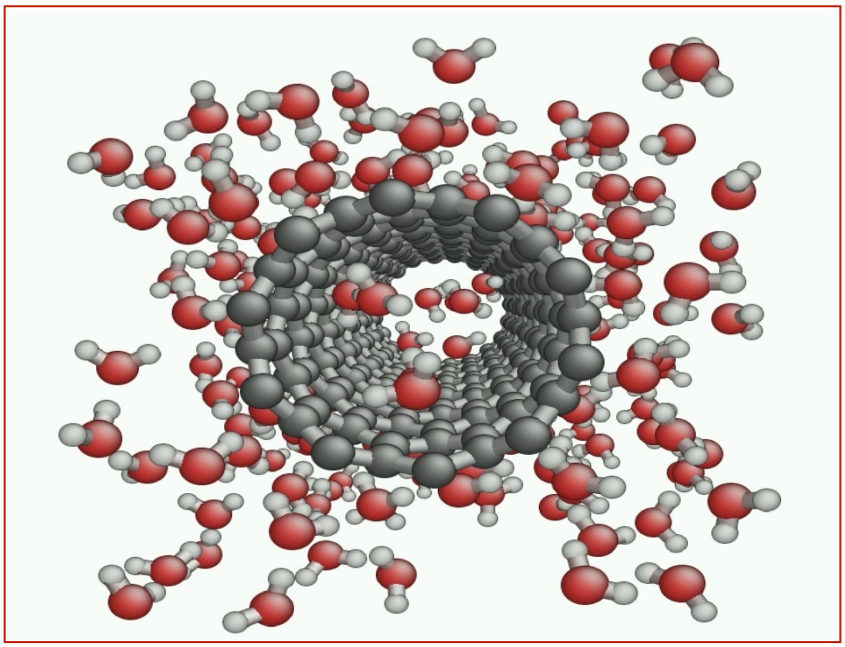
Uniform Description System for Materials on the Nanoscale



Prepared by the CODATA-VAMAS Working Group
On the Description of Nanomaterials
www.codata.org/nanomaterials

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Preface

Beginning in 2012, CODATA, the International Council for Science: Committee on Data for Science and Technology **(**www.codata.org**)**, and VAMAS, an international pre-standardization organization concerned with materials test methods **(**www.vamas.org**)**, established a joint working group to foster the development of a uniform description system for nanomaterials to address the growing diversity and complexity of nanomaterials being developed and commercialized.

The Working Group (WG) was formed following a 2012 workshop held in Paris co-sponsored by ICSU and CODATA. The international working group includes representatives from virtually every scientific and technical discipline involved in the development and use of nanomaterials, including physics, chemistry, materials science, pharmacology, toxicology, medicine, ecology, environmental science, nutrition, food science, crystallography, engineering, and more. Many international scientific unions have actively participated.

Following its work plan, the WG surveyed requirements for a description system. Over 40 responses were received that provided important insights into potential uses for a Uniform Description System for Nanomaterials (UDS). Based on the workshop and the survey an initial draft Framework for the UDS was developed and made available for further comment and modification. That initial Framework was reviewed by the Working Group at a second workshop held in Paris in May 2013.

To continue development of the draft UDS and to obtain more complete input from all the scientific communities and variety of researchers and industries involved with nanomaterials, the CODATA-VAMAS Working Group convened three international conferences:

- April 2014, North Carolina (USA)
- April 2014, Paris (France)
- September 2014, Beijing (China)

The workshops reviewed the draft Framework in great detail from a multi-disciplinary point of view. New information categories were added and detailed subcategories and descriptors were defined.

Based on these workshops and two years of work and meetings by an international, multi-disciplinary expert group, Version 1 of the UDS has been drafted and is presented in the following document. The document is provided in hopes that it will be directly applicable for developing data formats, reporting research results, and other uses.

The Chairs of the WG, John Rumble, Steve Freiman, and Clayton Teague, extend our thanks to all workshop participants for their many comments, recommendations, and critiques that contributed significantly to the evolution of the UDS Framework that brought it to this latest version.

Guide to this Document

This version of the CODATA-VAMAS Uniform Description System for Materials on the Nanoscale (UDS) is divided into several sections that serve a variety of purposes.

Sections I through VII, XI, and XII as well as Appendix A provide an introduction, background, and discussion of the approach and philosophy behind the UDS.

Most of the remaining sections can be read and used directly without reference to these first seven sections. We provide the table below as a guide to the use.

Using the UDS: Major Information Categories Used to Describe a Nanomaterial		
Information Category	**Section**	**Description**
General Identifiers	VIII	The general terms used to name and classify a nanomaterial
Characterization of		A set of measurement results that taken together uniquely describes the physical, chemical, structural and other characteristics of a nanomaterial
An individual nano-object	IX	
A collection of nano-objects	X	
Production	XIII	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	XIV	A set of detailed information about specification documentation according to which a nanomaterial has been produced or documented

Each of these sections contains one or more tables that define a set of descriptors with detailed definitions that can be used directly to describe individual nano-objects or collections of nano-objects. These descriptors are intended to provide guidance in describing a nanomaterial in research papers, database schemas, ontologies, regulations, modeling software, classification systems, sharing and exchanging property data, and many other uses.

As noted, this is Version 1.0 of the UDS. We expect that over time the UDS will be updated and expanded as users implement it in different ways.

Errors, improvements, and suggestions should be sent to udsnano@udsnano.org.

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I. Introduction

This document is Version 1.0 of the Uniform Description System for Materials on the Nanoscale (UDS) as prepared by the CODATA-VAMAS Working Group (WG) on the Description of Nanomaterials. This version is based on a Framework for the UDS as previously developed by the CODATA-VAMAS WG [1].

II. Background

Following discovery by experimentation or design, the process of using a new material goes through stages. First it becomes the focus of research and development (R&D) with the intent of understanding how it behaves and then demonstrating such understanding through control of various parameters to give predictable behavior. During this discovery process, the need grows to describe the material accurately to the group researching it. There eventually comes the time when it is necessary to describe the material to a much larger group of people.

The above process has been followed during the past 20 years of growing interest in nanomaterials, a group of novel materials that offer great promise for vastly improved properties and functionalities caused by nanoscale features. As the first wave of nanomaterials is being incorporated into products and new nanomaterials are continually being developed, they have become of great interest to a wide diversity of stakeholders ranging from researchers to product manufacturers to health and environmental experts to regulators and legislatures to consumers and the general public. All new materials offer both the promise of benefits and the potential of risks; nanomaterials are no different.

What is clear about nanomaterials is that the combination of small scale, exotic behaviors, and significant commercial value brings an interesting challenge: How do we know exactly which nanomaterial is under discussion as well as which of its features are important? Nanomaterials are larger than ordinary inorganic, organic, and biochemical molecules with significantly more features that provide a wide variety of functionalities. At the same time, the description methods for “bulk” materials are insufficient to describe the nanoscale features such as form, quantum effects, and surface properties that make nanomaterials interesting. Further, nanomaterials are of great interest to a wide group of scientific disciplines, product developers, and user communities, all of which need to communicate effectively with one another.

To restate the challenge: How can one describe a nanomaterial accurately on a multi-disciplinary, multi-user basis, recognizing that the science and technology of nanomaterials continues to evolve? The Uniform Description described herein attempts to answer that question.

III. Definitions

Several terms are used throughout this document and are defined as follows:

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

Note 1: A descriptor conveys both the semantics of the results as well as the result itself. A general model of a descriptor is given in Appendix A.

Information category: A set or group of related descriptors that represents a property, characteristic, or feature of an object

Note 1: Information categories may be hierarchical and contain subcategories (referred to as such), each containing a set of descriptors.

Note 2: Information categories and their subcategories are constructed to convey understanding of the structure, properties, features, and performance of an object.

Note 3: A descriptor may occur in more than one information category. It is the responsibility of the owner of data or information resources using an information category to ensure that data and information redundancy is adequately addressed.

Nano-object: A material with one, two, or three external dimensions in the nanoscale (as defined in ISO/TS 80004-3:2010(en), 2.2)

Collection of nano-objects: A group of two or more nano-objects

Note 1: A collection of nano-objects can contain identical or different nano-objects.

