UNIVERSITY OF BIRMINGHAM | COLLEGE OF LIFE AND ENVIRONMENTAL SCIENCES

Integrating the codata Uniform Descriptor System into extension of InChI for nanomaterials

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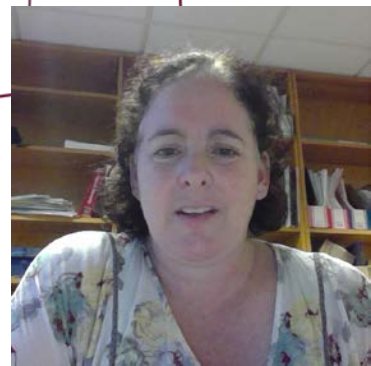
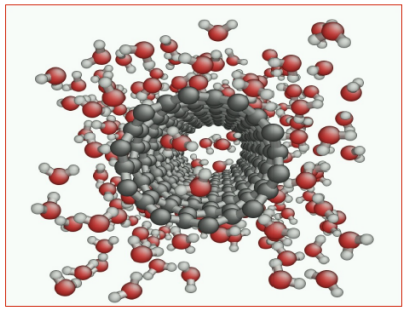


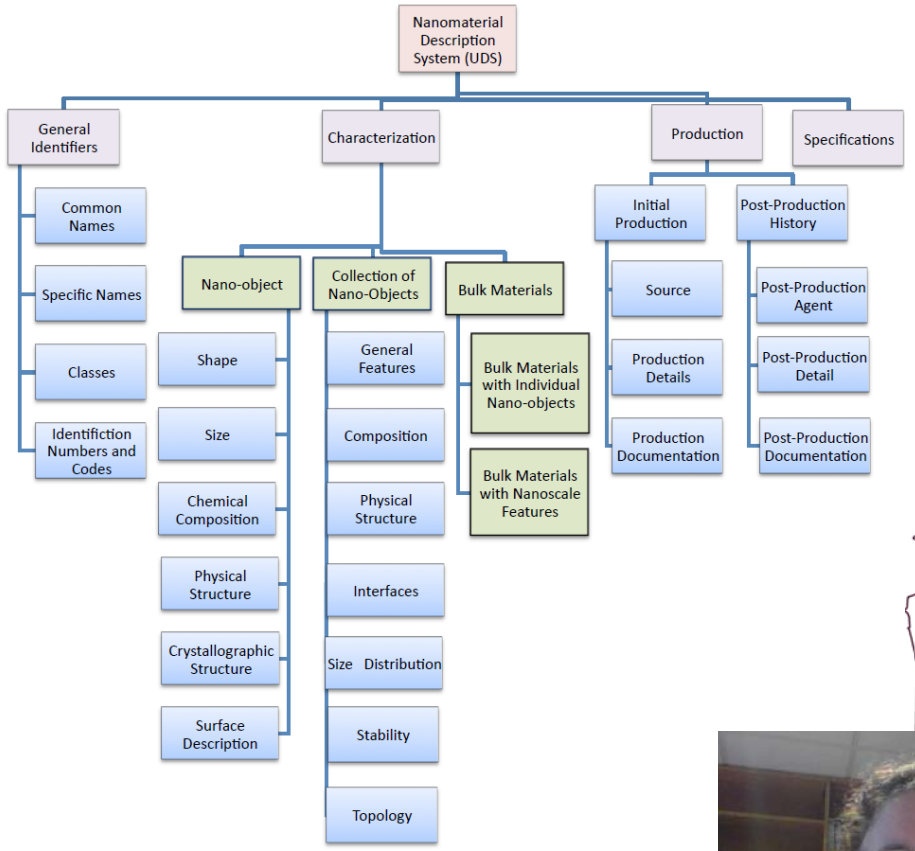
The Uniform Description System for nanoscale materials

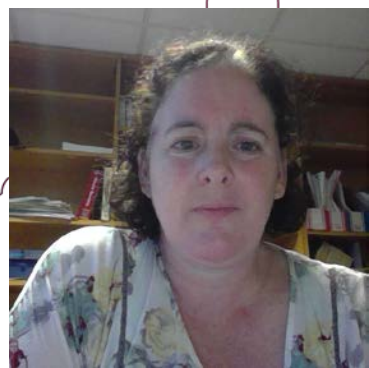
Uniform Description System for Materials on the Nanoscale



