NanoCommons

Nano-Knowledge Community

Introducing the InChI for Nanomaterials (NInChI)

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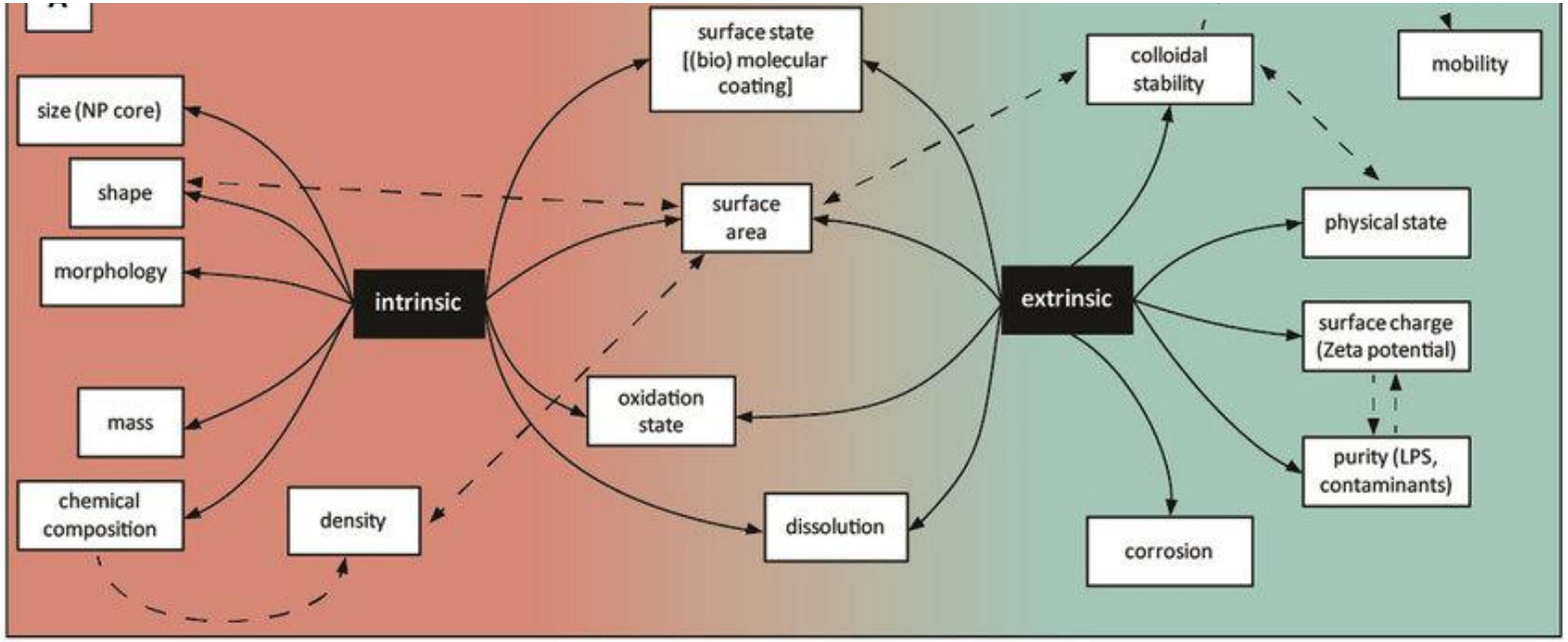
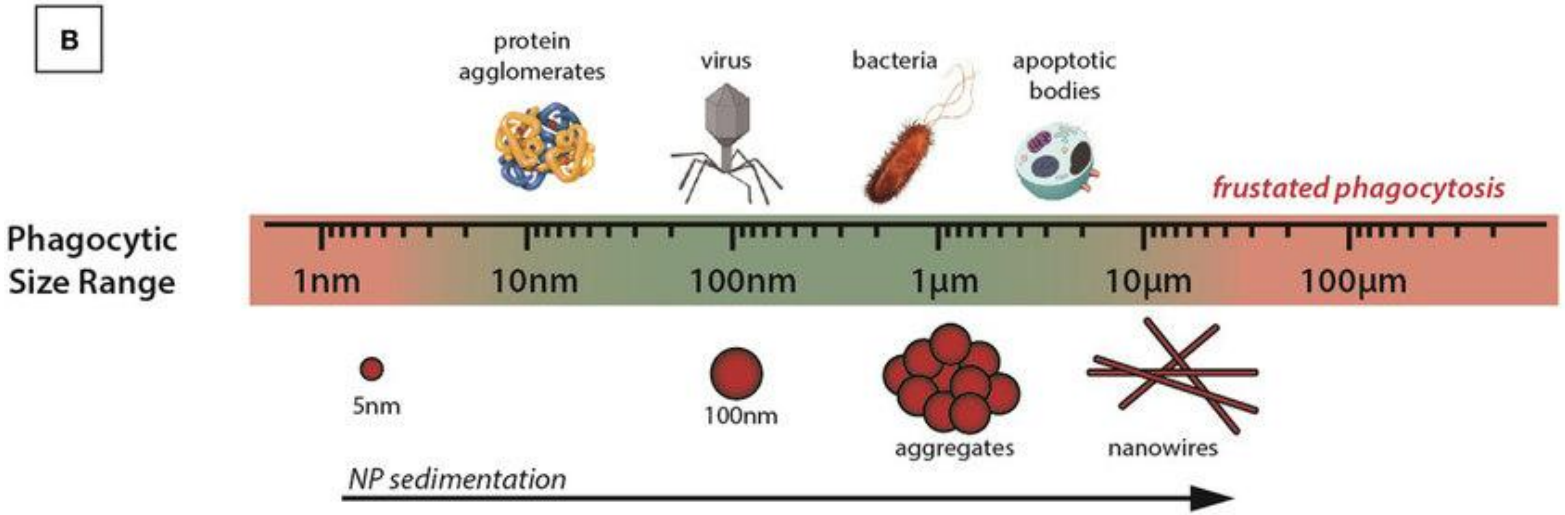
Dr. Antreas Afantitis, Novamechanics Ltd.