Note 2: The nano-objects within the collections can be associated in a variety of ways, including but not limited to direct bonding, van der Waals attraction, electrostatic interactions, or third party mediation (e.g. catalyst).

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

Note 1: A bulk material may have internal and surface features discernable on 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

IV. Background

The approach taken herein has been to identify the broad types of information that are used throughout the nanomaterials community to describe a nanomaterial as completely as possible. The goal has been to establish the uniqueness of a nanomaterial so it is clear which nanomaterial is being described and to allow the establishment of the equivalency of two nanomaterials to whatever level is desired. The terms *equivalency* and *uniqueness* are described in the definitions in Section III.

This approach was chosen so that the majority of the terms and concepts used in the description system are readily understandable to the scientists, technologists, and lay persons involved in nanotechnology. It is anticipated that the description system will be used by many different users groups, including informatics experts who design and implement data and information resources using the latest informatics tools such as information modeling, ontologies, and semantic web technology. Such efforts will likely uncover some ambiguities and redundancies, and that knowledge can be fed back into updates and evolution of this description system.

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 inadequate 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 dot" convey important information, identification of a specific nanomaterial requires more. Instead, for complete specificity, all relevant information categories need to be used. Many situations require this level of specificity including the development of regulations, standards, purchasing, and testing.

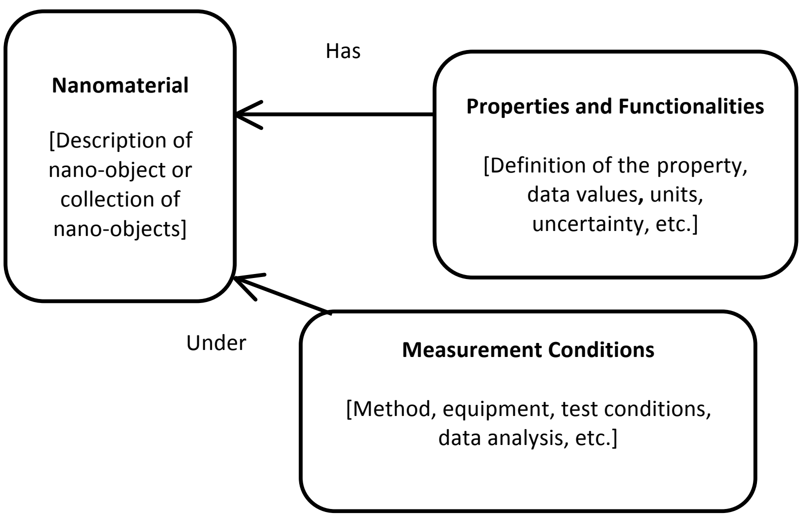
One can imagine that in the future a numbering system will evolve that traces back to specific values of the descriptors included in the information categories of the UDS.

V. Use of the Uniform Description System

The purpose of the Uniform Description System is to allow users, regardless of discipline, type of nanomaterial, or application, to use a common method for accurately describing a nanomaterial. Possible uses include the following:

Nanoinformatics: As researchers improve the quality and reproducibility of property measurements on nanomaterials, many groups will build data collections of measurement results. Users in turn will want to use multiple data resources to gain access to all available information. The UDS provides a backbone for building the database schemas and ontologies that are at the core of a nanoinformatics resource so that information from different resources can be compared and contrasted correctly.

In developing a data resource for nanomaterials, the required information can be divided into three major types as shown in Figure 1. A nanomaterial has a set of properties and functionalities determined under certain measurement conditions. The UDS specifies the information categories and descriptors that should be used for the description of the nanomaterials (upper left box). The UDS should be useful as data resources develop schemas and ontologies for describing a nanomaterial. The information categories and descriptors for the properties and functionalities and measurement conditions, however, are not covered by the UDS and need to be defined by other systems, schemas, or ontologies.



Regulatory actions: The UDS provides a methodology that allows regulators to define precisely and accurately the specific nanomaterial(s) being regulated. Ambiguous and ill-defined terms such as carbon nanotubes are not adequate for regulations. For example, certain forms of titanium oxide have toxic effects; other forms do not. Simply declaring titanium oxide as a species to be regulated without additional specificity of its form would be incorrect.

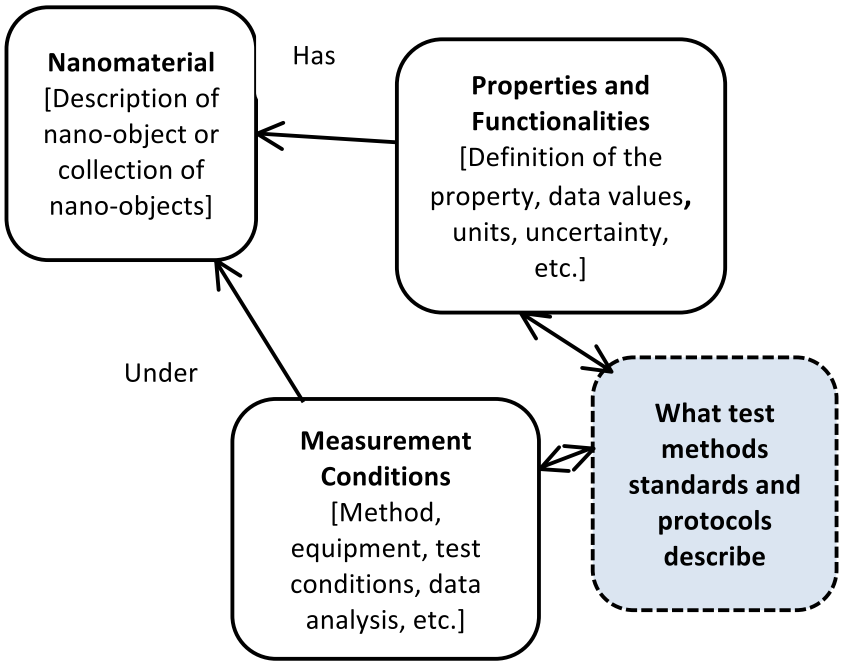
The basis for regulatory actions with respect to nanomaterials is risk assessment: Is the use of a nanomaterial in a product or food likely to cause harm to the user, the public, or the environment. These are legitimate concerns, but they need to be addressed using the best available science. Unfortunately today risk assessment is not a precise science. The testing of actual and potential nanomaterials is very challenging, first because of the large number of nanomaterials and second because small changes in a nanomaterial, such as its physical structure or surface coatings, can significantly change its interactions with biological and environmental systems, especially at the lowest (molecular and cellular) level.

Consequently it is critical that in assessing potential risk, i.e., unwanted and negative interactions, we are able to identify the mechanism by which these negative interactions operate. Scientifically that means understanding the factors (independent variables) about a nanomaterial that cause the negative interaction. For example, how does the chemical composition, or shape, or surface charge distribution affect the properties of a nanomaterial? Lacking detailed knowledge of cause and effect, regulators may find it convenient to issue regulations on an entire class of nanomaterials instead of a specific nanomaterial. In doing this, many nanomaterials of high value in terms of functionality or performance enhancing capability could be unscientifically removed from commerce, a result equally undesirable as ignoring real risk.

The UDS can play an important role in facilitating scientifically sound risk assessment through its definition of the important features of a nano-object or collection of nano-objects that need to be viewed as independent variables that are carefully controlled during risk assessment experiments. It is critical that researchers carefully document the exact nanomaterial being tested so its behavior can be accurately correlated with specific features of the nanomaterial itself.

Indeed one of the attractions of nanomaterials is the ability to fine tune them through atomic and molecular engineering to alter the shape, size, or surfaces, which in turn alters their properties, functionalities, or reactivity. Documenting the results of that engineering accurately is one of the major goals of the UDS.

Standards developers: The UDS provides standards developers with a structure to help identify critical areas for standardization as well as the research needed to address those areas. For example, the description of the surface of a nano-object and the topology of a collection of nano-objects are areas in which no consensus approach yet exists to describe the complexity of nanomaterials.



