US-EU Communities of Research – Characterization Initiatives

Vladimir Lobaskin
University College Dublin, Ireland

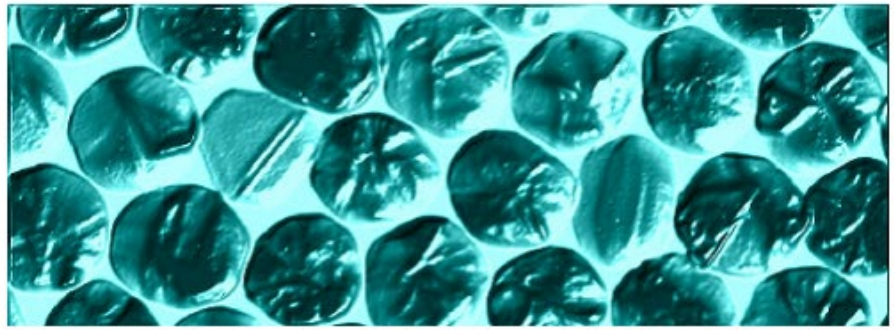
US — EU
Nanotechnology Communities of Research (CORs)

Welcome!

The U.S.-EU Nanotechnology Communities of Research (CORs) provide a platform for scientists to collaboratively identify and address key research needs through community-led activities such as telecons, webinars, publications, and annual in-person meetings. There are currently seven CORs addressing questions about the potential environmental, health, and safety (EHS) implications of nanomaterials and one Nanomanufacturing COR. Each COR has one U.S.-based co-chair and one EU-based co-chair. More information about these communities is available via the links below.

NanoEHS Communities of Research

Nanomanufacturing Community of Research



NanoEHS CoRs

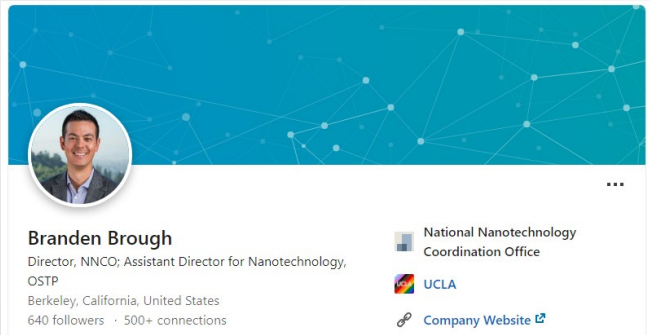
- **Who:** NanoEHS scientists and other interested stakeholders from academia, government, industry, and NGOs in the U.S., EU, and third-party countries.
- **What:** A platform for scientists to develop a shared repertoire of protocols and methods to overcome research gaps and barriers and to enhance their professional relationships.
- **Where:** Video- and/or teleconferences and annual workshops.
- **Why:** To address environmental, health, and safety questions about nanomaterials and to collaboratively advance the field.
- **How:** The communities will be largely self-run with the EC and the U.S. National Nanotechnology Coordination Office providing administrative support.
- Contact: Rhema Bjorkland (rbjorkland@nnco.nano.gov) for more information. Web: http://us-eu.org