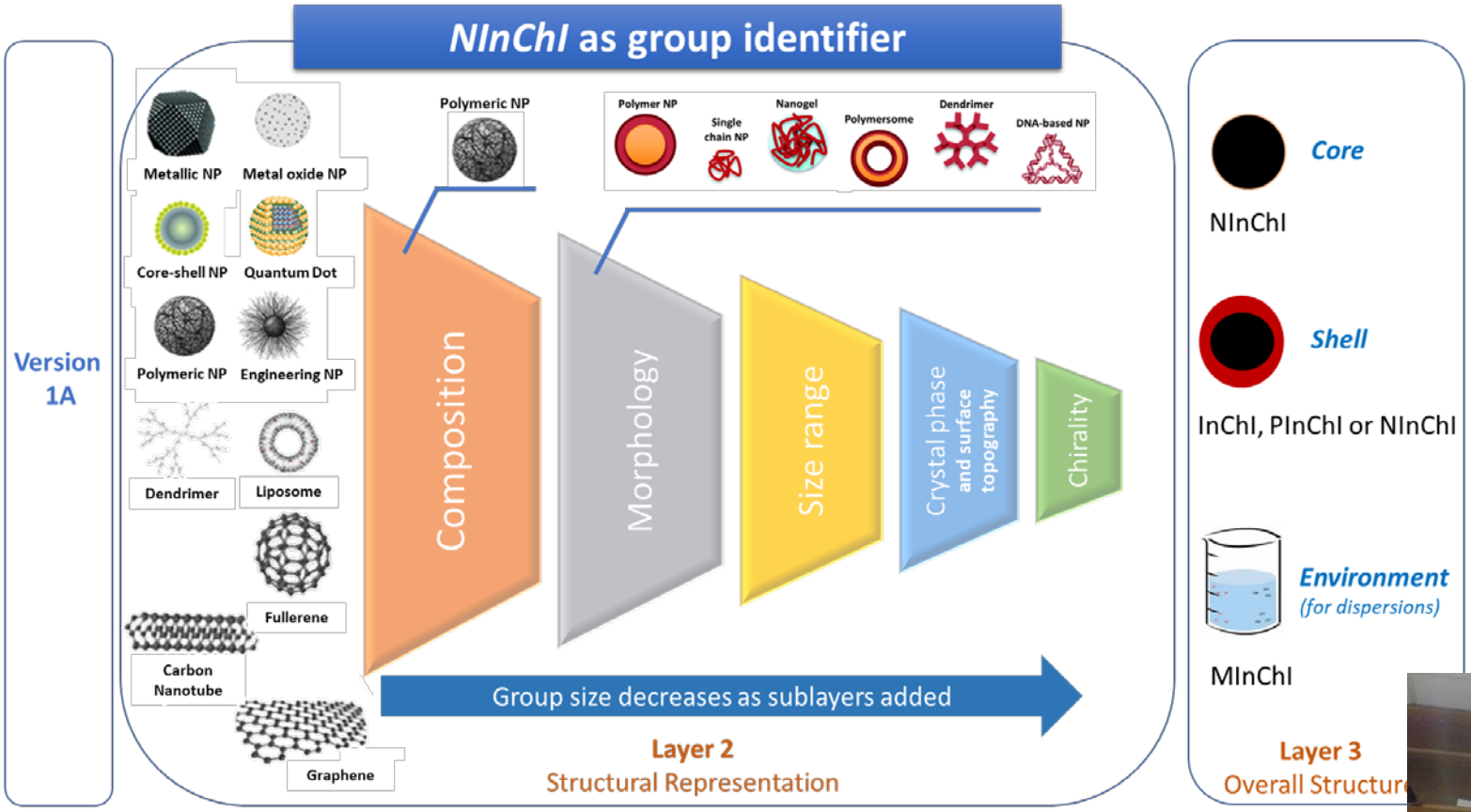
Prepared by the CODATA-VAMAS Working Group
On the Description of Nanomaterials
www.codata.org/nanomaterials

Version 1.0
1 February 2015

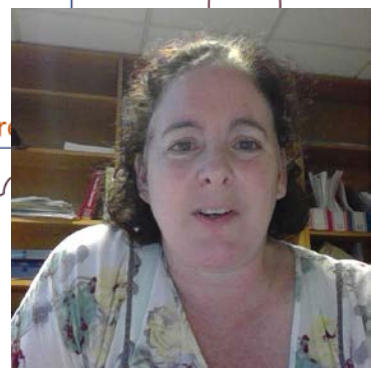




Alpha version of specification of Nanomaterials in InChI



https://doi.org/10.3390/nano10122493



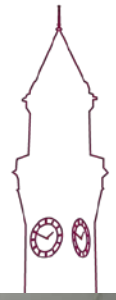
Task Group to integrate and align

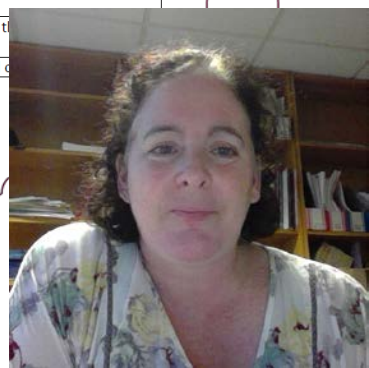
Planned activities (Two years)

- Dataset curation by members to develop sets of real-world nanomaterials libraries to **challenge** the implementation and coding of the NInChI
- Virtual hackathons with nanomaterials experts and the IUPAC NInChI working group experts to develop workable suggestions for how to **encode** these different aspects, some of which are likely to be non-canonical and poorly characterized or understood.
- Workshop (hopefully face to face) in Cyprus in June 2022 as satellite event to the NanoCommons final conference and "Nanoweek" of activities. The CODATA-InChI Trust NInChI session will be a key milestone in the roadmap towards implementation of NInChI as an **official standard extension of IUPAC InChI Trust.**

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 t nano-object
Type of surface charge	Charge sign, magnitude, full c





Membership & alignment with IUPAC and international efforts

Expected Outputs and Outcomes

- Curated and well-documented (full metadata) nanomaterials descriptions and associated characterization data (where available) and the associated NInChIs.
- Descriptions of the decisions made and how the NInChIs were generated.
- Description of the alignment with the other InChI working groups for mixtures and reactions especially with respect to standardising what information is provided in the core NInChI versus what is in the Auxiliary Information, and why.
- Guidelines of using NInChI as part of the UDS.
- Support community understanding and adoption of the NInChI standard in due course.
- Report from stakeholder workshop on user feedback and real-world considerations of the NInChI.

Membership

- Open to all, with EU, US, Canada, Brazil, China, South Africa and South Korea participation already.
- Strong linkages already established with IUPAC and the InChI Trust, which are growing to include other IUPAC activities such as the working group on chemical connectivity etc.
- Other Unions such as IUCr, IUTox, IUPAP, would be invited to join.
- Link to IUPAC Committee on Publications and Cheminformatics Data Standards will be made.

Vote and Join!

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NanoCommons
Nano-Knowledge Community

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