More importantly, as shown in Figure 2, the UDS interfaces with the test methods and protocols developed by the standards development committees. As these groups develop test methods and protocols for determining the properties and functionalities of nanomaterials, systems for describing the measurement conditions and properties must be developed to facilitate sharing of property data electronically.

Correlation of properties with nanomaterial features: The descriptors in the UDS can be considered as independent variables that affect in some way the properties of a nanomaterial. To be able to predict properties, one must identify and understand all the major variables that affect that property. The UDS provides a rigorous framework for systematically identifying and reporting the relationship between a feature (independent variable) and a property (dependent variable), which is of particular importance to health, safety, and environmental issues.

As discussed above under regulatory actions, the UDS has been designed to describe accurately all features of a nanomaterial so that they can be correlated with properties. This is especially true with respect to testing or research efforts that systematically vary one or more features (variables) to determine the resulting effect on a property. While this approach is important in maximizing potential positive performance (greatest strength, least reactivity, etc.), it is also critical for identifying and eliminating negative effects, such as toxicity or persistence.

Researchers: As new nanomaterials are discovered and formed, an accurate description is necessary so that future researchers are able to perform studies on the same nanomaterial. Already the scientific literature is being written with ambiguities present. One that commonly occurs is the use of the @

symbol to indicate both when a molecule or nano-object is inside or attached to a second molecule or nano-object. The UDS provides guidance to journals to avoid such ambiguities in the literature.

Purchase of nanomaterials: The complexity of nanomaterials precludes their specification by a simple name or formula. Purchasers of nanomaterials want to know exactly what they are getting, and providers of nanomaterials want to be able to clearly state what they are providing. The UDS provides a system to meet both needs.

Prediction of properties and evaluation of materials for use: The adoption of nanomaterials for use in products and other applications depends on the availability of reliable data about their performance under specified conditions. The UDS provides a mechanism for consistent reporting of data as well as the use of data from multiple sources in design and performance prediction software.

VI. Framework

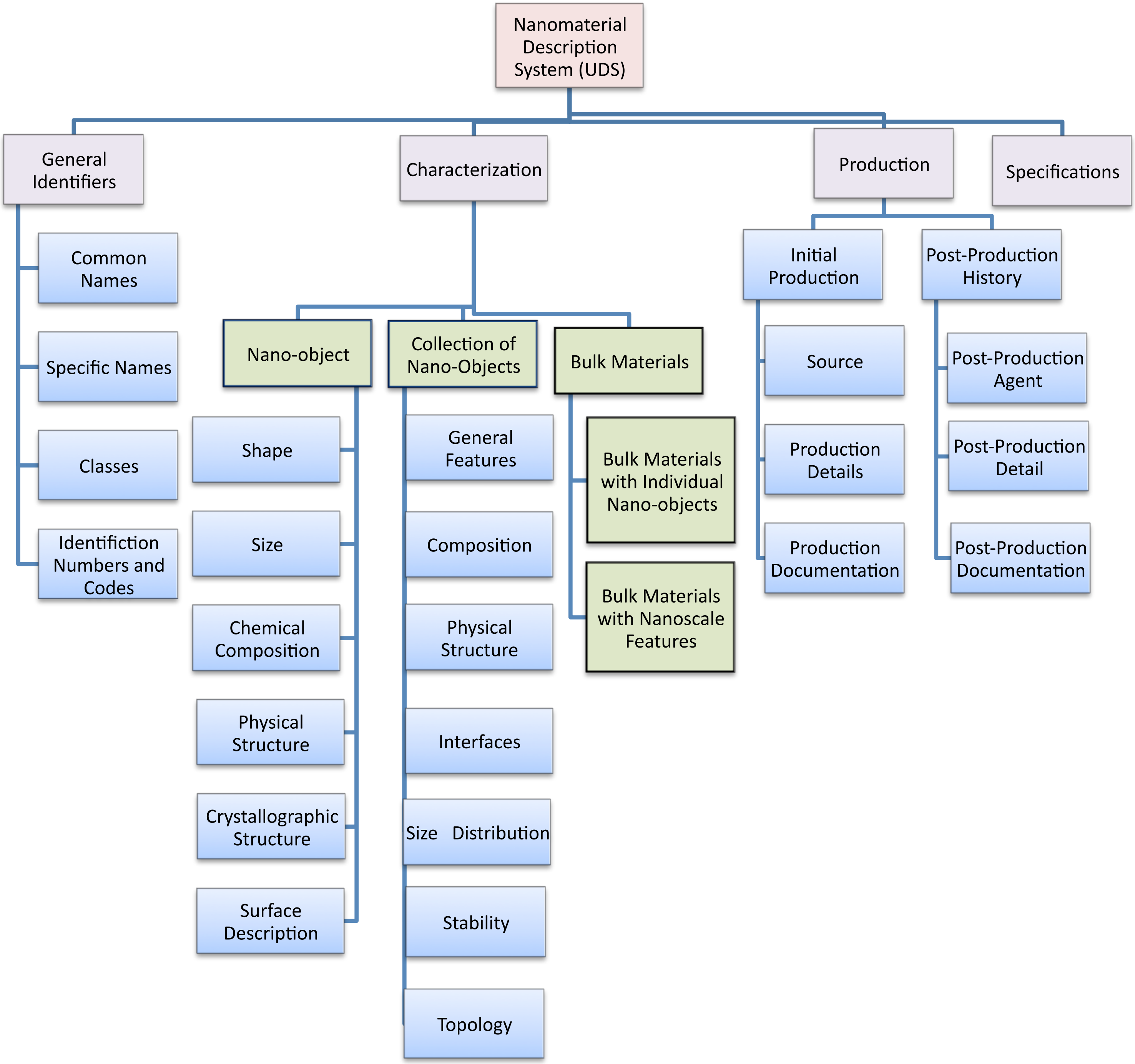
The first step in the development of the UDS was a survey of a large variety of user communities as to their need, as well as the convening of a series of interactive workshops to obtain consensus on the approach. There were also interactions with standards committees such as ISO Technical Committee 229 Nanotechnologies [2] and ASTM Committee E56 on Nanotechnology [3] as well as groups such as the OECD Working Party on Manufactured Nanomaterials [4]. Based on this preliminary work, a Framework of the information used by different disciplines in their nanomaterials work was created as shown in Figure 3. The Framework integrated existing approaches that have focused on specific detailed aspects of nanomaterials, such as size, shape, structure, etc. The final Framework, which is available at www.codata.org/nanomaterials, defined four major information categories used to describe nanomaterials as shown in Table 1.

Table 1. Major information categories used to describe a nanomaterial

Major Information Categories Used to Describe a Nanomaterial	
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

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 system is not hierarchical except that subcategories refer back to the main categories. Different users of the description system will use different subcategories and descriptors to a lesser or greater extent. These categories and subcategories can be used to create an ontology for nanomaterials that can be used to support many different types of applications.

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.


Nanomaterial Description System (UDS)
General Identifiers
Characterization
Production
Specifications
Common Names
Specific Names
Classes
Identifiction Numbers and Codes
Nano-object
Collection of Nano-Objects
Bulk Materials
Shape
Size
Chemical Composition
Physical Structure
Crystallographic Structure
Surface Description
General Features
Composition
Physical Structure
Interfaces
Size Distribution
Stability
Topology
Bulk Materials with Individual Nano-objects
Bulk Materials with Nanoscale Features
Initial Production
Post-Production History
Source
Production Details
Production Documentation
Post-Production Agent
Post-Production Detail
Post-Production Documentation

VII. Types of Nanomaterials

Throughout this document, the term *nanomaterials* is used to mean *materials on the nanoscale*. While a variety of definitions of nanomaterials exist, two major international standard definitions have been adopted. This Framework is intended to be compatible with both definitions.

The ISO TC229 definition [5] of a ***nanomaterial*** is as follows:

> *"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 [6] of a ***nanomaterial*** is as follows:

> *"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 %.*

In establishing the UDS, the rich array of actual and potential nanomaterials requires considerable detail to be differentiated from one another. It is extremely useful, however, to divide nanomaterials and the objects that contain them into four major types:

- An individual nano-object
- A collection of nano-objects
  - Identical nano-objects
  - Different nano-objects
- A bulk material containing individually identifiable nano-objects
- A bulk material that has nano-scale features

Each type of nanomaterial requires slightly different sets of information to describe it completely.

