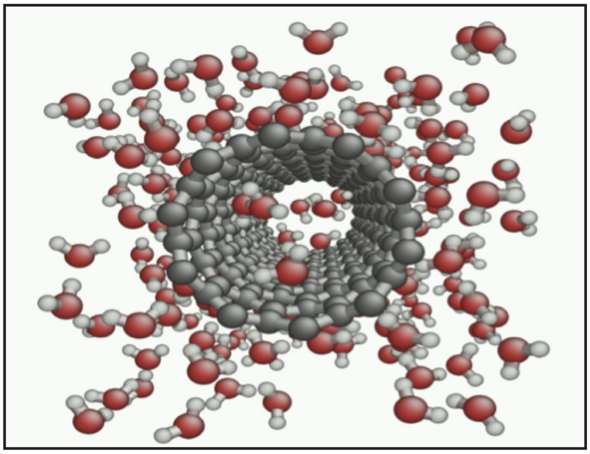
# Towards a Uniform Description System for Materials on the Nanoscale

*by John Rumble, Steve Freiman, and Clayton Teague*

**When is a chemical not a chemical? When is a material not a material? The answer to both questions can be considered the same: When the procedures and rules chemists and materials scientists have developed to describe those substances no longer work. One area where this occurs is in the world of nanomaterials.**



These substances, containing hundreds of thousands to hundreds of millions atoms (with leeway at both ends of that range), have rapidly evolved the potential to impact virtually every area of our physical world—health, food, engineering, transportation, energy. In many cases, nanomaterials are already part of our world.

Yet unlike chemical and "normal" engineering materials, there is no accepted way to describe nanomaterials such that we know exactly which nanomaterial is being discussed, reported on, regulated, bought, or put into a commercial product. Simple chemical nomenclature does not suffice—nanomaterials have solid-like aspects beyond normal chemistry. Systems used for engineering materials, such as ceramics, metals, and polymers, do not capture the nanoscale features of form, size, surfaces, etc., that impart special properties to nanomaterials.

Further, nanomaterials are the subject of intense interest in many disciplines, from chemistry, physics, and material science to food, medicine, and nutrition. The user communities are equally diverse, including researchers, product designers, purchasers, regulators, health experts, and many others. These users need to discuss and describe nanomaterials accurately. Nanomaterials themselves are not homogeneous except for their nanoscale size. Single-walled carbon nanotubes, quantum dots, titania nanoparticles, and thin film perovskites share little, except for their intriguing and exciting nanoscale-derived properties.

So what can be done to describe nanomaterials in a way that meets the needs of diverse scientific disciplines, user communities, and nanomaterials themselves? During the last three years, a CODATA [1]-VAMAS [2] Working Group (WG) on Nanomaterials has worked on a multidisciplinary, multi-user community, international basis to develop a Uniform Description System for Materials on the Nanoscale (UDS). Version 1.0 of the UDS was released 1 February 2015 and is publicly available for download, use, and comment at www.codata.org/nanomaterials.

The UDS has two primarily goals. The first is to describe nanomaterials uniquely, so that each is differentiated. The second is to determine when two instances of a nanomaterial are equivalent to whatever degree desired. The UDS was designed to meet both goals as well as to meet the needs of different disciplines and user communities for as many types of nanomaterials as possible. The CODATA-VAMAS WG is built on the work of many groups, including standards committees, database developers, and nanomaterials researchers.

Before describing the UDS in more detail, it is important to mention several import facets of the present version. As Chemistry International readers well know from the work of IUPAC nomenclature committees, a description system is never complete. As new substances are discovered and synthesized and new knowledge is discovered about the structure and function of these substance, description and nomenclature systems must be updated and extended. We anticipate the same for the UDS, especially as the field of nanomaterials is advancing so rapidly. New uses for a description system will also require changes. So the release of version 1.0 of the UDS is not the end of the process. Changes will be required and improvements suggested. The IUPAC community is well positioned to help with this process, and comments, suggestions, and improvements are welcomed.

## Definitions

**Nanomaterial:** There are two primary definitions of nanomaterial in wide use. The UDS applies to both definitions.

The ISO TC229 definition [3] of 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 [4] of a *nanomaterial* is: "*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 %."*

**Descriptor:** Numerical data or text that expresses the measurement, observation or calculational result of some aspect on an object.