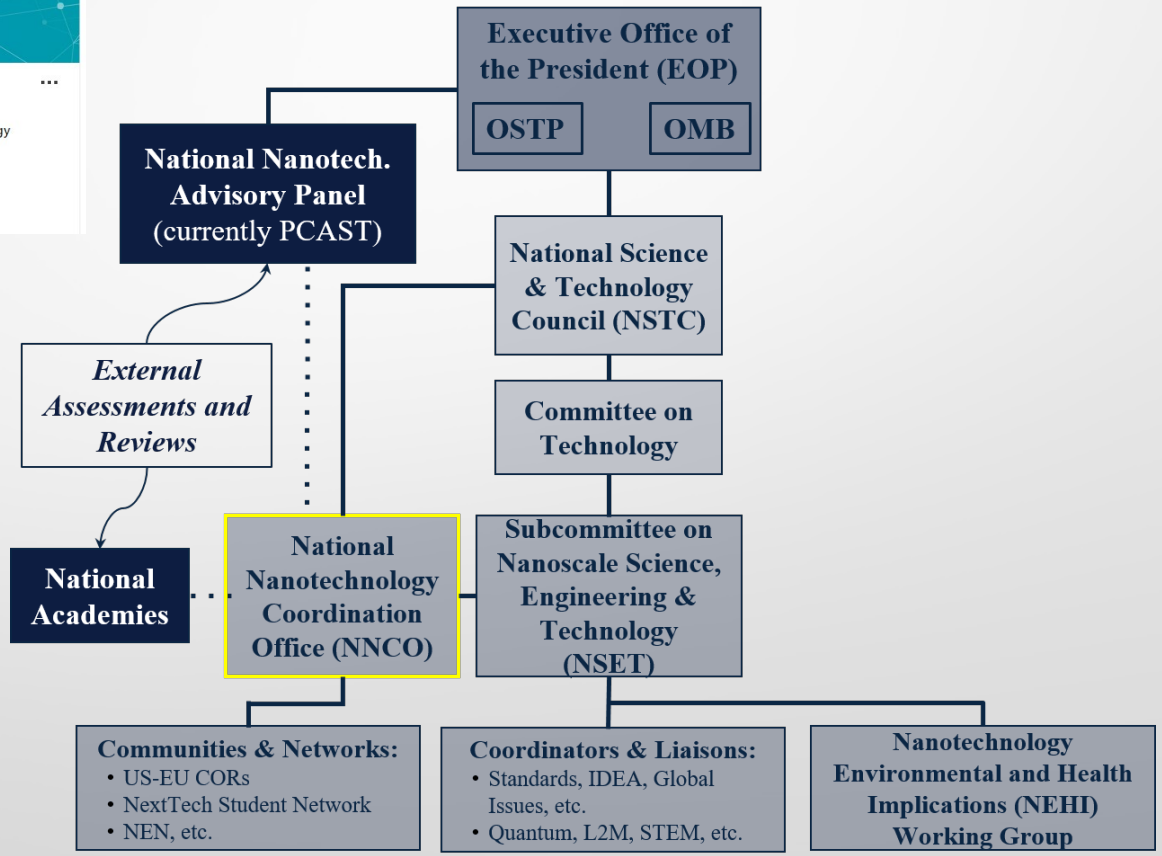
US-EU NanoEHS CoRs

- **Characterization**
  Co-chairs: Vladimir Lobaskin (EU) and Anil Patri (U.S.)
- **Databases and Computational Modeling for NanoEHS**
  Co-chairs: Fred Klaessig (U.S.) and Thomas Exner (EU)
- **Ecotoxicity**
  Co-chairs: Olga Tsyusko-Unrine (U.S.) and Susana Loureiro (EU)
- **Human Toxicity**
  Co-chairs: Arno Gutleb (EU) and Christie Sayes (U.S.)
- **Exposure through Product Life**
  Co-chairs: Christof Asbach (EU) and Paul Westerhoff (U.S.)
- **Risk Assessment**
  Co-chairs: Mark Wiesner (U.S.) and Keld Alstrup Jensen (EU)
- **Risk Management and Control**
  Co-chairs: Khara Grieger (U.S.) and Ulla Vogel (EU)

United States

National Nanotechnology Coordination Office (NNCO)





US National Nanotechnology Coordination Office: Structure and Connections

- Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the NSTC
- Nanotechnology Environmental and Health Implications (NEHI) Working Group

Connections:

- Environmental Protection agency (EPA)
- Department of Agriculture (USDA)
- Occupational Safety and Health Administration (OSHA)
- National Institute of Standards (NIST)
- Consumer Product Safety Commission (CPSC)
- National Institutes of Health (NIH)
- Food and Drug Administration (FDA)

US-EU NanoEHS CoRs
Annual meetings

- U.S.-EU NanoEHS Joint Workshop, October 11-12, 2018, Washington, DC, U.S.A.
- EU-U.S. NanoEHS CORs Workshop, October 15-16, 2019, Aix-en-Provence, France
- U.S.-EU NanoEHS COR Workshop: Bridging Insights and Perspectives September 16-17,2020, Virtual Meeting
- EU-U.S. NanoEHS CORs Workshop, Nanosafety Week, June 20-24, 2022, Limassol, Cyprus

US-EU NanoEHS CoRs Activities

- For individual CoRs, meetings organised by co-chairs at major conferences, e.g. SETAC Europe 2023 Main theme: Data-driven environmental decision-making
- Bi-monthly co-chairs web meetings
- Webinars
- Joint projects, e.g. EU NanoCommons, NanoSolveIT

US-EU NanoEHS CoRs
Discussion topics

- FAIRness of NM data (FAIR - Findable, Accessible, Interoperable and Reusable)
- Metadata stewardship
- Consistent NM representations, harmonization of ontologies and databases
- Detection and characterisation of micro and nanoplastics

EU Initiatives

Recent funding calls: focus on Data, IT and Modelling

- NanoSolveIT, NanoinformatiX, NanoCommons projects
- Advanced materials modelling and characterisation
- Adaptive multi-scale modelling and characterisation suites from lab to production