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. 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.

VIII. General Identifiers

As with all scientific fields, practitioners create formal and informal terminology to refer to aspects of the objects that are of interest, especially to be able 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, and
- Formal classifications as determined by rules or as assigned by an authority.

A. Common or Informal Names and Identifiers

Most physical objects have multiple names that have evolved through needs to name something that is being discussed. Common and informal names for all types of nanomaterials are no exception, and any implementation of the UDS needs to be able to include such names. One simple example is the multiplicity of acronyms used for single walled carbon nanotubes, i.e. CNT, SWNT, and SWCNT.

B. Formal Names and Identifiers, as Determined by Rules or as Assigned by an Authority

Formal chemical names can be assigned to chemical moieties through a series of rules established by authorities such as the International Union of Pure and Applied Chemistry [7] or by a commercial service such as the Chemical Abstract Services [8]. A number of similar systems are used for metals, alloys, polymers, and other engineering materials. Such systems are likely to be established for various types of nanomaterials in the future though it is likely that there will be multiple systems.

C. Informal Classifications Based on One or More Features

Most physical objects are put into informal classes based on one of more features, i.e., size, shape, content, functionality, etc. For nano-objects, classes commonly used are based on form (nanotubes), size (quantum dots), content (graphene), and many more. Such classes arise informally and have no rigorous definition.

D. Formal Classifications as Determined by Rules or as Assigned by an Authority

The proliferation of nanomaterials has led to the more formal assignment of classes by authorities such as ISO and other standard development organizations, commercial groups, regulators, and other organizations. These classes are based on form, size, content, and other aspects, with clearly (hopefully) definition for inclusion or exclusion. Table 2 includes some classes as defined and approved by ISO TC 229 on Nanotechnology. Of particular interest is the first entry *Nano-tree* that presents a broad classification scheme for nanomaterials.

Table 2. Examples of formal classes approved by ISO TC229

Examples of Formal Classes Approved by ISO TC 229		
Classification Term	Definition (without notes)	ISO Document
Nano-tree	Differentiates nanomaterials in terms of their internal/external structures, chemical nature, and physical, mechanical, biological, and other properties	ISO/TR 11360:2010(en)
Nanoparticle	Nano-object with all three external dimensions in the nanoscale	ISO/TS 27687:2008(en), 4.1
Nanoplate	Nano-object with one external dimension in the nanoscale and the two other external dimensions significantly larger	ISO/TS 27687:2008(en), 4.2
Nanofibre	Nano-object with two similar external dimensions in the nanoscale and the third dimension significantly larger	ISO/TS 27687:2008(en), 4.3
Nanotube	Hollow nanofibre	ISO/TS 80004-3:2011(en), 2.6
Nanorod	Solid nanofibre	ISO/TS 80004-3:2011(en), 2.7
Nanowire	Electrically conducting or semi-conducting nanofibre	ISO/TS 27687:2008(en), 4.6
Quantum dot	Crystalline nanoparticle that exhibits size-dependent properties due to quantum confinement effects on the electronic states	ISO/TS 27687:2008(en), 4.7
Nanostructured materials	One of five types: nanostructured powder; nanocomposite; solid nanofoam; nanoporous material; fluid nanodispersion.	ISO/TS 80004-4:2011(en)
Nano-onion	Spherical nanoparticle with concentric multiple shell structure	ISO/TS 80004-3:2010(en), 2.8
MNO	Nano-object intentionally produced for commercial	ISO/TS 13830:2013(en), 3.4

	purposes to have specific properties or composition	
Stealth nano-object	Nano-object specifically designed to avoid detection or rejection by the body's defence system	ISO/TS 80004-7:2011(en), 4.1
Manufactured nano-object	Nano-object intentionally produced for commercial purposes to have specific properties or composition	ISO/TS 12805:2011(en), 3.3
PCMNO	Products in which manufactured nano-objects are intentionally added, attached, or embedded	ISO/TS 13830:2013(en), 3.9
Engineered nanoparticle	Nanoparticle intentionally engineered and produced with specific properties	ISO/TR 27628:2007(en), 2.8
Nanoaerosol	Aerosol comprised of, or consisting of, nanoparticles and nanostructured particles	ISO/TR 27628:2007(en), 2.11
Nanostructured particle	Particle with structural features smaller than 100 nm, which may influence its physical, chemical, and/or biological properties	ISO/TR 27628:2007(en), 2.13

Classification schemes for nanomaterials are presently of great interest for regulatory purposes. These schemes can be based either on features of a nanomaterial or on a property thereof. The logic of classes based on features, such as size, chemical composition, etc., is that the feature correlates strongly with a desirable or undesirable property, especially those related to a risk, such as toxicity or environmental degradation. Many of the proposed classification schemes are simplistic, overlooking the complexity of nanomaterials and the multi-variable dependency of a "property" such as toxicity. Over time as the causal relationship of property to specific features is clarified, these classification schemes will become more accurate and therefore more useful.

E. Summary of General Identifiers

The general identification of objects such as nanomaterials plays an important role in any description system. These identifiers provide a convenient and efficient way to convey a set of information that is implied in a name or class name. Whether the identifiers arise from informal usage or are established for more formal reasons, implementations of the UDS must be able to include these data.

Information systems containing property data or literature references about nanomaterials will usually use these identifiers as major access points to their content. It is important to recognize the difference between formal and informal names and formal and informal classes in creating and using these information resources. In practice, the use of informal names and classes often is more common than their formal counterparts, sometimes leading to ambiguous, confusing, or even inaccurate designations that in turn hinder the location and retrieval of desired and pertinent data and information. Users and system designers need to recognize the potential problems.

IX. The Characterization of an Individual Nano-Object

It is at the scale of individual nano-objects that the complexity and uniqueness of nanomaterials is most clearly demonstrated. The term nano-object is defined in ISO TS 12805:2011, 3.1 as "*a material with one, two or three external dimensions in the nanoscale*."

The following six subcategories, as shown in Figure 2, comprise the characteristics of an individual nano-object relevant for its description. In the discussion that follows, the term "nano-object" refers to an individual nano-object.

A. Shape
B. Size
C. Chemical composition
D. Physical structure
E. Crystallographic structure
F. 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.

A. Shape

The characterization of the geometrical shape of a nano-object is critical as its properties and reactivity are strongly dependent on this factor. Considerable effort has gone into establishing standard definitions for many forms, and as new shapes are discovered, additional definitions are developed. The most common criterion for defining the shape of a nano-object is its general three-dimensional geometry.

ISO TC 229 has defined several common shapes including: nanoparticle, nanorod, nanotube, nanoplate, and nanocone. It is anticipated that ISO TC 229 will continue to standardize the terminology associated with the shape of newly discovered nano-objects.

To describe quantitatively the shape of a nano-object, several different descriptors are required as shown in Table 3.

Table 3. Descriptors for the shape of a nano-object

Descriptors for the Shape of a Nano-Object	
Descriptor	**Definition**
Subcategory: Shape Type	
Number of dimensions on nanoscale	The number of dimensions of the nano-object on the nanoscale (1 to 100 nm)
General shape	Common name of shape
ISO 229 shape name	Shape name as defined by ISO TC 229
Specific shape	Shape name with qualifiers
Type of thickness of a nano-object with one dimension at the nanoscale	The geometrical name of the shape taken perpendicular to the thickness
Cross-sectional view for nano-object with two dimensions at the nanoscale	For nano-object with two dimensions at the nanoscale, the geometrical name of the cross-section taken perpendicular to the non-nanoscale dimension
Number of layers (for nano-object with two or three dimensions at the nanoscale)	When relevant, the number of layers in the shape
Geometric regularity	Description of the geometrical regularity of the shape
Shape symmetry	Overall symmetry of the shape
Symmetry components	The number of and type of symmetry components
Subcategory: Shape Features (recurring)	
Type of feature	A features that occurs in the shape
Regularity of feature	The regularity of that feature
Number of feature	The number of occurrences of the feature
Symmetry of feature	The symmetry of the feature

B. Size

The dimensions needed to specify the size (internal and external dimensions) of different nano-objects vary according to the shape. In addition, some shapes have ambiguity in their definition, e.g., at what ratio of diameter to length can a rod also be considered a particle, similarly for plates. In many instances, the smallest dimension (such as wall thickness) is often given in terms of the number of atomic or molecular layers. In an ideal situation, each nano-object shape would have a well-defined set of size measurements to be reported so that property-size correlations could be made. To describe the size of a nano-object, several descriptors are required, as defined in Table 4.