**Information category:** a set or group of related descriptors that represent a property, characteristic, or feature of an object.

**Nano-object:** The ISO TC229 definition [5] of a *nano-object* is: *"A material with one, two or three external dimensions in the nanoscale".*

**Collection of nano-objects:** a group of two or more nano-objects that may function as a unit; a collection can be made of identical or different nano-objects.

**Bulk material:** A material that has all external physical dimensions larger than the nanoscale.

**Uniqueness:** The ability of a description system to differentiate one object (here a nanomaterial) from every other object (all other nanomaterials) and to establish which particular object (nanomaterial) is being described within the broad range of disciplines and user communities.

**Equivalency:** The ability of a description system to establish that two objects (nanomaterials), as assessed by different disciplines or user communities, are the same to whatever degree desired.

## Approach

The approach taken has been to identify the broad types of information used through the nanomaterials community to describe a nanomaterial as completely as possible. This approach was chosen so that the majority of the terms and concepts used in the description system are readily understandable to scientists, technologists, and lay persons involved in nanotechnology. The basic premise behind the Uniform Description System is that, unlike individual molecules, a nanomaterial cannot be uniquely specified by a simple, or even complex, name. Further, the description systems developed for metals, alloys, ceramics, polymers, and composites are also in an incomplete state for nanomaterials because of size, surface, shape, and other effects that significantly influence their properties. While simplistic terms such as "carbon nanotubes" or "quantum dots" convey important information, the identification of a specific nanomaterial requires more. For complete specificity, all relevant information categories must be used. Many situations require this level of specificity, including the development of regulations and standards, purchasing, and testing. One can imagine in the future a numbering system that traces back to specific values of the descriptors included in the information categories of the UDS.

The first step in the development of the UDS was a survey of a large variety of nanomaterial communities, including those representing medicine, toxicology, food science, chemistry, biology, etc., as to their needs, as well as the convening of a series of interactive workshops to obtain consensus on the approach. There were also interactions with standards committees such as ISO Technical Committee 229 Nanotechnologies [6] and ASTM Committee E56 on Nanotechnology [7] as well as groups such as the OECD Working Party on Manufactured Nanomaterials [8]. Based on this, a Framework was built for the information used by different disciplines in their nanomaterials work. The Framework integrates existing approaches that have focused on specific detailed aspects of nanomaterials, such as size, shape, structure, etc. The

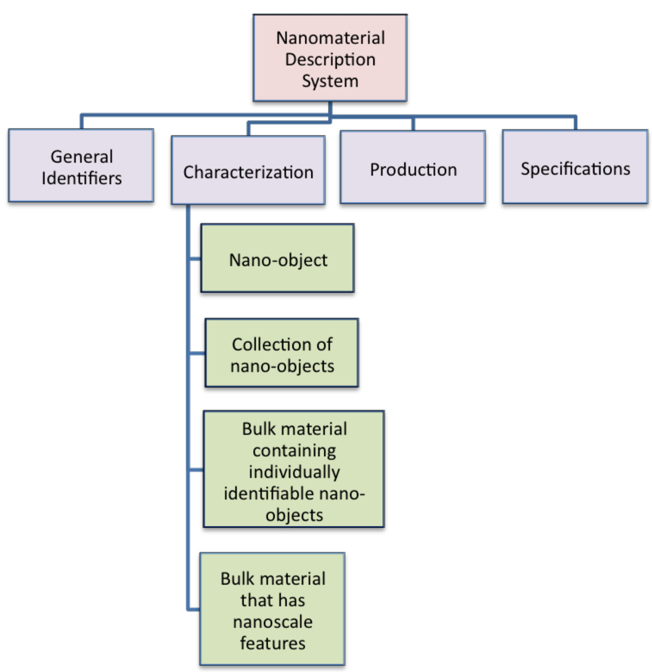



*Fig 1: Schematic of the information framework relevant to nanomaterials work.*

| Information Category | Description |
|---|---|
| General Identifiers | The general terms used to name and classify a nanomaterial. |
| Characterization | A set of measurement results that taken together uniquely describes the physical, chemical, structural and other characteristics of a nanomaterial. |
| Production | A set of general and specific information that describes the production of a nanomaterial. The production of a nanomaterial is assumed to have a distinct initial phase followed by one or more post-production phases. |
| Specification | A set of detailed information about specification documentation according to which a nanomaterial has been produced or documented. |

*Table 1. Information categories used to describe nanomaterials*

Framework is shown in Figure 1.