Dr. Thomas Exner, Seven Past Nine

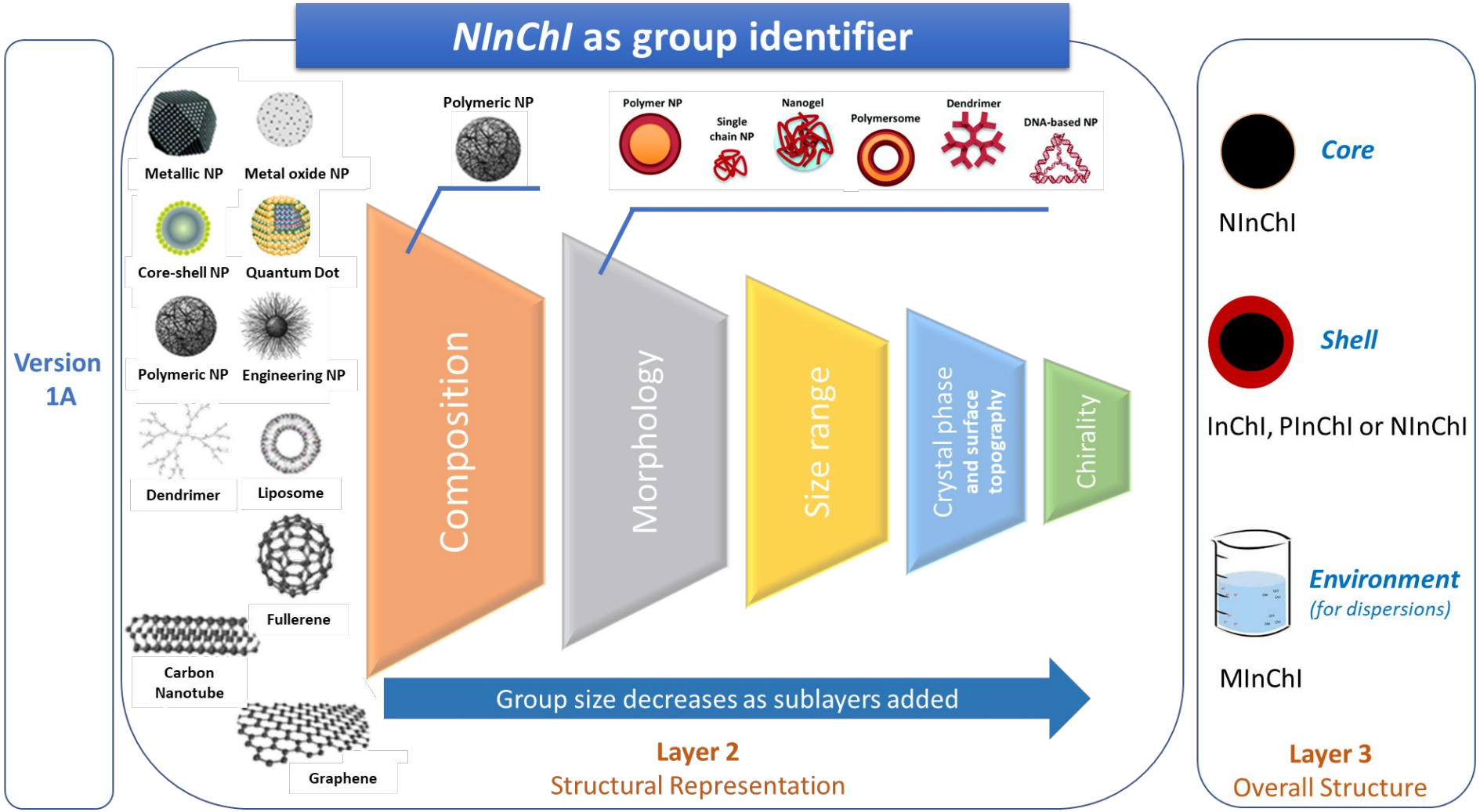
INTRINSIC VERSUS EXTRINSIC PROPERTIES OF NANOMATERIALS





https://www.frontiersin.org/articles/10.3389/fimmu.2017.00970/full

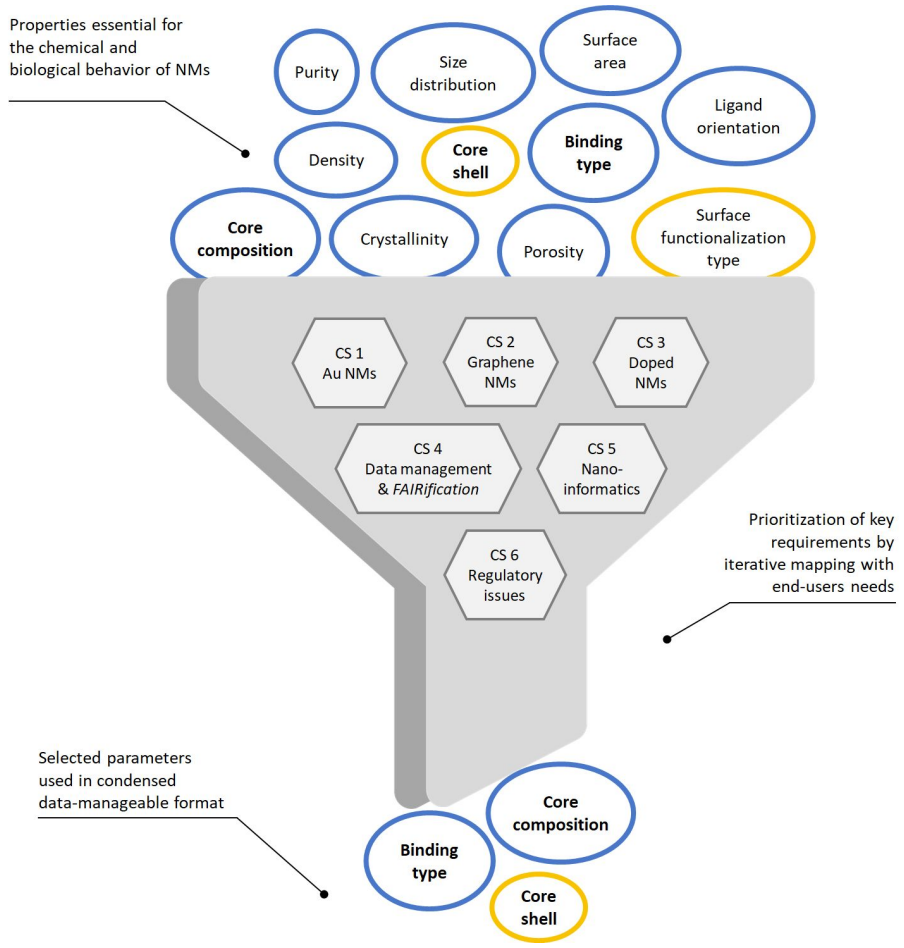
NInChI – enhancing interoperability of data – supporting "nanoforms"



NANOMATERIAL IDENTIFIER - InChI FOR NANO

Case studies

1. Library of Au NMs of different sizes and surface functionalities (ligands)
2. Library of carbon nanotubes
3. Complex chemistries and structures (Multi-metallics – doped / core-shell)
4. NM-related data management and incorporation into the FAIR data landscape
5. NInChI in Nanoinformatics
6. Regulatory challenges (e.g., nanoforms / sets of nanoforms)



BUILDING ON EXISTING InChI CONCEPTS

Component 1:
Composition: Au -> InChI=1S/Au
Morphology: shell -> sh
Size: thickness of 2 nm given as lower and upper radius -> 2t-9

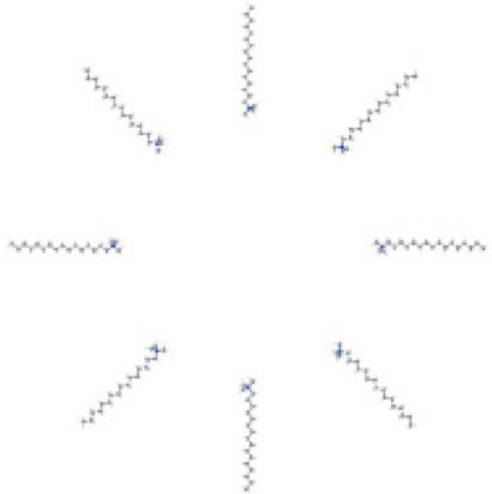
Part of NInChI for component 1: Au/msh/s1t-9