Table 4. Descriptors for the size of a nano-object

Descriptors for the Size of a Nano-Object	
Descriptor	**Definition**
Subcategory: Applicable Dimensions	
Names of dimensions	Names of appropriate dimensions for a specific shape
Dimensions	Measured or computed value for each dimension
Type of dimension	What dimension represents: Individual measurement, calculated, average, etc.
How measured	Measurement method
Subcategory: Derived Dimensions	
Aspect ratio (when applicable)	Ratio of the greatest to the least dimension
Maximum virtual diameter	Dimension of the diameter of the largest sphere that can be inscribed about a nano-object while maintaining contact at two points
Subcategory: Internal Dimensions	
Number of internal features	The number of internal features being reported
Feature name	Name of each internal feature
Names of dimensions	Names of appropriate dimensions for each individual internal feature
Applicable dimension	Measured or computed value for each dimension
Type of dimension	What dimension represents: Individual measurement, calculated, average, etc.
How measured	Measurement method

C. Chemical Composition

The chemical composition of a nano-object can be expressed in several ways, e.g., in terms of the principal atoms or molecules present, or as a percentage of various chemical moieties (functional parts of a molecule). When a nano-object has multiple internal structures, such as a core, shell, surface, or covering, the chemical composition for each structure should be given as needed. The chemical composition comprises the list of chemical components (on an atomic or molecular basis), their amounts, and their chemical bonding (including structural formula), when appropriate.

The International Union of Pure and Applied Chemistry (IUPAC) [7] is the major international authority for chemical nomenclature and is the appropriate body to try to extend current chemical nomenclature and bonding terminology to nano-objects. At the same time, other disciplines, such as food science and paint pigment technology, have developed specialized terminology to describe the chemical composition of materials and need to examine if their systems for describing chemical composition need to be extended.

This subcategory also includes chemical structural identifiers such as the IUPAC International Chemical Identifier (InChI) and those used by government and private company chemical databases and other chemical software. Chemical structural identifiers, by definition, contain embedded information from which all or part of the chemical structure of a nanomaterial can be deduced.

The chemical composition of a nano-object uses a number of descriptors as shown in Table 5.

Table 5. Descriptors for the chemical composition of a nano-object

Descriptors for the Chemical Composition of a Nano-Object	
Descriptor	**Definition**
Subcategory: Atomic Composition	
Number of different types of atoms present	Number of different types of atoms in the nano-object
Atoms present	A list of the component atoms
Composition percentage type	Basis of the composition percentage: number, mass
Composition percentage	Measured or computed value of each percentage
Type of composition	What atomic composition represents: Individual measurement, calculated, average, etc.
How measured	Measurement method
Subcategory: Molecular Composition	
Number of different types of molecules present	Number of different types of molecules in the nano-object
Molecules present	A list of the component molecules
Molecular formula	Chemical formula for each molecule present
Molecular name	Chemical name of each molecule present
Structural formula	Structural formula for each molecule present
CAS Registry Number	CAS Registry number for each molecule present
IUPAC InChI	The IUPAC InChI notation for each molecule present
Composition percentage type	Basis of composition percentage: number, mass
Composition percentage	Measured or computed value of each percentage
Type of percentage	What the percentage represents: Individual measurement, calculated, average, etc.
How measured	Measurement method

Subcategory: Chemical Moieties	
Number of different chemical moieties present	Number of different types of chemical moieties present
Chemical moieties present	List of chemical moieties present
Chemical moiety formula	Chemical formula for each chemical moiety present
Chemical moiety name	Chemical name for each chemical moiety present
Chemical moiety structural formula	Structural formula for each chemical moiety present
CAS Registry Number	CAS Registry Number for each chemical moiety present
IUPAC InChI	IUPAC InChI notation for each chemical moiety present
Composition percentage type	Basis of composition percentage: number, mass
Composition percentage	Measured or computed value of each percentage
Type of percentage	What the percentage represents: Individual measurement, calculated, average, etc.
How measured	Measurement method

D. Physical Structure

Nano-objects can have internal structures depending on their complexity. Because nano-objects take so many different shapes and sizes, many different physical structure models are possible. Many nano-objects are layered, contain inhomogeneities, and have features such as holes, protuberances, and appendages. These structural characteristics need to be described in detail in terms of the composition of each component, its place in the overall structure, and other details. Some nano-objects are synthesized to have specific pore sizes, e.g., for catalytic purposes. The description of structural defects and impurities, whether intentional or unintentional, should include details of the amount, identity, and location of each defect or impurity.

At present, no general system exists for describing the physical structure of nano-objects or of physical models that could be used as a basis for a general system. Some classes of nano-objects, such as carbon nanotubes, have had their physical structure considered in detail. For a comprehensive approach to the description of the physical structure of nanocarbon, see [http://www.slideshare.net/AxelPeterMUSTAD].

The physical structure of a nano-object uses a number of descriptors as shown in Table 6. Additional aspects of physical structure can be described as their importance becomes apparent.

Table 6. Descriptors for the physical structure of a nano-object

Descriptors for the Physical Structure of a Nano-Object	
Descriptor	**Definition**
Subcategory: Layered Nano-Object	
Number of layers	The number of layers present
List of layers	List of the names of the layers
Order of layers	The order of the layers
Extent of layers	The physical extent of the layers, e.g. area, regularity
Geometry of layers	The 2-D geometrical shape of the layer
Composition of layers	The chemical composition of each layer: refer to the chemical composition descriptors
Thickness of layers	Measured or computed value of the thickness value
Thickness measurement method	Measurement method
Subcategory: Shell Structure	
Number of shells	The number of shells present
List of shells	List of the names of the shells
Order of shells	The order of the shells
Chemical composition of shells	The chemical composition of each shell: refer to the chemical composition descriptors
Thickness of shells	Measured or computed value of the thickness value
Thickness measurement method	Measurement method
Uniformity of shells	Completeness, regularity of thickness, etc.
Subcategory: Physical Features	
Number of physical features	The number of physical features present
List of physical features present	Names of the individual features in the nano-object
Types of physical features	Holes, protuberances, appendages, end cap, legs, etc.
Location of each individual physical feature	Location of each individual physical feature on the nano-object
Geometry of each individual physical feature	Geometrical shape of each individual physical feature
Dimensions of each individual physical feature	Appropriate dimensions for each individual physical feature
Regularity of the physical feature	Overall regularity on shape or location of the physical features
Subcategory: Defects	

Number of defects	The number defects present
List of defects	List of defects present
Types of defect	Type name for each individual defect
Location of each individual defect	Location of each individual defect on the nano-object
Geometry of each individual defect	Geometrical shape of each individual defect
Dimensions of each individual defect	Appropriate dimensions of each individual defect
Regularity of each individual defect	Overall regularity of the location of the defects
Subcategory: Entrapment	
Number of entrapped species	Number of species that are entrapped
Names of entrapped species	List of names of entrapped species
Type of entrapped species	What kinds of species are entrapped: atoms, molecules, moieties, other nano-objects, etc.
Chemical composition of entrapped species	The chemical composition of entrapped species: refer to the chemical composition descriptors
Concentration of entrapped species	The amount of species entrapped
Type of entrapment	How the species is entrapped
Regularity of entrapment	Does entrapment repeat? If so, how and how often?
Subcategory: Additions	
Type of addition	Type of addition: Corona, single molecule, other nano-object, etc.
Name of addition	Name of the addition
Species type in addition	The species comprising the addition: atoms, molecules, moieties, other nano-objects, etc.
Chemical composition of addition	The chemical composition of the addition: refer to the chemical composition descriptors
Type of addition	How the species are added: bonding, etc.
Geometry of addition	Geometry of the addition
Uniformity of addition	Completeness of coverage, uniformity of thickness, etc.