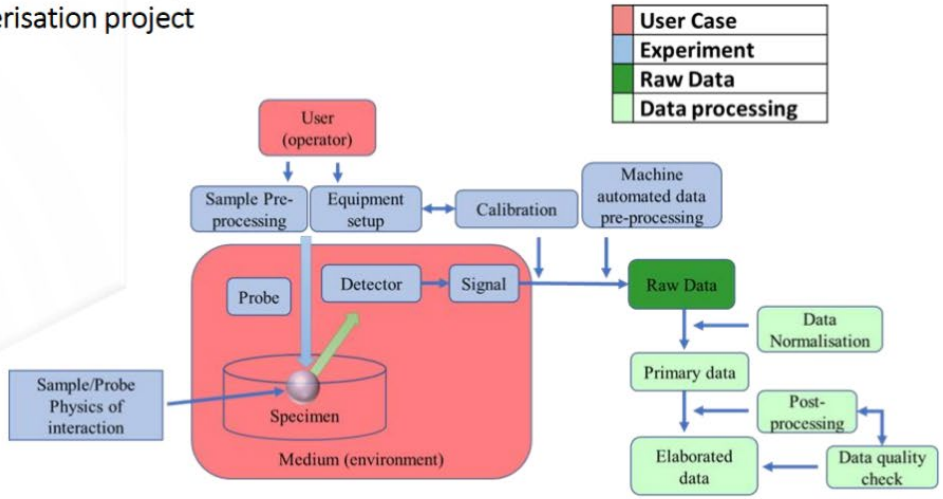
Collaborative networks

- European Materials Characterisation Council (EMCC)
- European Materials Modelling Council (EMMC)
- EU NanoSafety Cluster: https://www.nanosafetycluster.eu/

EU EMCC: Characterisation Data (ChaDa)

Standardised documentation (CHADA)

A common language and formal approach
how to log a characterisation project



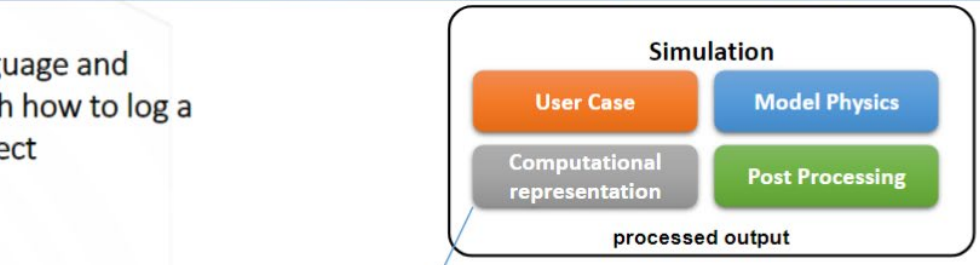
CWA 17815 "Materials characterisation - Terminology, metadata and classification "

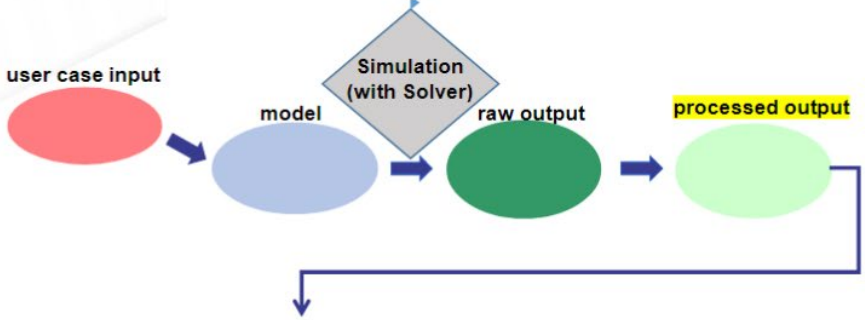
https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/ICT/cwa17815.pdf

EU EMMC: Modelling Data (MoDa)

Standardised documentation (MODA)

