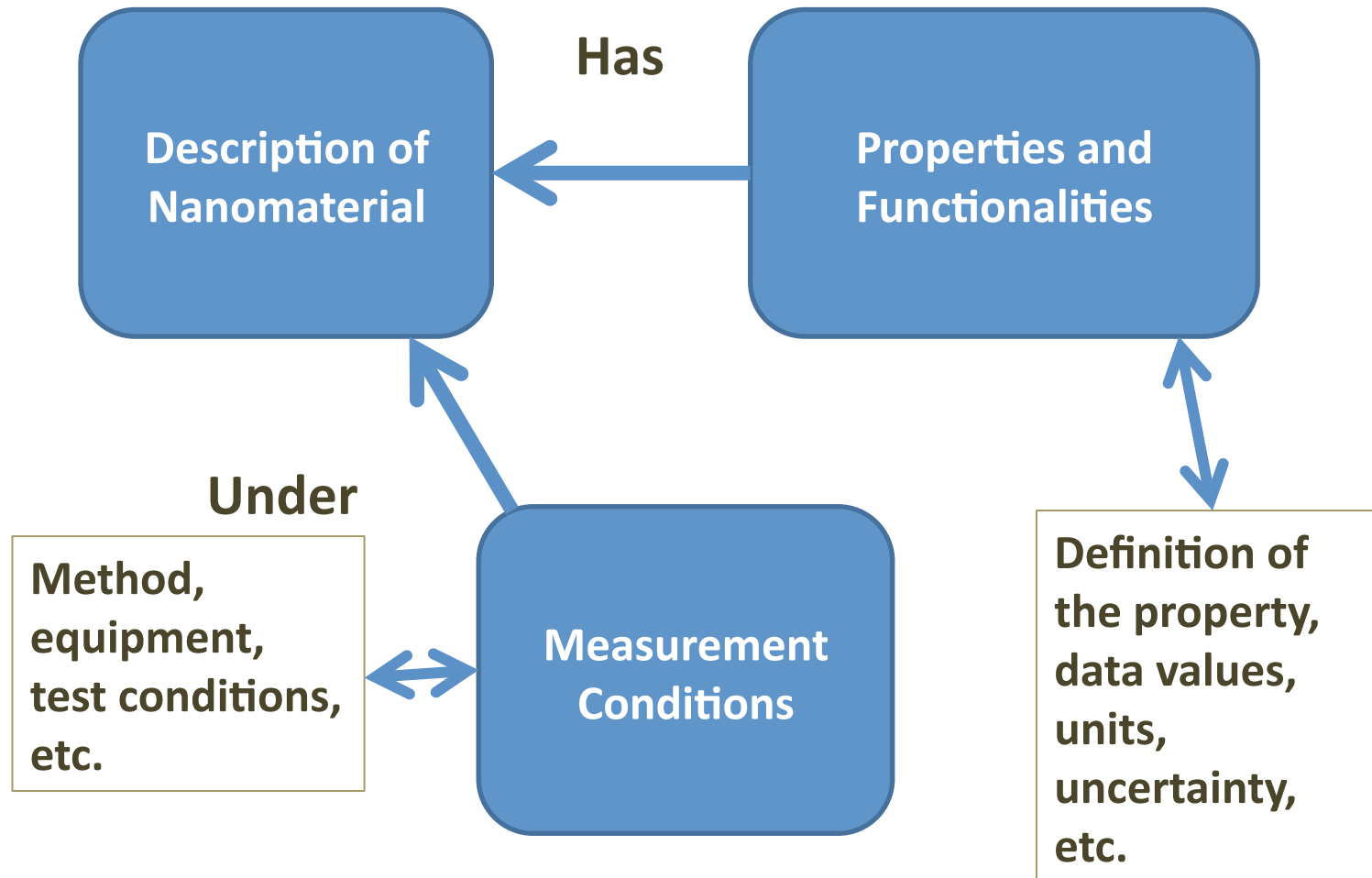
## **The European Commission definition of a *nanomaterial*:**

- ***“A natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50 % or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm - 100 nm.***
- ***“In specific cases and where warranted by concerns for the environment, health, safety or competitiveness the number size distribution threshold of 50 % may be replaced by a threshold between 1 and 50 %.***

