

Nanoinformatics ~2010

NanoWG White Paper (part of NCI's caBIG effort)

- Modeling requires large data sets;
- One 'master' database unlikely due to maintenance costs and need for on-going curation;
- Laboratory databases will need to communicate, to federate, to be **findable, accessible**;
- Nanoparticle Ontology (NPO) meant as a template **interoperable** with bioinformatics databases
- ASTM standard

Nanoinformatics Inflection Point

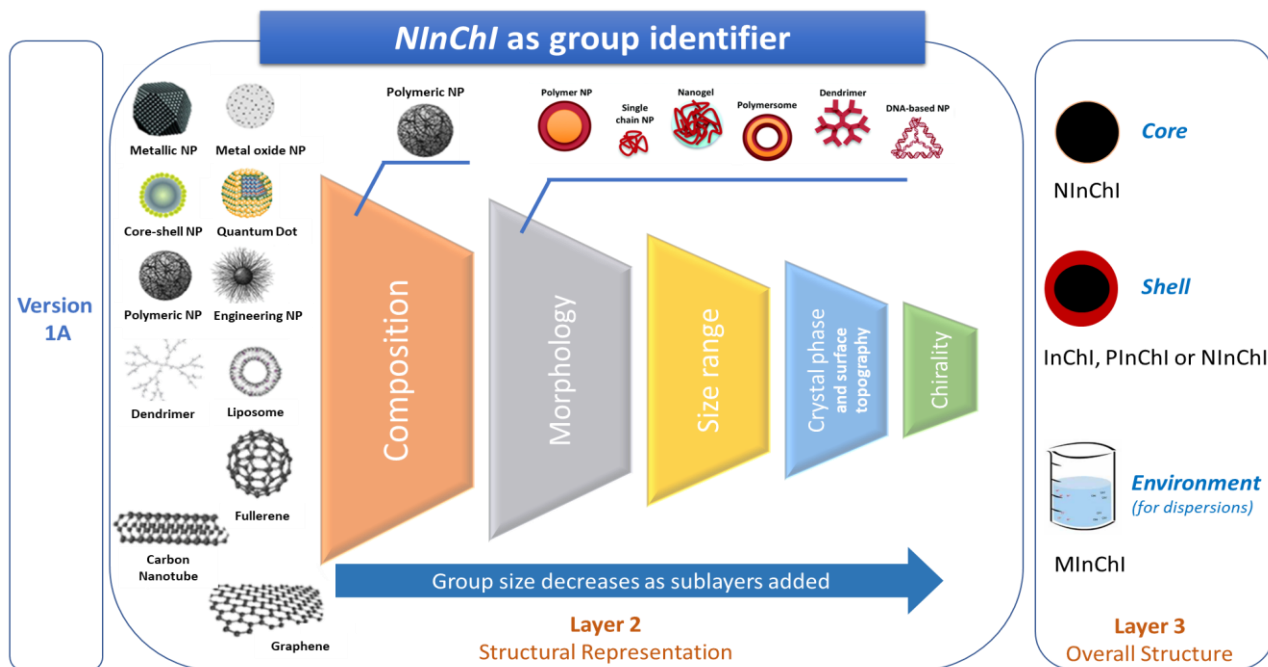
- NPO part of US discussion (CEIN and CEINT), but not used beyond caNanolab, **access** issues
- NPO incorporated into eNanoMapper along with other ontologies (ChEBI)
 - Data repository for EU-projects (**access** issues)
 - Has a regulatory focus (GHS, harmonized procedures)
 - Reports processed data more than lab measurements
- Not a 'large data set' useful for modeling
- Once again an uncoordinated landscape of locally administered databases

Current Informatics Directions

- Candidates for Persistent Identifiers
 - Chan: 2-90H(6)-(Pb,S)-[(Amn,Alk)]-O (90 nm PbS cube aminoalkane cap)
 - Nanomaterial Registry (US, administered by RTI)
 - NM #s at JRC repository and trade names
 - Demokritou: GNP003 (gold nanoparticle 003)
 - NaKnowbase (EPA): doi of the source publication
 - **European Registry of Materials (ERM): project-specific, covering also undisclosed nanomaterials**
- Persistent identifier
 - ISBN – semi-structured plus dedicated fields
 - NInChI machine-readable unit of ontology separate from the database structure

NInChI

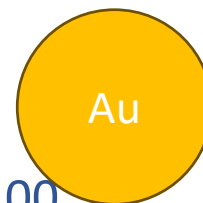
Jonathan Goodman:
The (N)InChI is a representifier = an incomplete representation and a good identifier



30nm gold nanoparticles (with citric acid stabilisation from synthesis)

NInChI=0.00.1A/Au/Nmsp/Ns0:15rxyz-9/Nk225!

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/Nmmol/No100/Ny1>2



30nm gold

NInChI=0.00.1A/Au/Nmsp/Ns0:15rxyz-9/Nk225!

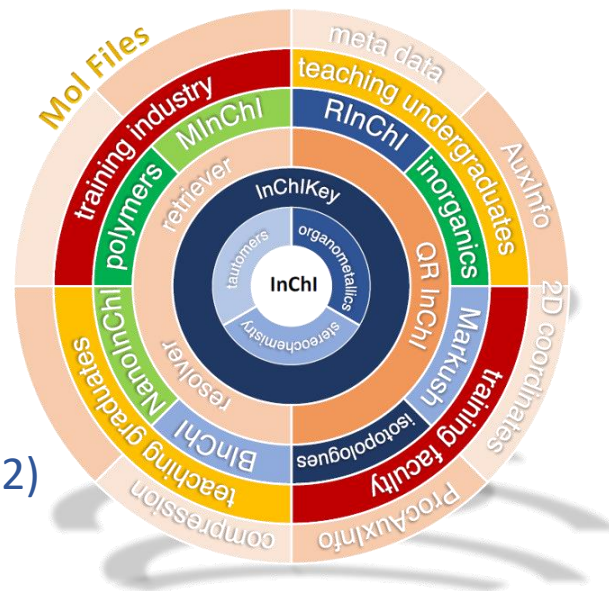
C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)
/Nmmol/No100
/Ny1>2

NInChI=0.00.2A/Au&

C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)
/Nn1>2/Nmsp&mol/Ns0:15rxyz-9& /Nk225& /No &100

NInChI=0.00.3A/InChI=1S/Au/Nmsp/Ns0:15rxyz-9/Nk225&

InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)/Nmmol
/Ny1>2/No &100



Morphology, size and crystallinity are properties of an entity (e.g. core)
Occupation is properties of multiple entities (e.g. ligands on surface of core)