VAMAS

Nanoparticle Populations

Technical Working Area 34

Call for Participation

Project 17

Line notation and unique identifiers for nanomaterials and groups of nanomaterials

Objectives

Clear, unambiguous reporting of the identity of a nanomaterial is a complex and not completely solved task. A standardized line notation encoding important physicochemical characteristics will improve this situation. It could replace other suboptimal unique identifiers and provide better machine readability. Specific objectives are:

Identify and agree on a set of characteristics needed to be encoded in the line notation.

Generate a technical specification and software implementation compatible with the chemical line notation InChI and its extensions endorsed by IUPAC.

Test the line notation on a set of diverse nanomaterial classes to guarantee broad applicability but also to define the applicability domain of the identifier.

Background

VAMAS and CODATA jointly developed the Uniform Description System (UDS) for materials at the nanoscale to define minimal reporting guidelines for physicochemical characterizations of nanomaterials. This can be used as the basis for a line notation, which encodes all this information (or parts of it) in a compact form that is easy to extract from different documents, enabling comparisons, supporting searches for specific nanomaterials and corresponding data, and identifying similar materials. A first prototype was published recently as an extension of the InChI.

Standardization needs

The new line notation (NInChI) will improve the UDS by providing a unique identifier for a material or group of materials and, at the same time, a summary of the major characteristics of the material and its provenance. Standards based on the UDS should be updated accordingly.

Work Programme

- Dataset curation to develop sets of real-world nanomaterials libraries to challenge the implementation and coding of the NInChI as much as possible.
- Monthly virtual hackathons with nanomaterials experts and IUPAC NInChI working group experts to develop workable suggestions for how to encode different aspects of nanomaterials descriptors.
- Face-to-face workshops.

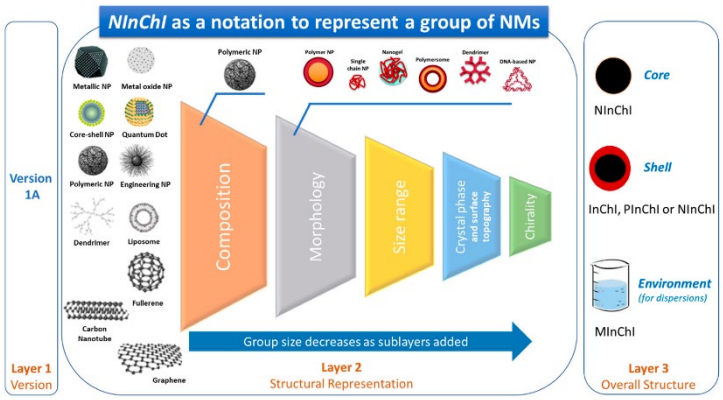

Illustration of the *NInChI*a notation to represent a particular group of NMs (reproduced from Lynch at al., https://doi.org/10.3390/nano10122493)

Deliverables and Dissemination

- Specification of a line notation for nanomaterials (NInChI, multiple development cycles) as extension to the IUPAC International Chemical Identifier (InChI).
- Standard implementation to be used in data management and reporting tools
- Update(s) of the UDS to integrate the NInChI and additional reporting requirements identified during the development of the NInChI.
- Update of ASTM E3144-19 and other standards based on UDS to include NInChIs and other reporting requirements.

International Participation

Current participants include volunteers from countries on all continents. Anyone with expertise in specific nanomaterial classes, standards for nanomaterial characterization, and machine-readable identifiers and representations is welcome.

Funding: Participants fund their own involvement in the project. Organization of workshops can be supported.

Status: The project started in 2022. Additional participants are welcome.

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