Component 2:
Composition: Si -> InChI=1S/O2Si/c1-3-2
Morphology: sphere -> sp
Size: diameter of 20 nm -> 20d-9
Space group: amorphous -> 000

Part of NInChI for component 2: O2Si/c1-3-2/msp/s20d-9/k000

Layer 1: 1A
Layer 2: /Au/msh/s2t-9!O2Si/c1-3-2/msp/s20d-9/k000
Layer 3: /y2&1 (ordering from inside out)

CTAB-capped gold nanoparticles, diameter = 20 nm



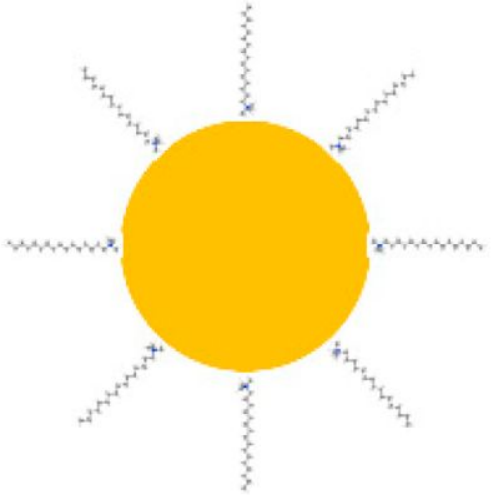
Component 1:
Composition: Au -> InChI=1S/Au
Morphology: sphere -> sp
Size: diameter of 20 nm -> 20d-9
Space group: not specified

Part of NInChI for component 1: Au/msp/s20d-9

Component 2:
Composition: Si -> InChI=1S/C19H42N.BrH
/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)4;
/h5-19H2,1-4H3;1H/q+1;/p-1
Morphology: none
Size: none
Space group: none

Part of NInChI for component 2: C19H42N.BrH
/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)4;
/h5-19H2,1-4H3;1H/q+1;/p-1

Layer 1: 1A
Layer 2: /Au/msp/s20d-9
!C19H42N.BrH
/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)4;
/h5-19H2,1-4H3;1H/q+1;/p-1
Layer 3: /y1&2 (ordering from inside out)



Other examples

Polystyrene-coated silica, diameter = 20–100 nm:

NInChI=0.00.1A/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2/z200-1-8!1S/O2Si/c1-3-2/msp/s20:100d-9/k000/y2&1

Chiral single-wall nanotube of the (3,1) type with 0.4 nm diameter:

NInChI=0.00.1A/C/mtu/s4d-10/w(3,1)/y1

TiO_2 nanoparticle of 2 nm in the anatase form doped with 5% HfO_2:

NInChI=0.00.1A/2O.Hf&2O.Ti/n{1&2}/g{5wf-2&}/msp/s2d-9/k{I 41/a m d}/y1

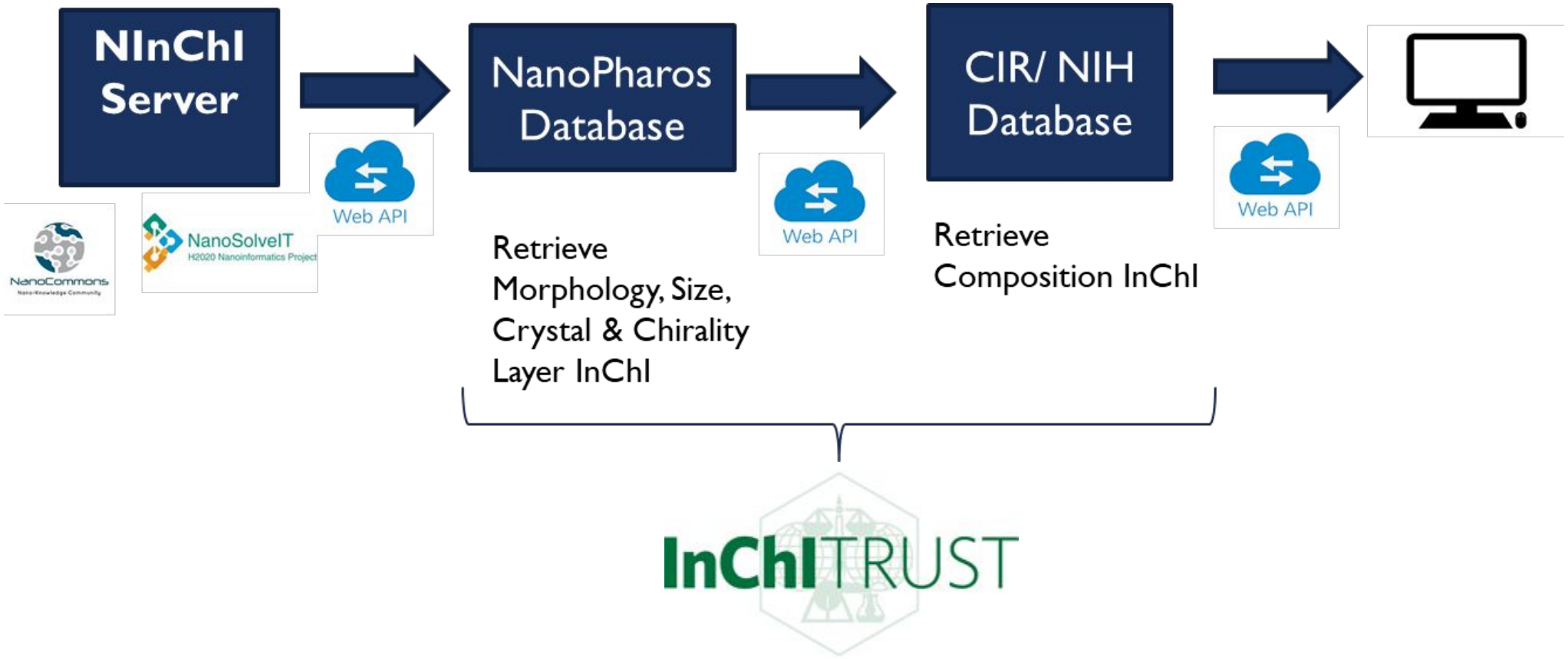
TECHNICAL IMPLEMENTATION

NInChI Server

Example with two components

https://enaloscloud.novamechanics.com/nanocommons/NInChI/

TECHNICAL IMPLEMENTATION

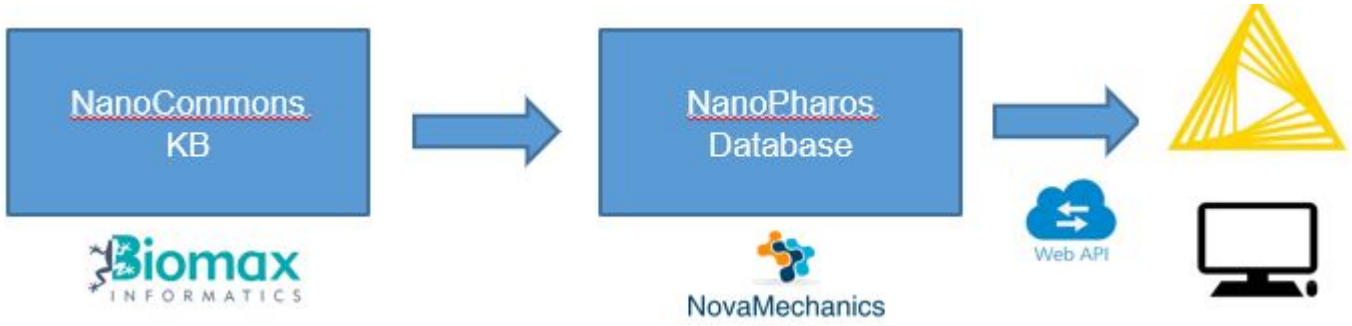


Future Plans: Include theses steps in the InChi software

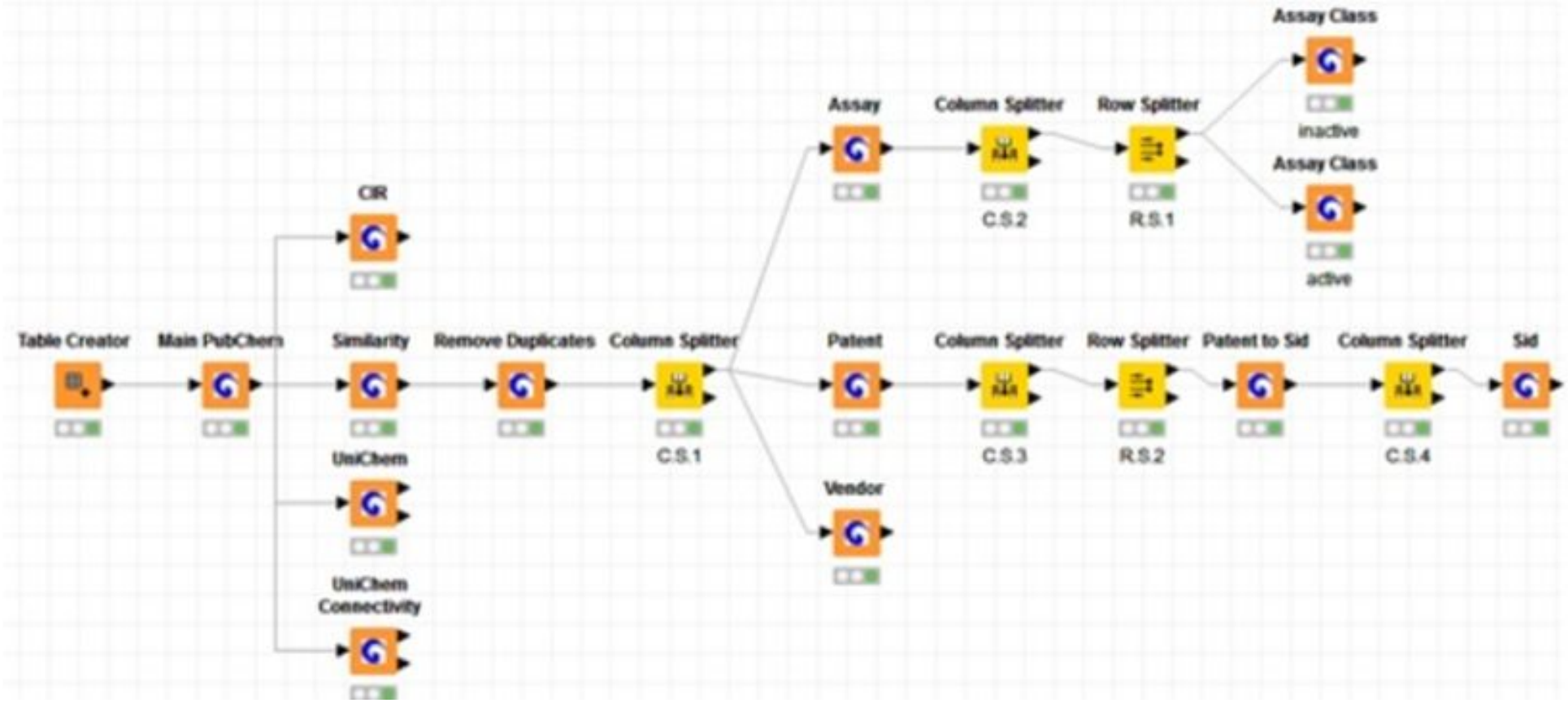
Under Development - NInChI KNIME node

Advantages

- Enable high throughput calculation of several NInChI simultaneously
- Access Nanomaterials Databases through APIs for Look up search (currently compatible with NanoCommons & NanoSolveIT KBs)
- Direct integration with nanomaterials descriptor calculation tools
- Direct integration with image analysis tools



Blend >35 databases together with the aid of InChi, why not for NInChI



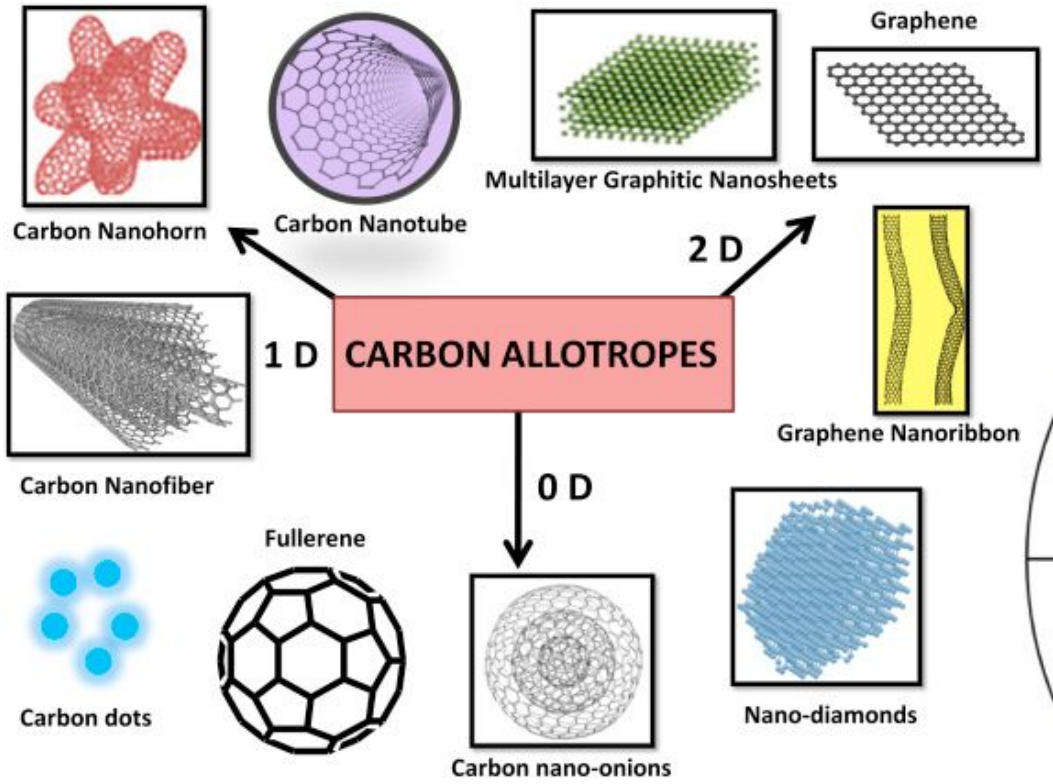
NInChI WORKING GROUP - TERMS OF REFERENCE