A common language and formal approach how to log a simulation project



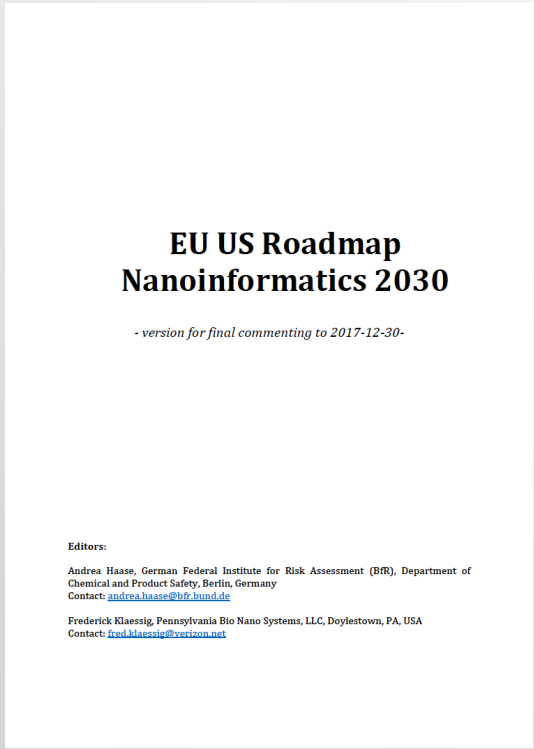


MODA for <user-case>
Simulated in project <acronym>

	OVERVIEW of the SIMULATION		
1	User Case		General description of the User Case. Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated. No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.
2	Chain of Models	Model 1	Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently. Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm). All models should be identified as electronic, atomistic, mesoscopic or continuum.
		Model 2	Please identify the second model.
		Data-based model	If data-based models are used, please specify.
3	Publication Peer-Reviewing the data		Please give the publication which documents the data of this ONE simulation. This article should ensure the quality of this data set (and not only the quality of the models).
4	Access conditions		Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).
5	Workflow and its rationale		Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently. This should include the reason why a particular aspect of the user case is to be simulated with a particular model.

US-EU Characterisation CoR Nanoinformatics Roadmap

Simplified Data Flow proposed in the NanoInformatics 2030 Roadmap



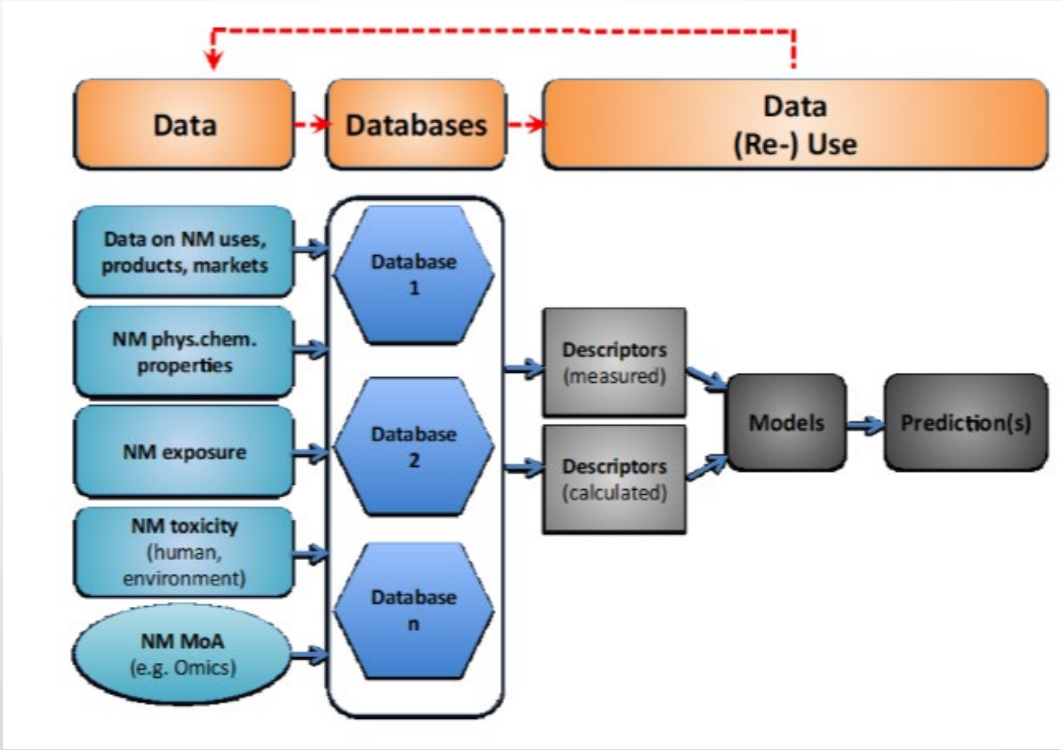
EU US Roadmap Nanoinformatics 2030

- version for final commenting to 2017-12-30-

Editors:

Andrea Haase, German Federal Institute for Risk Assessment (BfR), Department of Chemical and Product Safety, Berlin, Germany
Contact: andrea.haase@bfr.bund.de

Frederick Klaessig, Pennsylvania Bio Nano Systems, LLC, Doylestown, PA, USA
Contact: fred.klaessig@verizon.net



US-EU Characterisation CoR Recent activities

Nanomaterials **2020**, 10, 2493;
doi:10.3390/nano10122493

InChI for Nano: Extension of IUPAC InChI
A universal way to record the NM characteristics across different methods and map nanoforms