The final Framework defines four major information categories used to describe nanomaterials as shown in Table 1. Each of these information categories contains numerous subcategories that in turn contain the descriptors that provide the detailed information and data comprising a complete description system.

The UDS identifies the various types of information and data that can be used to describe a nanomaterial. It does not, however, prescribe which pieces of information and data must be reported; that will be determined by the reason for describing a nanomaterial, which in turn is determined by the community receiving the information and data. It should also be noted that additional descriptors may become necessary as our knowledge of the properties of nanomaterials increases.

In establishing the UDS, the rich array of actual and potential nanomaterials requires considerable detail in order to differentiate one from another. It is extremely useful, however, to divide nanomaterials and the objects that contain them into four major types, each of which requires slightly different sets of information to describe completely:

1. An individual nano-object
2. A collection of nano-objects
3. A bulk material containing individually identifiable nano-objects
4. A bulk material that has nano-scale features

It must be recognized that the distinction between bulk materials of types 3 and 4 may be difficult to determine and the use of information categories related to those types will depend on the application and discipline. The majority of "products" made from nanomaterials will primarily belong to one of these types. At the same time, the functionality of nanomaterials may really take place as an individual nano-object or as a collection of a small number of nano-objects that have separated in use from the bulk material that originally contained it. This is especially true for bio-medical functionality. It should be noted that the applicability of the UDS is not limited to engineered or manufactured nanomaterials but is also pertinent to naturally occurring nanomaterials. In the following sections these information categories are examined in much greater detail.

## Information Categories and their Subcategories

### General Identifiers

As with all scientific fields, practitioners create formal and informal terminology to refer to aspects of objects that are of interest, especially in order to aggregate items of interest into classes. Such identifiers include:

- Common or informal names and identifiers
- Formal names and identifiers as determined by rules, or as assigned by an authority
- Informal classifications based on one or more features
- Formal classifications as determined by rules, or as assigned by an authority

### Characterization of an individual nano-object

It is at the scale of an individual nano-object that the complexity and uniqueness of nanomaterials is most clearly demonstrated. The following six subcategories comprise the characteristics of an individual nano-object that are relevant for its description. In the following discussion, the term "nano-object" refers to an individual nano-object:

- Shape
- Size
- Chemical composition
- Physical structure
- Crystallographic structure
- Surface description

Some of these subcategories have well defined methods for quantifying information about their details, whereas other subcategories do not, a situation that will change as new methods for characterizing aspects of nanomaterials evolves.

### The characterization of a collection of nano-objects

Perhaps the most important type of nanomaterials from the viewpoint of actual applications is a collection of nano-objects, created either deliberately or through chance interactions. In most cases, the reactivity of individual nano-objects means that on a practical scale, it is difficult to produce, manipulate, and use an individual nano-object in isolation from all other nano-objects. Clearly there are exceptions, such as in applications being explored in the manipulation of quantum dots or individual atoms to create qubits for quantum computing applications.

A collection of nano-objects may be homogeneous, composed of one type of nano-object, or heterogeneous, composed of two or more different types of nano-objects. A collection may be tightly associated and act as an unit, or simply an assemblage of non-interacting nano-objects. All collection types are characterized in the same manner, using seven categories:

- Composition
- Physical Structure
- Interfaces
- Surface
- Size Distribution
- Stability
- Topology

A collection is differentiated from the third and fourth types of nanomaterial in that it contains only nano-objects, whereas the other types of nanomaterials are bulk materials containing nanomaterials or bulk materials with features on the nanoscale. Because of the wide diversity of possible collections, considerable thought must be given to the details accurately describing a collection, and in many situations, the description will be made on the basis of an average or representative collection rather than each individual collection. The implications of this approach are significant. The correlation of properties with collection features may be difficult. In a distribution of collections, individual collections away from the average might exhibit different levels of reactivity and properties than those that are average. Indeed, over time the description of a distribution of collections might be a new level of description for the UDS. For the present, we assume that the UDS is being used to describe one specific collection.