- Is a nanomaterial an extension of a molecule, or is a molecule a component of a nanomaterial?
- Is the nanomaterial InChI canonical?
- Can developments of the core InChI, including improved descriptions of organometallics and inorganics, fit easily into the Nano InChI without requiring substantial reprogramming?
- Does the Nano InChI describe nanomaterials in a way which is globally accepted, or might take up in some regions be higher than in others?
- How should the Nano InChI software interact with the core InChI software?

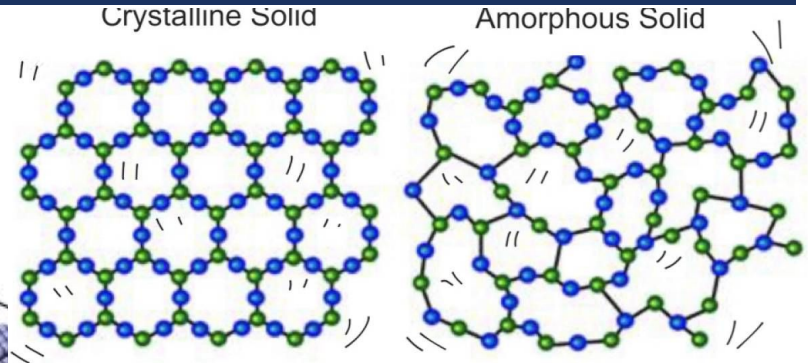
Questions arising from InChI conference (22-24 March 2021)

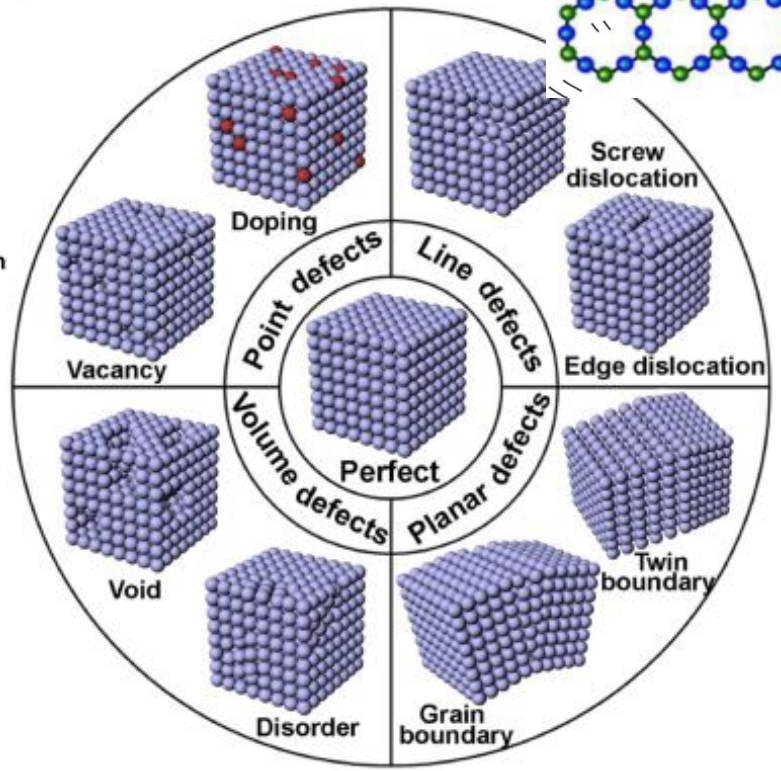
- Are there ways to include metal-organic frameworks?
- Are non-integer atom counts supported? Again this is more a question of the representation of the chemical constitution of the components.
- Different/specific types of NMs - is there a need to have more specific NInChIs?
- Dispersed NM?
- Group identifiers versus individual substance identifier - precedent here from Markov structures for example

Key requirements to capture in the NInChI?



Dimensionality, layers, chirality, defects, rigidity

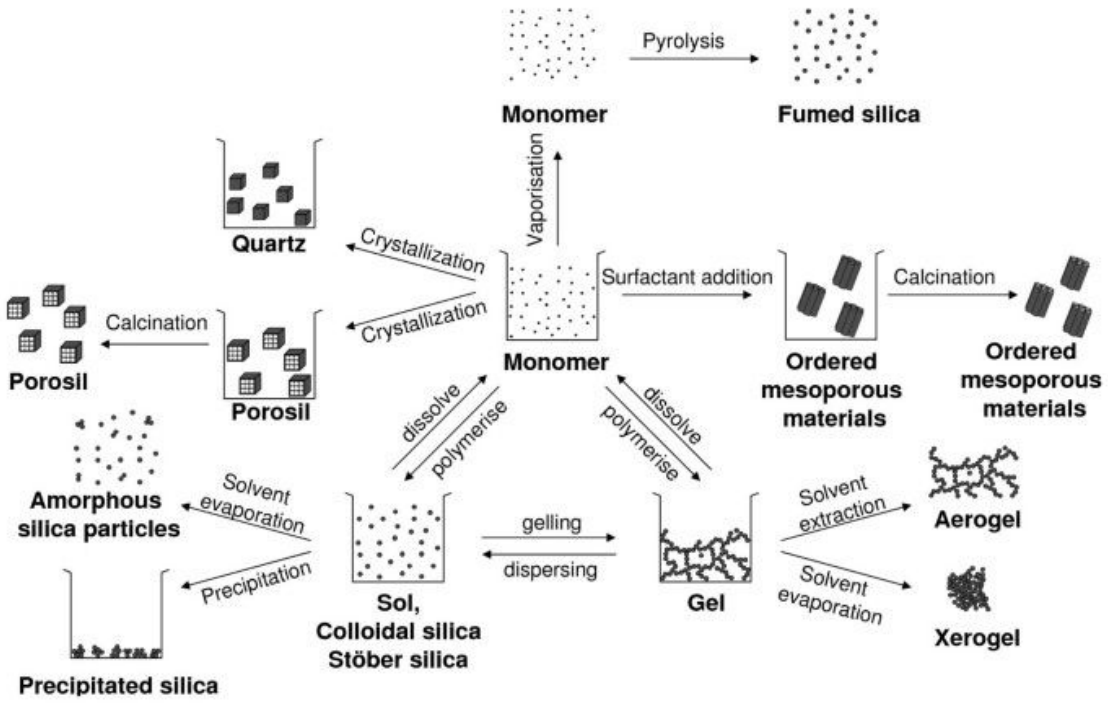




Crystal phases, phase boundaries, homogeneous / heterogeneous mixtures, defects, interfaces, vacancies etc.