# The Information Used for Reporting Data

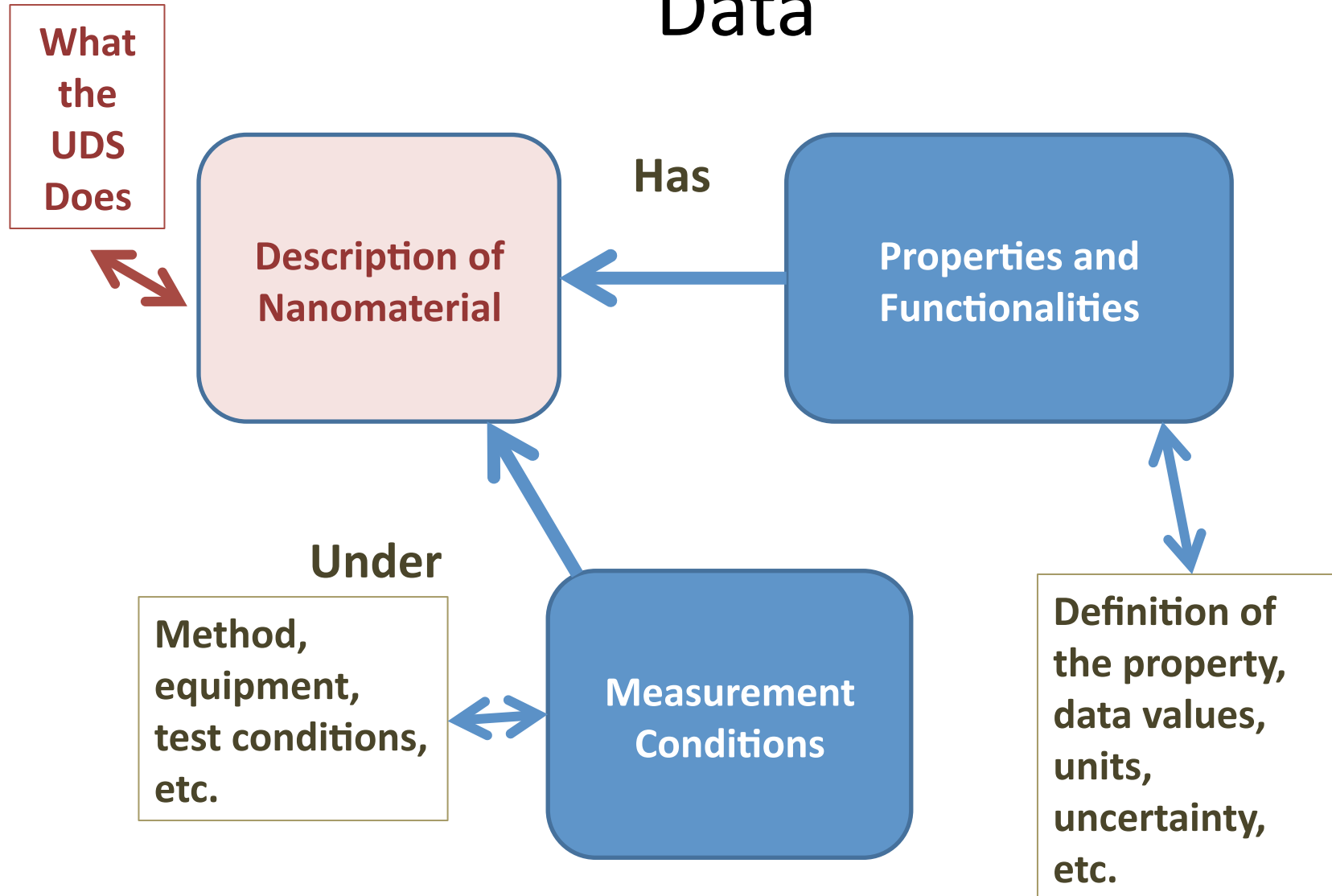


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# What does it mean to “identify” a nanomaterial?

- **Uniqueness:** The ability of a description system to differentiate one nanomaterial from all other nanomaterials and to establish which particular nanomaterial is being described within a broad range of disciplines and user communities
- **Equivalency:** The ability of a description system to establish that two nanomaterials, as assessed by different disciplines or user communities, are the same to whatever degree desired.

# Approach

## Reviewed work of

- **Nanotechnology committees  
ISO, ASTM, OECD**
- **Nanoinformatics resources  
(NPO, NMR)**
- **Materials data standards and  
databases**
- **Modeling of engineering  
information**
- **Survey of nano community**

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## Concluded

- **Must be systematic**
- **Use terminology nano-  
community understands**
- **Take advantage of existing  
work (IUCr, IUPAC, ISO)**
- **Break model into manageable  
pieces (ASTM E49, CEN/  
SERES, ISO 10303)**
- **Define things carefully**

# Using the Categories

- **Detailed descriptors** included in version 1.0 of the UDS
- **Use existing details** where exists
  - ISO TC 229 (shape), IUPAC (chemistry), IUCr (crystal structure), EU (size distribution), others
- **Some areas need extensive work** to define quantitative descriptors
  - Surface description, topology, physical structure, stability
- UDS can be used as **roadmap for identifying areas where better descriptions are required**

# Review and Future

**WG has involved over 80 experts from 15 countries**

- **14 international unions are members**
- **Representatives from ISO, ASTM, OECD**
- **Funding from International Council for Science (ICSU)**
  - **Travel and workshops**
- **Five international and regional workshops held**
- **Presentations at numerous conferences/blogs/etc.**
- **Available at [www.codata.org/nanomaterials](http://www.codata.org/nanomaterials)**

**Next steps**

- **This Workshop**
- **Publication after revision (NIST Practice Guide?)**
- **Standards Publication?**