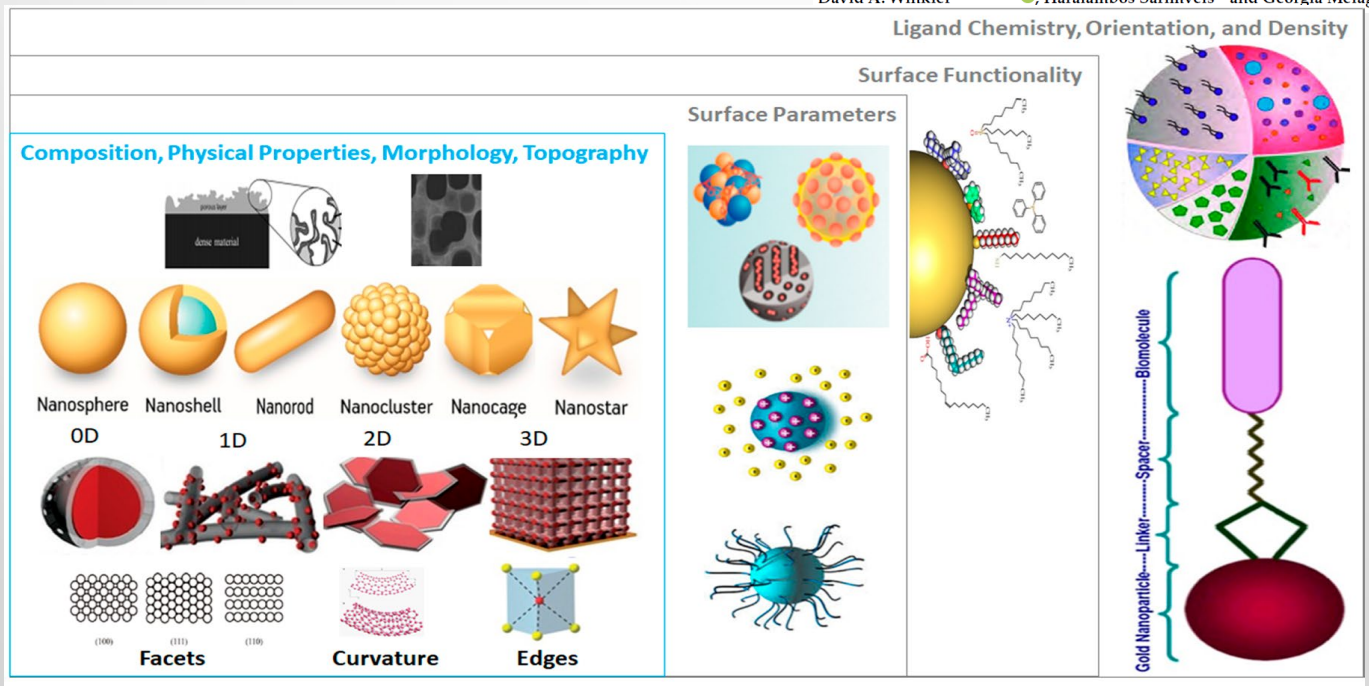
nanomaterials

MDPI

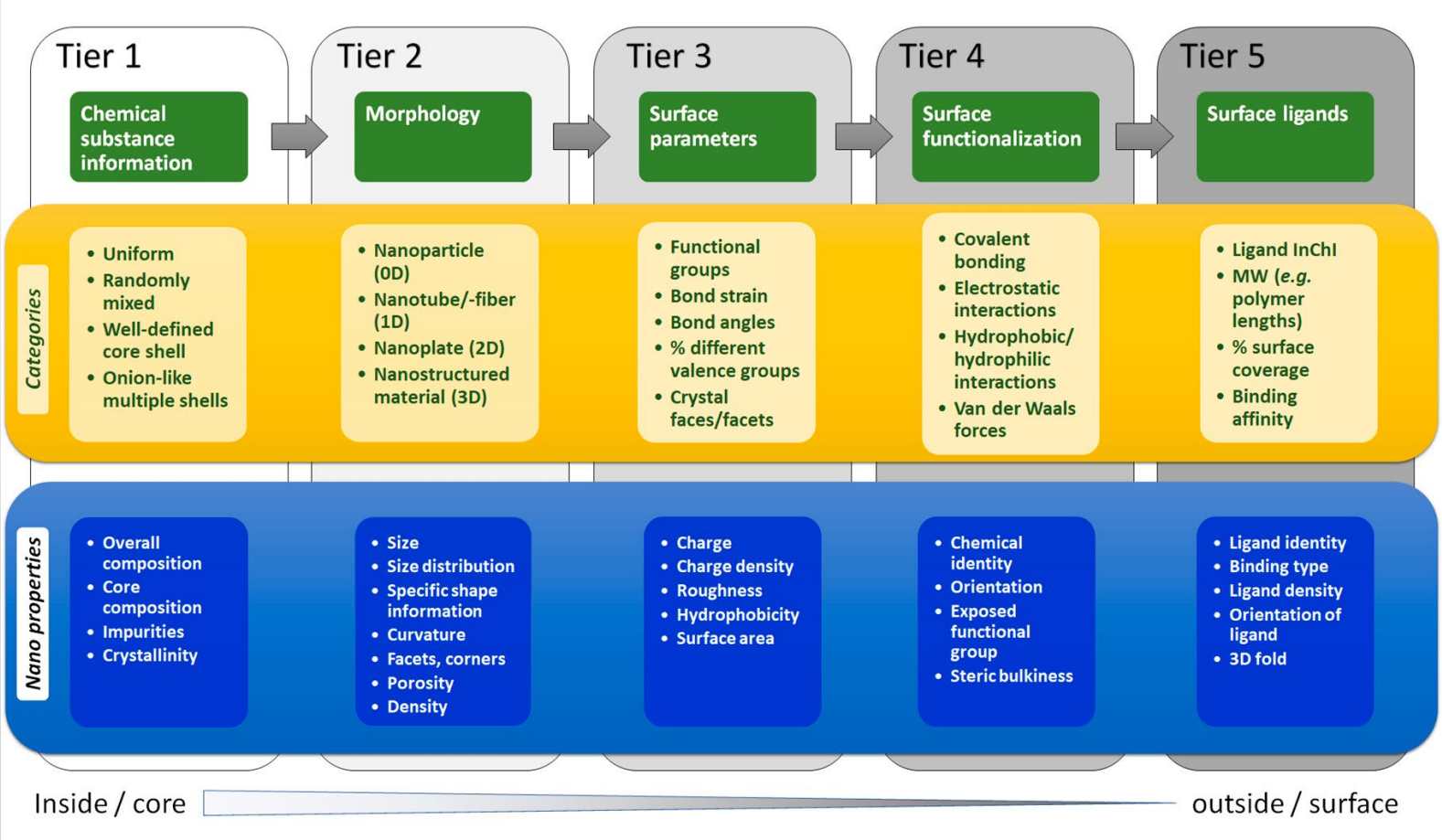
Article

Can an InChI for Nano Address the Need for a Simplified Representation of Complex Nanomaterials across Experimental and Nanoinformatics Studies?

