



ICSU - CODATA Workshop on the Description of Nanomaterials

Ministère de l'Enseignement Supérieur et de la Recherche 25 rue de la Montagne-Sainte-Geneviève 75231 Paris France

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The promise of nanotechnology is great, and every industrial country is making significant investments to realize its economic potential. Nanomaterials are a key foundation for progress in nanotechnology, and many scientific and engineering problems are being overcome. One significant challenge in advancing progress on nanomaterials arises from the large number of scientific disciplines that have an interest, including chemistry, materials science, molecular and cellular biology, medicine and health science, environmental science, as well as many others.

The International Council for Science (ICSU) and CODATA, the ICSU Committee on Data for Science and Technology, are sponsoring a two-day round-table workshop designed to bring together international scientific experts from these diverse fields to review the present status of developing description systems for nanomaterials and *to bring the views of their respective scientific communities to the attention of groups actively engaged in developing standardized nanomaterials descriptions*. As a result of the workshop, it is expected that scientific unions, national and international standards development organisations, and other groups will be activated to work cooperatively in addressing the complex issues associated with description of the full range of possible nanomaterials.

The workshop will feature overview presentations from experts in various aspects of nanomaterials, summaries of ongoing description development work, and small discussion groups to identify needed future actions. The workshop will be on an invitation basis and held in Paris on 23-24 February 2012. Approximately 50-60 attendees are expected.

Workshop Technical Focus

One key factor in the commercialization of any material, including all types of nanomaterials, is the development of an accepted method for describing the material. The potential value of nanomaterials makes the development of a nanomaterials description systems of great importance. We use the following definitions related to nanomaterials.

Nanoscale: The size range from approximately 1nm to 100 nm.

Note 1: Properties that are not extrapolations from a larger size will typically, but not exclusively, be exhibited in this size range. For such properties the size limits are considered approximate. [From Technical Specification ISO/TS 27687: 2008 on nanotechnologies]

Note 2: The lower limit in this definition (approximately 1 nm) is introduced to avoid single and small groups of atoms from being designated as nano-objects or elements of nanostructures, which might be implied by the absence of a lower limit.

Nano-object: A material with one, two or three dimensions in the nanoscale

Nanoparticle: Nano-object with all three dimensions in the nanoscale

Nanomaterial: A material with any dimension in the nanoscale *or* having internal structure *or* surface structure in the nanoscale. This definition includes nano-object and nanostructured material. [From ISO TC229]

1. The importance of description systems in commercializing nanomaterials

For a material to be commercially adopted, users and producers must be confident that they both know exactly what material is under consideration. The material must be produced with consistency and reproducibility. Often this is done by the development of material specifications by Standards Development Organisations. An accepted robust description system is fundamental to adoption of material. Further, an accurate method for describing a material is critical for making improvements to a material, its properties, or manufacturing processes.

2. What information has to be specified?

The basic information for describing most features of any material is independent of the type of material. One has to specify information on the naming conventions, composition, structure, connectivity and association of individual components (including chemical bonding), processing methods, and defining properties. Material description systems vary dramatically across material classes, from pure chemicals to complex biological materials, but the fundamental types of information are the same regardless of class. Nomenclature systems for materials such as chemicals, engineering materials (metals, alloys, ceramics, polymers, and composites), biological species, and bio-molecules have taken decades or even centuries to develop. Such systems also vary widely from country to country.

Nanomaterials represent a new class of materials, more complex than individual molecules, yet with a complexity significantly different from macroscopic materials such as engineering and biological materials. Their reach into different disciplines brings an additional layer of complexity in that a successful description system must be usable by a wide variety of physical science, engineering, biological, medical, and environmental disciplines and compatible with other description systems used in those fields.

3. Challenges in developing a nanomaterials description system

The first of course is the diversity of materials, When looking at aggregation of hundreds to tens of thousands of atoms, with both ionic and covalent bonding as well as micro-structural characteristics, it is not always clear if a nanomaterial is inorganic, organic, biological, or engineering material. As a consequence, the notion of a single nanomaterial description system may need to be replaced by a need for multiple compatible systems.

A second concern is the maturity of producing nanomaterials. The production of single-walled carbon nanotubes is a case in point. At present aspects related to the uniformity and reproducibility of these nanotubes are still partially an art and the nanomaterial itself still highly dependent on processing parameters not yet fully understood. The role of processing information in describing this particular nanomaterial (carbon nanotube) is clearly important. Every different process will likely yield a different material, as with ceramics.

Similar to all commercial materials, there are many uses of the description system: regulatory development, purchasing requirements, medical therapies, environmental, health and safety issues, public perception, and research and development. A central question is it possible that a single unified nanomaterial description can be developed to satisfy these and other uses.

A third issue is the need for an open access database containing key terminology and knowledge. If such a database is created, should it focus just on terminology and data important across disciplines, or should it contain all available terminology and data.

The ICSU-CODATA Workshop on the Description of Nanomaterials will address these and other challenges. ICSU is uniquely positioned to mobiles knowledge and resources of the international scientific unions who are concerned with nanomaterials, their use, and their impact, bringing a multi-disciplinary perspective to the challenges outlined about. OECD, through its ability to involve the world's major economic player has access to governmental expertise working on nanotechnology. CODATA, as the major international scientific and technical data organization, brings decades of expertise on how the tools of the information revolution can be used to address the problems defined above.

The Workshop recommendations and report will be published in the CODATA Data Science Journal.