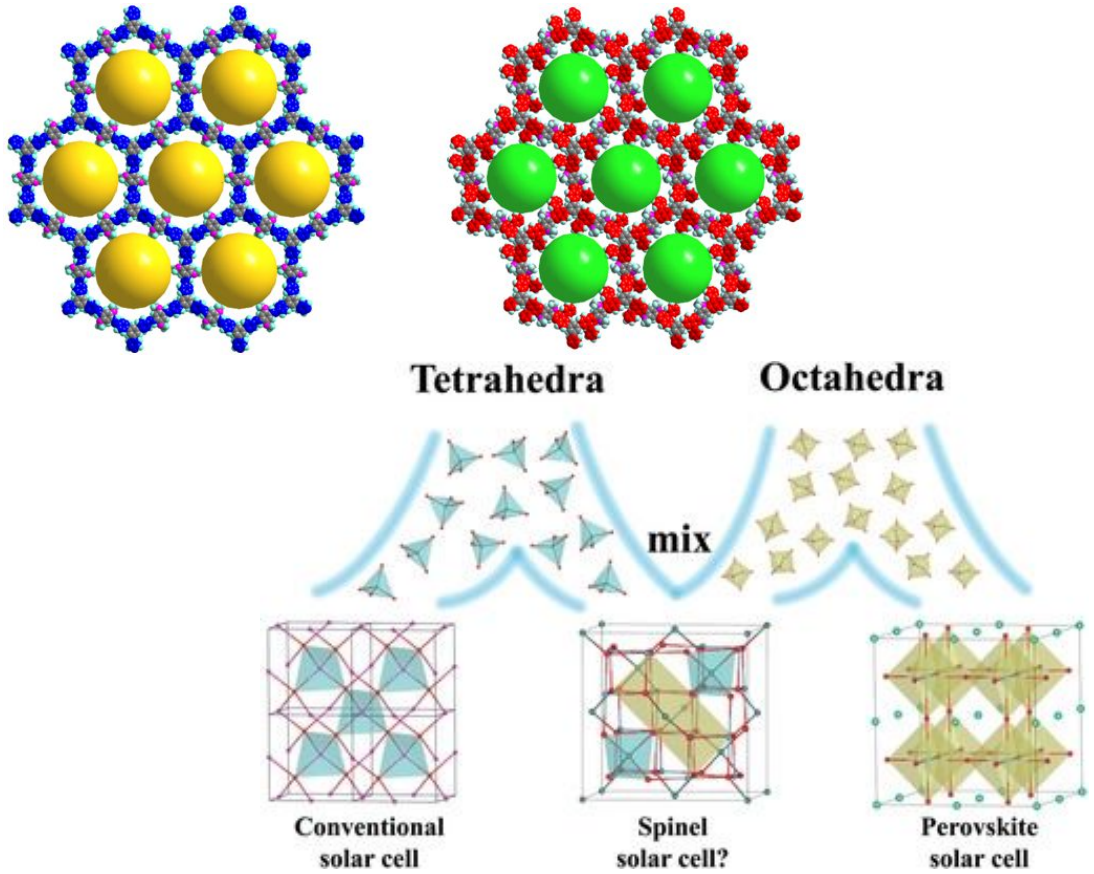
Intentional introduction of defects, lower oxygen contents etc. for

Key requirements to capture in the NInChI?



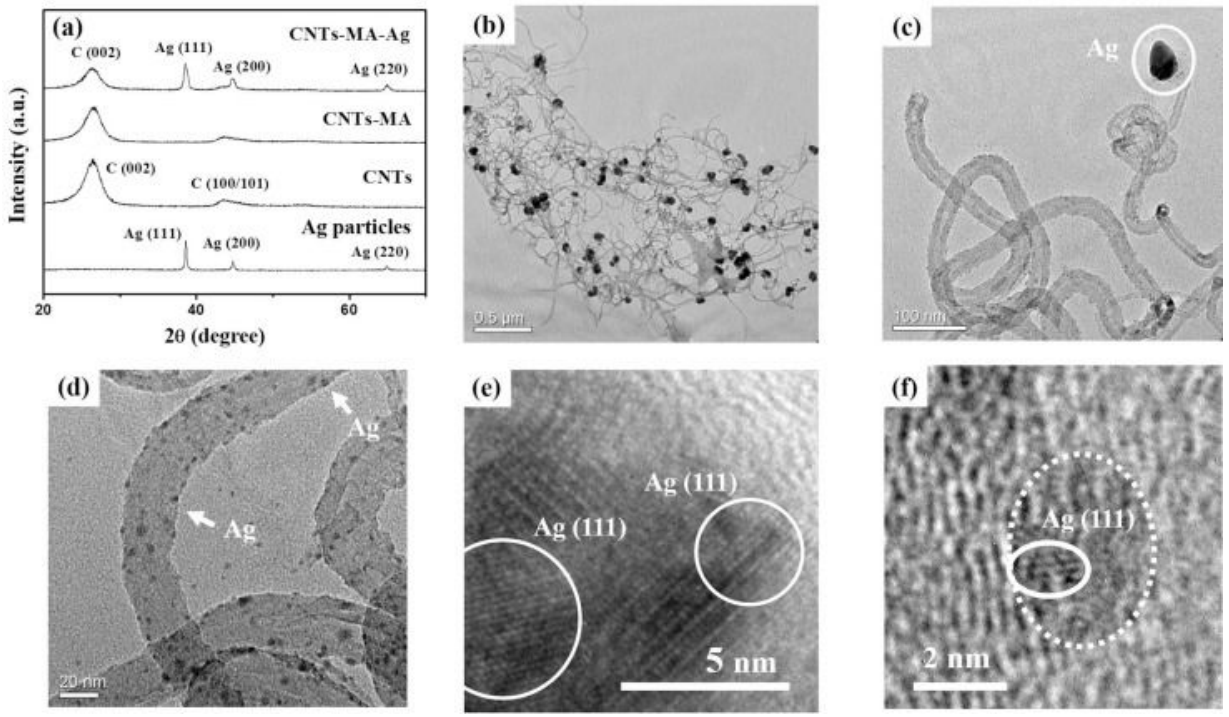
Form, associated liquid / gas, solid or dispersion, heterogeneous or homogeneous mixture etc.