E. Crystallographic Structure

The crystallographic structure of nano-objects is very important. A nano-object can have multiple physical structures within it, each with a different crystallographic structure. It can be amorphous, polycrystalline, or crystalline. When the physical structure of a nano-object has multiple components, layers, etc., each distinct region can have a different crystallographic structure. The International Union of Crystallographers (IUCr) has developed a comprehensive system for describing the details of crystallographic structure that can be used and extended for nano-objects. Subcategories and descriptors for crystallographic structure of a nano-object are given in Table 7.

Table 7. Descriptors for the crystal structure of a nano-object

Descriptors for the Crystal Structure of a Nano-Object	
Descriptor	**Definition**
Subcategory: Physical Structure Identification	
Physical structure name	Name of the physical structure within the nano-object that is being described by its crystal structure
Physical structure type	Structure type: layer, shell, surface, etc.
Physical structure location	Location of the physical structure within the nano-object
General nano-object type	Metal, polymer, etc.
Subcategory: Unit Cell Information	
Crystal system	The crystal system of the physical structure (one of seven)
Brevais lattice	The Brevais lattice of the physical structure (one of 14)
Space group	The space group
Miller indices	The appropriate Miller indices
Subcategory: Basic Unit Cell Parameters	
Cell length a	Cell length *a* appropriate for the crystal system value
Cell length b	Cell length *b* appropriate for the crystal system value
Cell length c	Cell length *c* appropriate for the crystal system value
Cell angle alpha	Cell angle *alpha* appropriate for the crystal system value
Cell angle beta	Cell angle *beta* appropriate for the crystal system value
Cell angle gamma	Cell angle *gamma* appropriate for the crystal system value
Cell volume	Measured or calculated cell volume
Cell measurement temperature	Temperature at which crystal structure data were measured

F. Surface Description

Structured surfaces on the nanoscale are produced to have unique and useful electronic and photonic properties. Because of the reactivity of one or more surfaces in a nano-object, it will have adherents on its surface, especially when it is in a biological or environmental fluid. These surface structures may also manifest themselves as an altered external shape. The description of the surface structure of a nano-object is important, and that description needs to include surface charge and surface attachments. The surface description structure of a nano-object uses a number of descriptors as shown in Table 8.

Table 8. Descriptors for describing the surface of a nano-object

Descriptors for Describing the Surface of a Nano-Object	
Descriptor	**Definition**
Subcategory: General Surface Description	
Overall surface structure	Description of overall surface: regular, irregular, coated, cleaned, etc.
General reactivity of surface	Description of surface reactivity: hydrophobic, hydrophilic, conductive
Cleanliness of surface	Description of cleanliness: cleaned, deliberately coated, environmentally coated, etc.
Surface Treatment	
Type of surface treatment	Oxidation, chemical, plasma assisted, etc.
Treatment process	Refer to description of post-production processing
Resulting coating composition	Use chemical composition descriptors
Coating thickness	Measured or calculated coating thickness
Coating completeness	Percentage coverage of the coating
Coating uniformity	Description of uniformity or lack thereof: gaps, thickness variability, compositional variability, geometrical variability, etc.
Subcategory: Surface Geometry	
Topological variations	Nano-scale topographic variations along one dimension or two dimensions in the plane of a nanoplate, along the axis of a nanorod, around the periphery of a nanorod, or on the surface of a nanoparticle.
Periodicity of variations	Periodic or random variations along either one or two dimensions of the nanoplate's plane or in the dimensions mentioned for a nanorod or a nanoparticle; more generally the variations may be random with some specified correlation length.
Specific surface area	Measured or calculated specific surface area
Measurement method	Method used to measured and/or calculate specific surface area
Detailed of measurement	Description of equipment, analysis method, assumptions, etc.
Surface steps	If present, description of steps and their size
Subcategory: Surface Electronic Properties	
Surface charge model	Description of the model of the surface charge of a nano-object
Type of surface charge	Charge sign, magnitude, full or partial

Charge distribution	Distribution of charge about a surface
Measurement method	Method used to measure or calculate surface charge
Subcategory: Other Surface Properties	
Property name	Wettability; phononic; optical; color; other
Property value	Property value
Measurement method	Method used to measure or calculate property

X. Characterization of a Collection of Nano-Objects

Perhaps the most important type of nanomaterial from the point 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 of all other nano-objects. Clearly there are exceptions when one considers applications such as are being explored in the manipulation of quantum dots for creating qubits for quantum computing applications. Collections can be characterized using the eight categories of information listed below.

A. General Features
B. Composition
C. Physical Structure
D. Interfaces
E. Surface
F. Size Distribution
G. Stability
H. Topology

A collection is differentiated from the third and fourth types of nanomaterial (Sections XI and XII respectively) 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. There remains the ambiguity of an individual nano-object that has acquired adherents, either as a full corona or partial coverage. In these cases, using the information categories for an individual nano-object is preferred.

A. General Features

A collection of nano-objects may be homogeneous, composed of one type of nano-object, or heterogeneous, composed on two or more different types. Because of the wide diversity of possible collections, considerable thought must be given to the details of accurately describing a collection, and in many situations, the description will be made on the basis of an *average* or *representative* 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 levels of reactivity and properties different than those that are *average*. The descriptors used to describe the general features of a collection are given in Table 9.

Table 9. Descriptors for the general features of a collection of nano-objects

Descriptors for the General Features of a Collection of Nano-Objects	
Descriptor	**Definition**
Type of collection	Type of collection being described: specific, average, representative, etc.
Collection sampling	If average or representative collection, how was sample obtained
Homogeneity of collection	The number of different types of nano-objects present in the collection

B. Composition

The composition of a collection of nano-objects is established by specifying the nature of each type of nano-object present and the amount thereof. The collection can range from completely homogenous, that is, comprising identical nano-objects of the same shape, size, and composition, to completely inhomogeneous, that is, an intentional or random mixtures of different nano-objects that vary in terms of composition, shape, size, and other characteristics. The descriptors used for composition are given in Table 10.

Table 10. Descriptors for the composition of a collection of nano-objects

Descriptors for the Composition of a Collection of Nano-Objects	
Descriptor	**Definition**
Subcategory: Composition Overview	
Number of different nano-objects present	The number of different nano-objects present in the collection
List of nano-objects present	A list of nano-objects present; they may be designated as primary or trace constituents
Homogeneity	Description of the uniformity of the constituent nano-objects in an collection
Degree of inhomogeneity	A measure of the lack of uniformity of the constituent nano-objects in the collection
Subcategory: Nano-Object Description (recurring for each component nano-object)	
Name	From the General Identifiers for a nano-object as specified in that information category
Other general identifiers	From the General Identifiers as specified in that information category
Shape	From Characterization as specified in that information subcategory for a nano-object
Size	From Characterization as specified in that information subcategory for a nano-object

Chemical composition	From Characterization as specified in that information subcategory for a nano-object
Physical structure	From Characterization as specified in that information subcategory for a nano-object
Crystallographic structure	From Characterization as specified in that information subcategory for a nano-object
Surface description	From Characterization as specified in that information subcategory for a nano-object
Production	From Production as specified in that information category
Post-production processing	From Post-Production Processing as specified in that information category

C. Physical Structure

The physical structure of a collection is characterized by the arrangement of the individual nano-objects within it. The structure may be totally regular, partially regular, or random, with each situation requiring different types of information. It is assumed that some of the dimensions of the collection could be on the micrometer (10^{-6} m) scale. Because the number of nano-objects on the micro-scale could number in the millions, the structure on those dimensions is likely to be characterized qualitatively. The collection itself has distinct boundaries that are both well-defined and detectable. When describing a collection of objects, one needs to specify the following information:

- What objects are present?
- Where are they located in absolute geometric space?
- Are the objects regularly arranged?
- If so, what is their shape and what are the dimensions of that shape?
- Does the regularity extend in one, two, or three dimensions?
- If less than three dimensions, is the additional regularity in the other one or two dimensions?
- How are the objects associated with each other within the shape?
- If the regularity is only partial, are the non-regular portions random or regular themselves?
- If the structure is totally random, does that randomness extend in one, two, or three dimensions?
- Do the boundaries of the collection have the same structure as the interior of the collection?