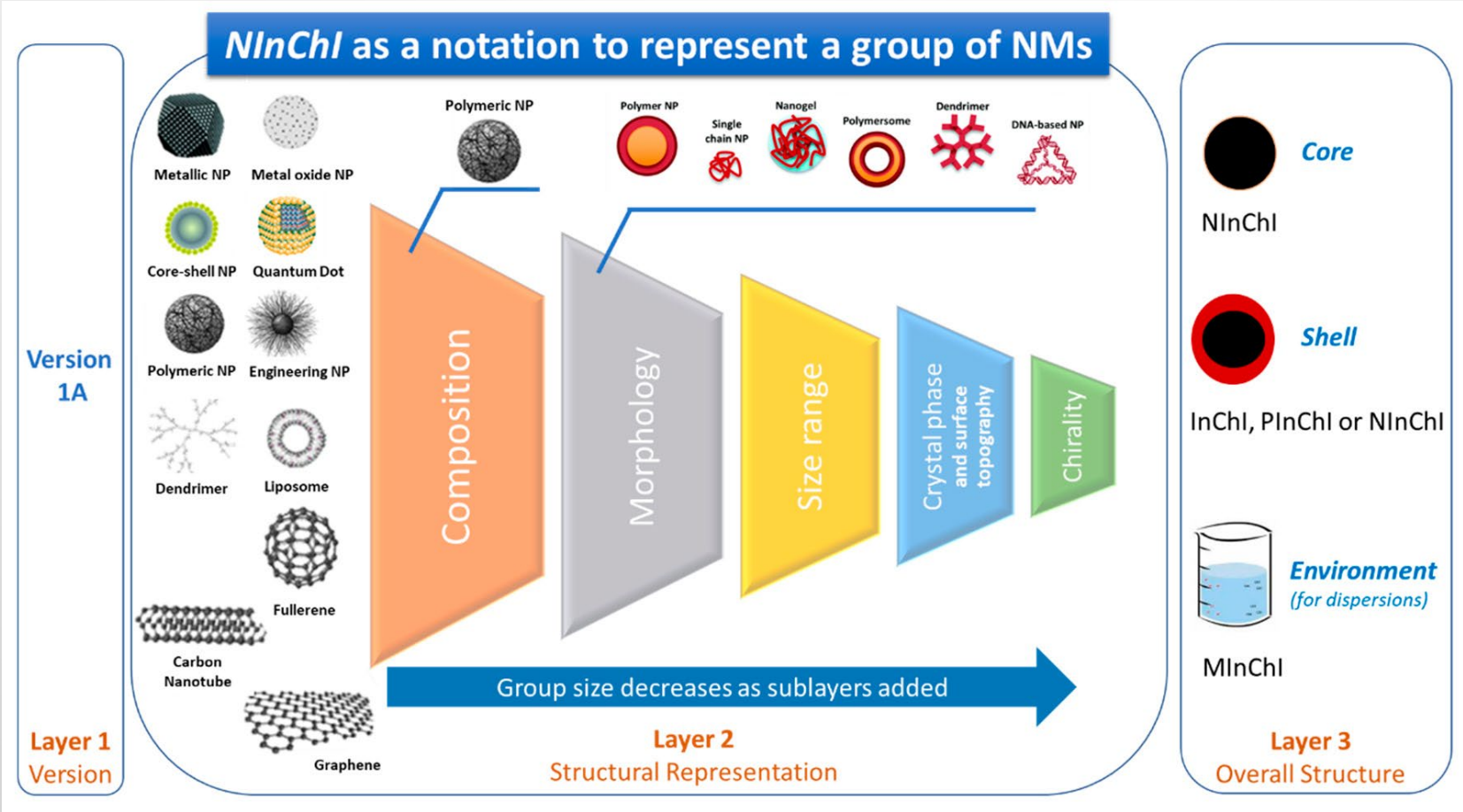
Iseult Lynch [1,*], Antreas Afantitis [2], Thomas Exner [3], Martin Himly [4], Vladimir Lobaskin [5], Philip Doganis [6], Dieter Maier [7], Natasha Sanabria [8], Anastasios G. Papadiamantis [1,2], Anna Rybinska-Fryca [9], Maciej Gromelski [9], Tomasz Puzyn [9], Egon Willighagen [10], Blair D. Johnston [11], Mary Gulumian [8,12], Marianne Matzke [13], Amaia