Metal organic Frameworks



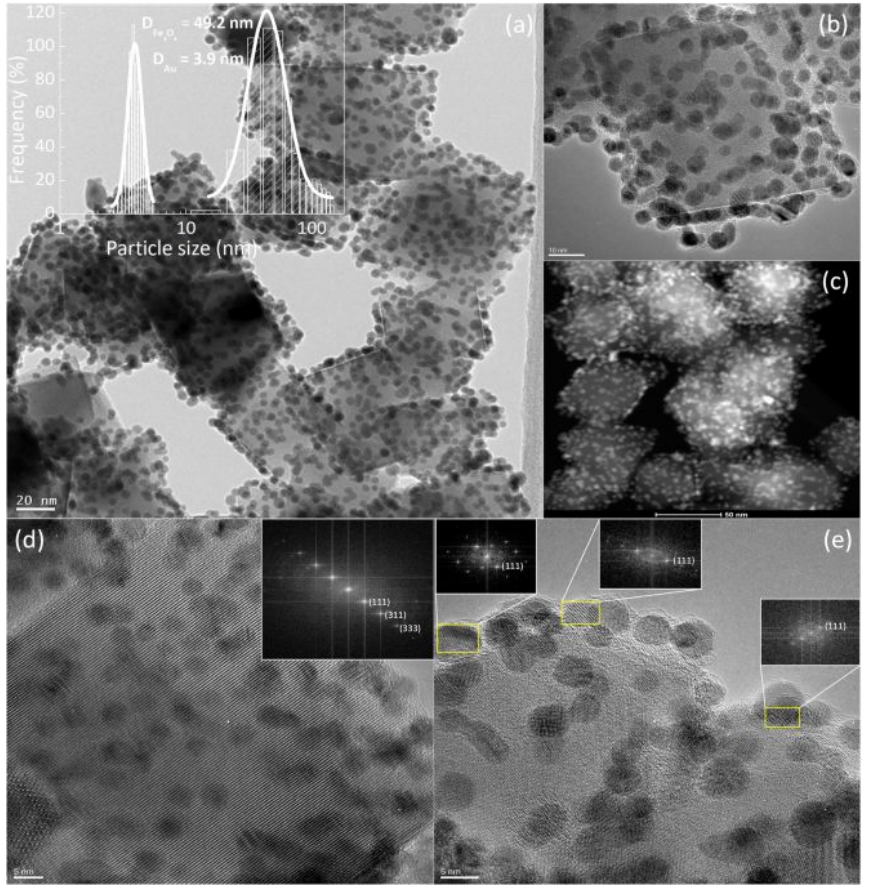
Alkyl halide perovskite materials

Some challenges to consider……



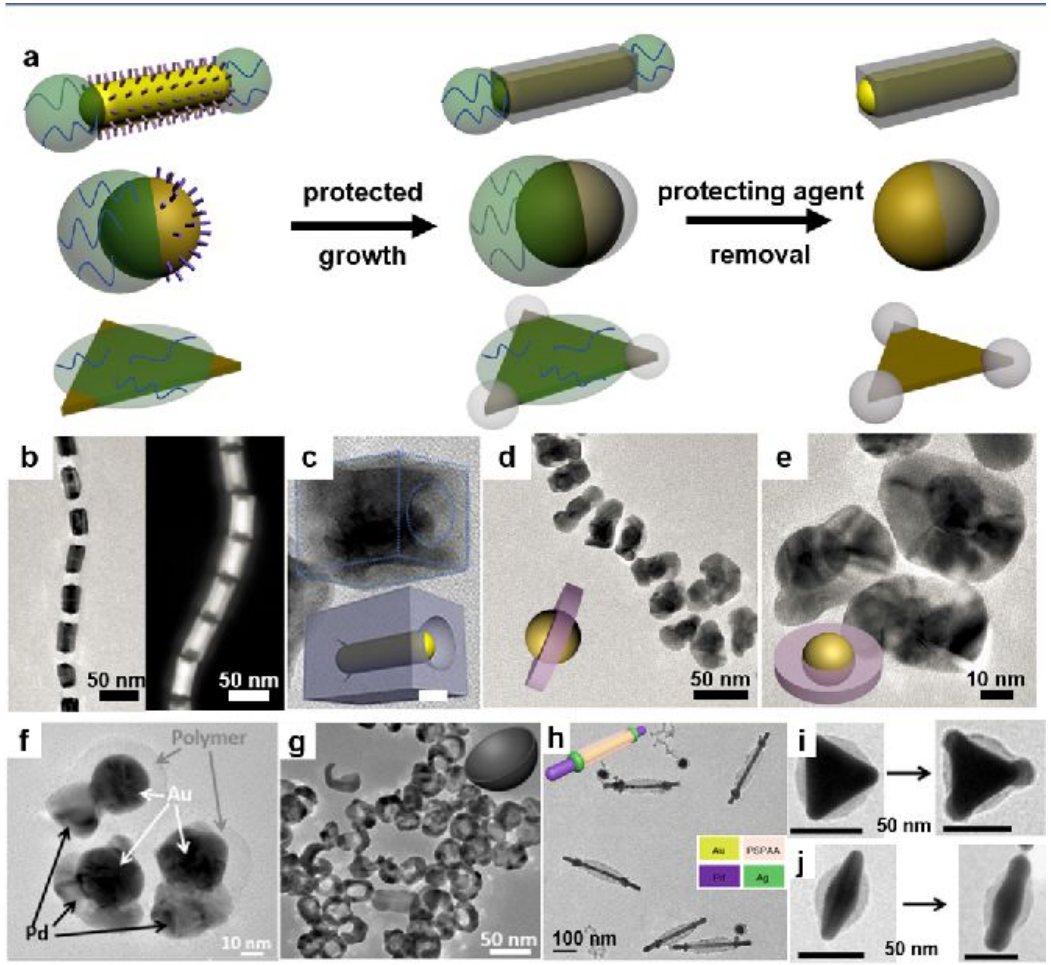
Hybrid materials - e.g. silver NM functionalised CNTs

- **Distribution, relative %, surface or inside tubes etc.?**



Gold NP-decorated iron oxide nanomaterials for hyperthermia

A lot beyond our current scope…..



Very complex shapes

Symmetry-breaking nanomaterials

What can we exclude from first iteration of NInChI standard?

Nanostructured surfaces / nanocomposites

Inverse NMs (nano holes in a bulk material),

Nanoporous materials ?

Dynamic properties (extrinsic properties) such as dissolution, agglomeration, and protein corona formation were also excluded for now, although it seems likely that these could be added using a modified reactions extension of InChI, in which reactions are considered to be transformations, or added via AuxInfo files associated with NInChI..