The description of the composition and structure of the surface of a collection of nano-objects is addressed in a separate section. The descriptors for physical shape are given in Table 11.

Table 11. Descriptors for the physical structure of a collection of nano-objects

Descriptors for the Physical Structure of a Collection of Nano-Objects	
Descriptor	**Definition**
Subcategory: Physical Structure Overview	
Number of nano-objects in the collection	The number of individual nano-objects in the

	collection
List of nano-objects present	The names of the nano-objects present in the collection
List of types of nano-objects in the collection	The names or classes of nano-object types in the collection
The number of each type of nano-object in the collection	The number of each type of nano-object in the collection
Collection general shape	The overall shape of the collection, if applicable
Collection size	The dimensions of the collection
Subcategory: Physical Structure Arrangement	
Regularity of arrangement	If the nano-objects are regularly arranged, what is the arrangement
Degree of and completeness of regularity	The regularity and completeness throughout the collection
Dimensionality of regularity	One-, two-, or three-dimensions
Geometrical arrangement, if any	The geometry of arrangement of the objects, if applicable
Subcategory: Structure Within Regular Shape (recurring)	
Substructure shape name	Name of a substructure within the collection
Substructure shape dimensions	Dimensions of the substructure
Substructure shape boundary	Description of the boundary of the substructure
Subcategory: Association of Nano-Objects in a Collection	
Nano-object association	Description of the association (bonding or otherwise) among the nano-objects in the collection

D. Interfaces

By their very nature, collections have a variety of interfaces among individual nano-objects as well as among subsets within the whole. Characterizing the details of these interfaces can be a difficult task as the internal physical structure, as described in the last section, is usually only partially regular and usually incompletely characterized. In addition, the regularity often is in just one or two dimensions rather than three dimensional. Consequently the description of the interfaces is often qualitative rather than quantitative.

An interface within a collection is defined as the boundary between two distinct regions. An interface is described by its location, the two regions on either side of the boundaries, the boundary area, and the type and strength of the interaction. Clearly as the size of the interfacing region grows, the description can become more qualitative. Greater inhomogeneity in a collection means the greater the number of interfaces that must be described. In many cases, the interface description is done qualitatively as the technology to examine individual interfaces deep within collection does not yet exist.

Collections may be prepared by treating the surface or boundary of individual nano-objects. The interface description then needs to include surface preparation as well as a description of residues, accidental or intentional. The set of descriptors for interfaces is given in Table 12.

Table 12. Descriptors for the interfaces within a collection of nano-objects

Descriptors for the Interfaces within a Collection of Nano-Objects	
Descriptor	**Definition**
Subcategory: Interface Overview	
General type of interface	Common name of type of interface (no standardized terminology available)
Interface preparation of nano-objects	Method used to prepare interface for establishing the collection, if applicable
Number of different types of interfaces	Number of different types of interfaces, if applicable
Subcategory: Description of Individual Interfaces (recurring)	
Interface name	Name of specific interface
Interface dimensions	Dimension of interface, if applicable
Interface boundary structure	Structure of the interface
Nano-objects forming interface	Name of nano-objects forming the interface
Residues on interface	Type and amount of residue on interface, if any
Method of residue determination	Method for determining type and amount of residue
Intentional or random	Indication of whether residue was intentionally placed or not
Uniformity of interface	Degree of uniformity of interface

E. Size Distribution

The distribution of sizes of the nano-objects within a collection is a key determinant of its overall properties. It may be desirable to have a very uniform size of nano-objects within the collection; in other situations, a wide distribution of sizes is needed. Considerable research has gone into developing technology to determine sizes across the range of nano-scales and types of nano-objects [9]. The size distribution descriptors are given in Table 13.

Table 13. Descriptors for the size distribution of a collection of nano-objects

Descriptors for the Size Distribution of Nano-Objects within a Collection	
Descriptor	**Definition**
Subcategory: Size distribution overview	
Distribution of sizes	List of sizes or size ranges that occur in the collection and their percentages
Range of sizes	Maximum and minimum size of participating nano-objects
Average size	Average size of nano-objects in the collection
Medium size	Medium size of nano-objects in the collection
Method of determination	Method used to determine the size distribution
Media in which determined	Media in which the size distribution measurement was made
Other experimental variables in size distribution measurement	Equipment used and other experimental parameters, dependent on method

F. Stability

Once a collection of nano-objects is created, its stability is a key factor. Instability arises primarily for three reasons:

- The collection is inherently unstable and will break apart spontaneously,
- The collection is subjected to unexpected conditions such as temperature changes, violent motion, unanticipated reactions, etc., and
- The collection is intentionally exposed to a reactive species.

The lack of stability may be expected or unexpected, and these situations require different descriptions as shown in Table 14.

Table 14. Descriptors for the stability of a collection of nano-objects

Descriptors for the Stability of a Collection of Nano-Objects	
Descriptor	**Definition**
Subcategory: Stability Overview	
Type of instability	Inherent, heat-sensitive, time-sensitive, reactive, environment sensitive, etc.
Expected or unexpected	Whether instability was expected or unexpected
Subcategory: Inherent Instability	
Name of instability	Actual name of instability
Type of decay	Mechanism of instability
Half-life of decay	Timed half-life of instability
Method of monitoring	Method for monitoring decay
Decay products	Names or types of decay products
Subcategory: Reactive Instability	
Name of reaction	Name or type of reaction

Media required	Media needed for reaction to occur
Reaction products	Name or type of reaction products
Stabilizing agent	Name or type of media that can be used to make collection stable
Concentration required	Amount of stabilizing agent needed
Subcategory: Instability Caused by Change of Conditions	
Name of instability	Name or type of instability
Condition that causes transformation	Name or type of the cause of instability
Condition parameters required	Conditions that foster the instability

G. Topology

Topology is the description of the overall connectivity and continuity of a collection of nano-objects or its components (where each component can be one or more nano-objects) or both. This includes the relative position in space of the components, e.g., totally or partially internal or external to each other, and their connectedness and boundaries, done in such a way that a correlation between the topological shape and the properties of a collection of nano-objects can be ascertained.

Topology by its very nature provides qualitative descriptions on nanomaterials. There are few direct applications of topology, but as is happening with molecular biology, researchers are finding situations in which functionality can be correlated to homeomorphism, that is the ability to transform one object (surface) into another without cutting or attachment. Another example is the application of knot theory that studies linear structures that are tied together such that the ends cannot be undone. At present there is no system under development to describe systematically the topological features of a collection of nano-objects.

XI. 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 different properties from the 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 from 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 contained therein?*

One can define two extreme situations. The first is when individual nano-objects or collections thereof separate from the bulk materials during use or other application and move around freely, outside the confines (boundaries) of the bulk material. In this situation case, the UDS can be used to describe the separated nano-objects, including a description of their production (i.e., the separation of the nano-object from the bulk material).

The other extreme situation is that the use or application of the bulk material does not involve any separation of the nano-objects from the bulk material. In this situation, the issue is what additional information is needed to fully characterize the bulk material, including contained 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 to account for these in-between cases may be necessary.

XII. A Bulk Material Having 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.

XIII. 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. A set of descriptors for the initial production phase and a generic post-production phase are given below.

A. Initial Production

The initial production information category contains the information relevant to how a nanomaterial was initially synthesized, formulated, produced, or manufactured to achieve its primary structure and properties. The production of a nanomaterial in the context of a research or experimental environment is quite different from production in a commercial setting. The amount and type of the processing history information reported will vary greatly depending on the circumstances as well as the source of the information. Many companies share very few processing details, relying instead on highlighting "unique" properties of their materials. Publicly funded research papers, however, might contain more complete details.