Green Etxabe [13], Nathan Bossa [14], Angela Serra [15], Irene Liampa [6], Stacey Harper [16], Kaido Tämm [17], Alexander CØ Jensen [18], Pekka Kohonen [19], Luke Slater [20], Andreas Tsoumanis [2], Dario Greco [15], David A. Winkler [21,22,23,24], Haralambos Sarimveis [6] and Georgia Melagraki [2,*]



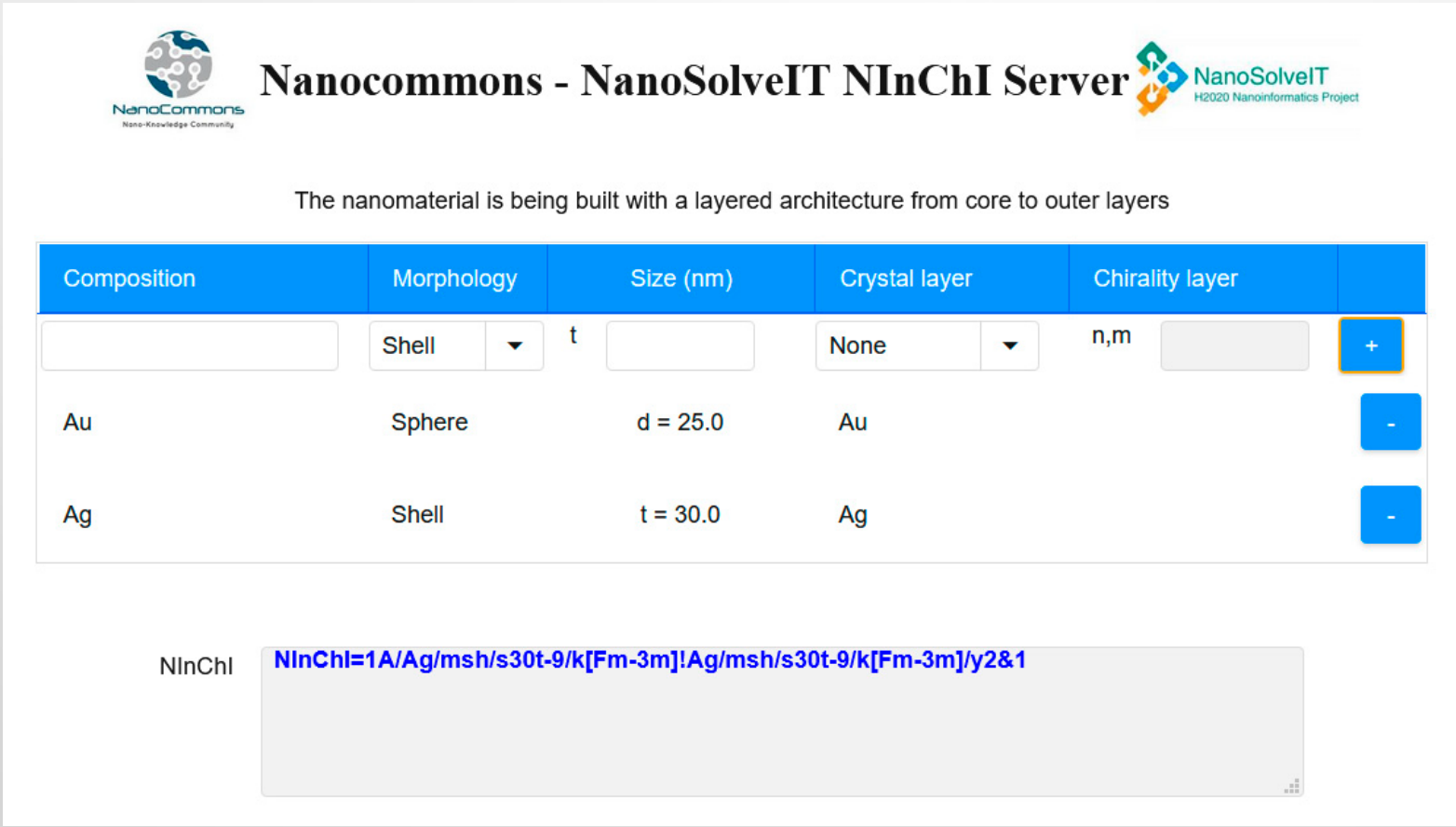
US-EU Characterisation CoR InChI for Nano