There remains the ambiguity of an individual nano-object that has acquired adherents, either as a full corona or as partial coverage. In these cases, using the information categories for an individual nano-object is preferred.

### A bulk material containing individually identifiable nano-objects

The Uniform Description System as discussed above is focused on the description of individual nano-objects or collections thereof. In many applications, however, nano-objects and collections of nano-objects will be placed in bulk materials, whether homogeneously or heterogeneously. When in service or during an application, the bulk material, which has most likely obtained new properties from the included nano-objects or collections, still functions as a bulk material.

We can differentiate between two types of bulk materials: solid phase and liquid phase. In liquid bulk materials, nano-objects and their collections are free to move around in the liquid, with interactions with other components of the liquid changing over time. The description of the nano-objects and their collections can be done by using the information categories and descriptors defined above. In solid bulk materials, the nano-objects and collections are more or less permanently locked in place and change locations slowly with respect to molecular time scales. Again, the description of the nano-objects and collections can use the tools above.

The question that then arises with respect to the description of this type of nanomaterial is the following: Does the bulk material have nano-scale features beyond those associated with the nano-objects or collections contained therein? One can define two extreme situations. The first is where individual nano-objects or collections nano-objects separate from the bulk materials during use or other application and move around freely, outside the confines of the bulk material. In this case, the

UDS is fully capable of describing the separated nano-objects, including a description of their production (i.e. by separation from the bulk material), if necessary.

The other extreme situation is where the use or application of the bulk material does not involve any separation of the nano-objects from the bulk material. In this case, the question becomes "what additional information is needed to fully characterize the bulk material as including nano-objects?" Aside from issues associated with the preparation of nano-objects before inclusion in the bulk material, or with the production process of the bulk material with nano-objects, current systems for describing bulk materials such as metals, alloys, ceramics, polymers, composites, food substances and others, should suffice.

Many cases between these two extremes are possible and as nanomaterials come into commerce, enhancements of the UDS may be necessary.

### A bulk material that has nano-scale features

The fourth type of nanomaterials that needs to be described is a bulk material that has nanoscale features, but does not have individual nano-objects or collections of nano-objects. At present the UDS does not describe these materials.

### Production

The production of a nanomaterial is assumed to have a distinct initial phase followed by one or more post-production phases. The post-production phase may simply be storage after initial production, or a more complex transformation. ISO TC 229 has produced ISO 80004-8:2013 which defines terminology applicable to nanomanufacturing. In addition, much effort is being made by several engineering communities to develop process models that are applicable to a wide variety of processes. As development of the Uniform Description System for nanomaterials progresses, these models need to be reviewed and utilized to the extent possible.

### Specifications

Specifications are a mechanism to define in detail how a nanomaterial is produced, purchased, or delivered. A specification is important for documenting the agreement between two or more parties as to the exact nature of the nanomaterial under consideration. Specifications can be informal or formal, and are often legally binding. Informal specifications are often used in the purchase of an object. They are developed by and agreed to by the parties involved. Formal specifications are developed by some competent organization on behalf of a cohort of interested parties so that they can be used by a simple reference.

Specifications can also contain information about the registration of a nanomaterial in a government, public, or private registration system, including the authority controlling the registration system. The fact that a nanomaterial is registered in such a system does not mean that it has specific properties or interactions; that information can only be determined by referring back to the registration system itself.

## Summary

The Uniform Description System as discussed above is now being widely reviewed by various communities working with and using nanomaterials. The UDS will continue to evolve over time as new knowledge is developed on how best to describe a nanomaterial accurately.

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**John Rumble <rumble@udsnano.org> is chair of the CODATA-VAMAS Working Group on Nanomaterials; Steve Freiman <freiman@udsnano.org> is the VAMAS Chair of the WG; and Clayton Teague <Teague@udsnano.org> is the Senior Nanotechnology consultant.**