The basic model of the production is as follows: A nanomaterial is produced from a set of starting materials using a production technique, specific recipe, and equipment under a given set of conditions. A production technique is the type of method used for producing a collection, e.g., mixing. The recipe specifies the starting materials and their actual amounts, the order of operations, and the conditions to be used. The reporting of the production of a nanomaterial uses a number of descriptors as shown in Table 15.

Table 15. Descriptors for the production of a nano-material

Descriptors for the Production of a Nano-Material	
Descriptor	**Definition**
Subcategory: Starting Materials	
Number of components	The number of starting materials
List of components used as starting materials	The names of all starting materials
Component Description	
Component name	Chemical name of the component
Component formula	Chemical formula of component
Component amount (absolute or percentage)	Amount of component, either in absolute quantity or percentage of all starting material
Component source	Source of component, supplier, etc.

Component purity	Purity of component
Component physical state	Physical state of component, liquid, gas, solution, etc.
Subcategory: Recipe	
Recipe name	Name of the recipe that specifies starting materials and conditions
Recipe source	Source of the recipe
Recipe documentation	Documentation of the recipe
Recipe details	Details contained in recipe
Changes from recipe	Deviations from standard recipe
Subcategory: Equipment (recurring)	
Equipment name	Name of equipment used in production
Equipment manufacturer	Manufacturer of equipment
Equipment role	Purpose of the equipment
Equipment set parameters	Initial setting of equipment parameters
Equipment model	Equipment model number
Calibration	Calibration details, when and how, etc.
Subcategory: Production Technique	
General description	Description of the production method
Documentation	Documentation of the production method
Source	Source of the production method
Variation(s) used	Variations from the standard production method
Subcategory: Conditions	
Temperature	Temperature(s) used
Media	Media(s) used
Media composition	Composition of media used
Pressure	Pressure(s) used
Other initial set parameters	Other initial conditions
Parameters monitored through production	Parameter monitored during production, e.g., concentration, temperature, etc.
Subcategory: Production Result	
Nanomaterials produced	Use information categories for nano-objects or collection of nano-objects as appropriate
Purity	Purity of nanomaterials produced
Composition	Amount of each nanomaterial produced
Yield	Amount of actual production compared to theoretical amount possible
Physical state	Physical state of nanomaterial
Date produced	Date produced

Location	Geographic or facility location of production
Producing organization	Organization that did the production
Batch number	Number of specific batch of nanomaterial
Production documentation	Other production documentation

B. Post Production History

In this subcategory, information of how a nanomaterial was subjected to initial post-production processing, stored, and transported. Information on exposure history provides a means to record the conditions to which a nanomaterial has been exposed subsequent to its being produced or being put into service. Because nanomaterials can be very reactive, this information is needed to establish that the nanomaterial continues to meet new or revised design criteria. The reporting of post-production history of a nanomaterial uses a number of descriptors as shown in Table 16.

Table 16. Descriptors for the post-production history of a nanomaterial

Descriptors for the Post-Production History of a Nanomaterial	
Descriptor	**Definition**
Subcategory: Post-Production Process	
Process type	Purification, storage preparation, actual storage, transportation preparation, actual transportation
Subcategory: Post-Production Process Recipe	
Recipe name	Name of the recipe that specifies starting materials and conditions for post-production process
Recipe source	Source of the recipe
Recipe documentation	Documentation of the recipe
Recipe details	Details contained in recipe
Changes from recipe	Deviations from standard recipe
Subcategory: Post-Production Equipment	
Equipment name	Name of equipment used in post- production
Equipment manufacturer	Manufacturer of equipment
Equipment role	Purpose of the equipment
Equipment set parameters	Initial setting of equipment parameters
Equipment model	Equipment model number
Calibration	Calibration details, when and how, etc.
Subcategory: Post-Production Technique	
General description	Description of the post-production method
Documentation	Documentation of the post-production method
Source	Source of the post-production method
Variation(s) used	Variations from the standard post-production method

Subcategory: Post-Production Conditions	
Temperature	Temperature(s) used
Media	Media(s) used
Composition	Composition of media used
Pressure	Pressure(s) used
Other initial set parameters	Other initial conditions
Parameters monitored through post-production	Parameter monitored during post-production, e.g., concentration, temperature, etc.
Subcategory: Post-Production Process Result	
Nanomaterial produced	Use information categories for nano-objects or collection of nano-objects as appropriate
Purity	Purity of nanomaterials produced
Composition	Amount of each nanomaterial produced
Yield	Amount of actual production compared to theoretical amount possible
Physical state	Physical state of nanomaterial
Date produced	Date produced
Location	Geographic or facility location of post-production
Post-producing organization	Organization that did the post-production
Batch number	Number of specific batch of nanomaterial
Post-production documentation	Other post-production documentation

XIV. 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 referred or used by 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.

ISO TC 229 has developed a standard on guidance for specifying nano-objects [10] that is:

"In response to the failure of specifications agreed between suppliers of manufactured nano - objects and their customers to ensure delivery of material that responds consistently to downstream processing or that is capable of generating consistent performance in the final product between batches and lots.

"This observed inconsistent performance of batches or lots of material has led to the conclusion that the cause has to be related to one or more of the following scenarios.

a) "The specification agreed between customer and supplier does not cover all material characteristics that have an influence on performance and/or processability, or it has been interpreted differently by the customer and supplier.
b) One or more material characteristic is currently being measured by an inappropriate technique.
c) *One or more measurement technique is being applied in an incorrect manner."*

In the case of nanomaterials, the specification itself contains well defined information about the nanomaterial and its properties, often including detailed information about production, shipping, and storage. Descriptors used in specifications are given in Table 17.

Table 17. Descriptors for a specification of a nanomaterial

Descriptors for a Specification of a Nanomaterial	
Item	**Definition**
Specification name	The name given in the specification document
Specification title	Title of specification document
Specification authority	Authority issuing specification document
Date of issue	Date of issue for specification document
Type of specification	Type of specification document [standard specification, regulation, company specification, purchase order, material list, etc.]
Version of specification	Version of the specification document
Identification number	When the number refers back to a document or reference source that specifies the nanomaterial

References

[1] www.codata.org/nanomaterials
[2] http://www.iso.org/iso/iso_technical_committee?commid=381983
[3] http://www.astm.org/COMMITTEE/E56.htm
[4] http://www.oecd.org/science/nanosafety/
[5] ISO/TS 800004-1:2010(E)
[6] http://ec.europa.eu/environment/chemicals/nanotech/#definition
[7] http://www.iupac.org/home/publications/e-resources/nomenclature-and-terminology.html
[8] http://www.cas.org/content/chemical-substances/faqs
[9] *Considerations on a Definition of Nanomaterial for Regulatory Purposes*, Göran Lövestam, Hubert Rauscher, Gert Roebben, Birgit Sokull Klüttgen, Neil Gibson, Jean-Philippe Putaud and Hermann Stamm, Reference Report by the Joint Research Centre of the European Commission, EUR 24403 EN (ISBN 978-92-79-16014-1)
[10] ISO/TS 12805:2011(en) Nanotechnologies — Materials specifications — Guidance on specifying nano-objects

Appendix A: Measurement Value

A.1 Introduction

Scientific data are the result of measurements made on one or more objects under circumstances that are controlled as much as possible. While a wide variety of measurements are possible, they generally may be classified as one of three types: Experimental, Observational, and Calculational. While there are similarities in how results are reported, the three types need to be described using significantly different information to describe the detailed procedures used. A number of models of measurement value results exist, many of which are more detailed than given below. Users are encouraged to use the models that most closely meet their information needs.

When measurement results are specified in the Uniform Description System for nanomaterials, the results should be considered a *measured value* as defined below.

A.2 Measured Value

Regardless of how generated, in the UDS, *measured value* explicitly includes the following additional items as listed in Table 18.

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Table 18. The content of a measured value

The Content of a Measured Value	
Item	**Definition**
Value	The measured result
Number of significant figures	Number of significant figures being reported
Unit	The unit of the value
Uncertainty	Statement of uncertainty about the value