US-EU Characterisation CoR InChI for Nano



US-EU Characterisation CoR
InChI for Nano



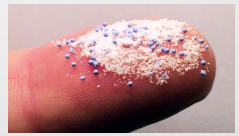
EU- US CoR Proposal for further actions (MNP)

1. Define Minimum level of reporting for publications on MNP (including additives, adsorbing pollutants)
2. Procurement of real-world samples (a public repository?)
3. Methods for robust reproducible characterization of pristine and aged MNP samples
4. Quantitative methods for exposure to MNP
5. SOPs / guidelines (e.g. California Water Board) for isolation, separation, characterization and quantitation and micro nanoplastics mixtures from complex matrices (water, sediments, food, feed, sea food etc).
6. Comprehensive database (e.g. eNanoMapper)
7. Inventory of projects and other resources (CUSP webpage)
8. Representative Test Material (RTM) / Benchmark material/test material in the absence of 'reference material standards (e.g. Hawaii Pacific Univ. Polymer Kit)
9. Models for release and adsorption of pollutants, morphology
10. New challenges from 3D printers

U.S. Interagency Nanoplastics Interest Group

- Formed in 2019 with the encouragement of the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council
- Staff support from the National Nanotechnology Coordination Office (NNCO)
- Purposes include:
  - Share information
  - Enhance collaborations and coordinate research
  - Minimize redundancies, leverage resources and capabilities
  - Understand knowledge gaps
- Thrust areas:
  - Collection & Characterization
  - Hazard, Exposure, & Risk Assessment
  - Reduction & Mitigation
- Participating agencies include FDA (chairing), EPA, DOI (USGS & USBR), NIST, CDC (ATSDR, NCEH, and NIOSH), DOL/OSHA, CPSC, DOD, USDA (FS and NIFA), DOE (Office of Science and EERE), NIH/NIEHS, NSF, NOAA (Marine Debris Program), State Dept., and NNCO.
- > 100 members; Meets once every two months

K.L. Law et. al., *Science*, **345**, 6193 (2014)



EU Efforts
Recent activities

CUSP International Conference 2023

When: 14th September 2023 (09.00-17.00)

Where: Jaarbeurs Centre, Utrecht, Netherlands.

Coordination with EU and US experts

- Contact CoR Co-chairs (Rhema Bjorkland)
- Take part in U.S.-EU NanoEHS CoR annual meetings
- Attend U.S.-EU NanoEHS CoR webinars
- NanoSafety Week – NSC annual meetings
- NSC Working Group F (Data) monthly web meetings

Meet us at conferences:

- SETAC meetings – special sessions
- 16th ICEENN, Plymouth, UK, 5 – 8 September 2023
- 23rd OECD WPMN meeting, Paris, France, 26-28 June 2023