Backup slides

ALPHA VERSION – PUBLISHED DEC 2020 – NInChI GENERATOR

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,*]

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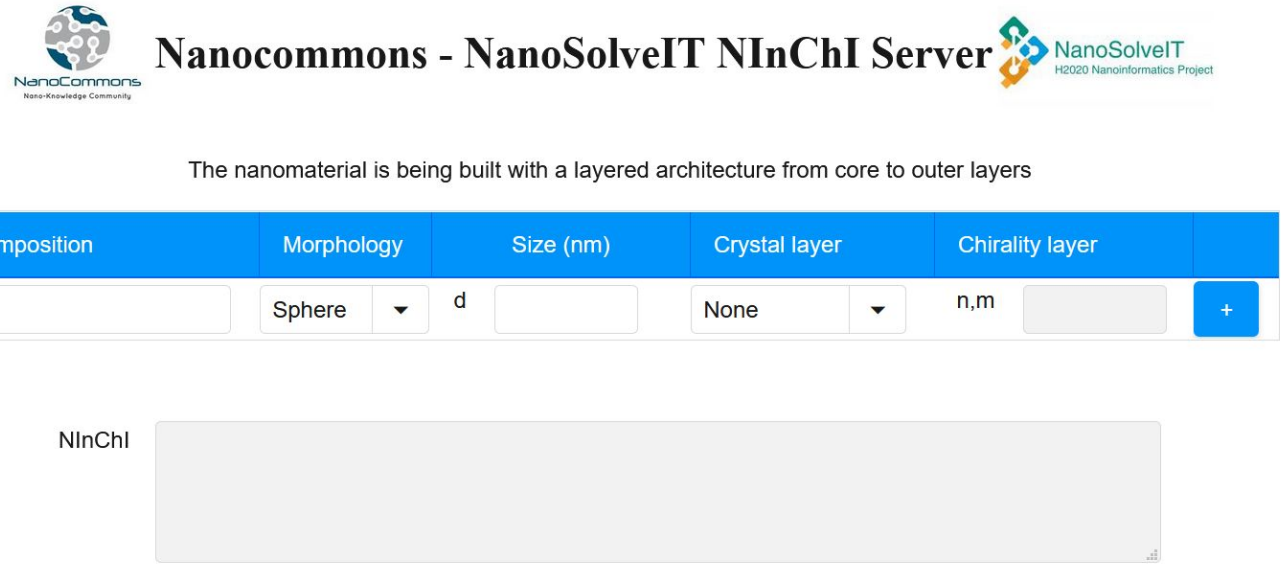
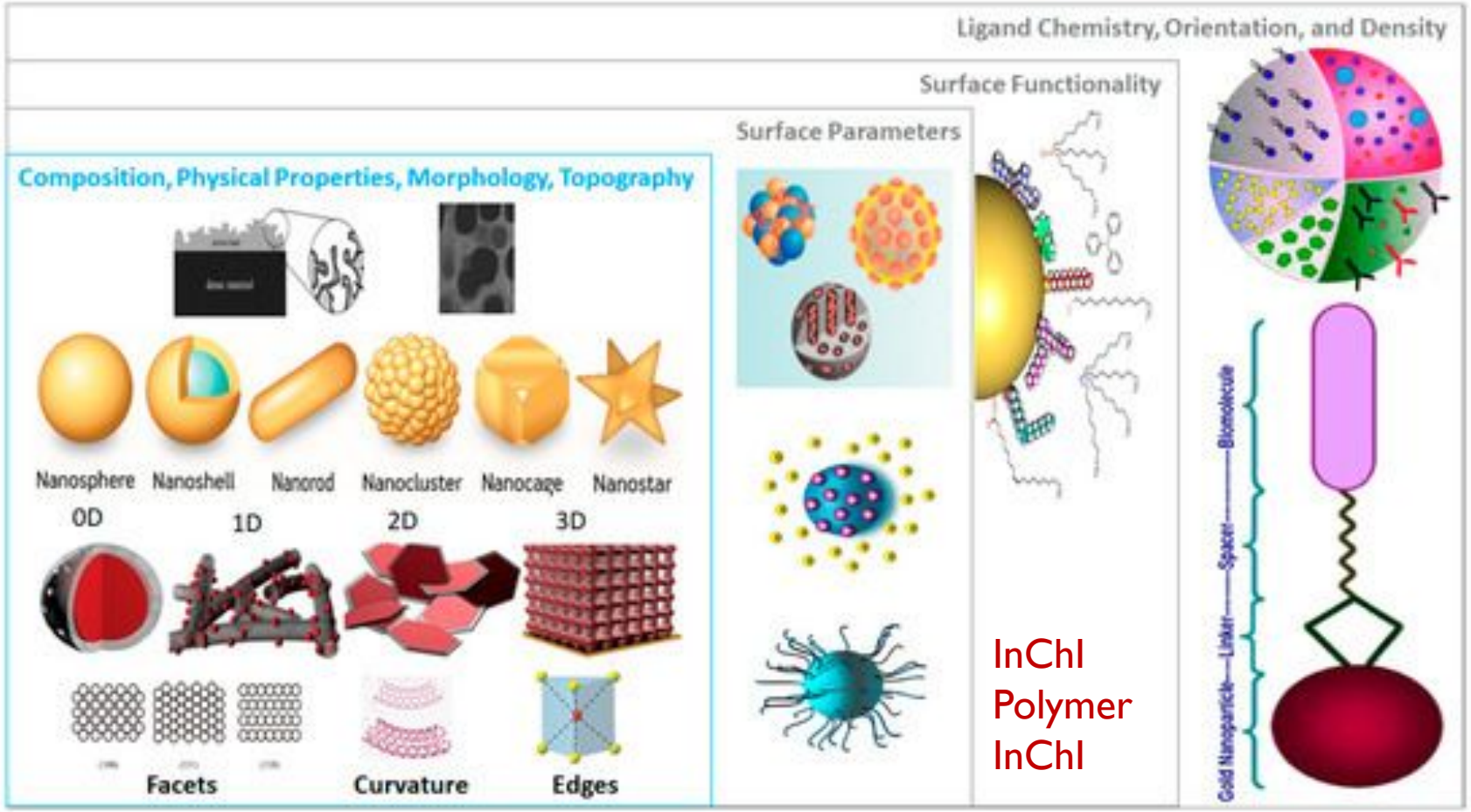
2 Nanoinformatics Department, NovaMechanics Ltd., 1666 Nicosia, Cyprus; afantitis@novamechanics.com (A.A.); melagraki@nvemechanics.com (A.T.)
3 Edelweiss Connect GmbH, Hochbergerstrasse 60C, 4057 Basel, Switzerland; thomas.exner@edelweissconnect.com



https://www.mdpi.com/2079-4991/10/12/2493

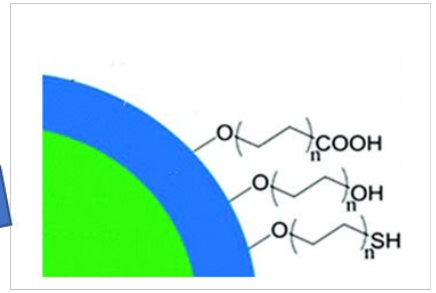
http://enaloscloud.novamechanics.com/nanocommons/NInChI/

CHALLENGES OF DISTINGUISHING NANOMATERIALS



- Crystal phase or mixed phases
- Chirality
- Dopants
- Defects
- Powder vs dispersion (Mixtures InChI)

NInChI AS A STRUCTURAL NANOMATERIAL IDENTIFIER



Core – Shell - Ligands

NInChI

1A/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2/z200-1-8!1S/O2Si/c1-3-2/**msp/s20:100d-9**/k000/y2&1

Layer 1 (version); Layer 2 (composition, morphology, size, crystal phase, chirality); Layer 3 – organisation of the constituents from inside to outside

nanomaterials

MDPI

Article - original research manuscript

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], Anna Rybinska-Fryca[9], Maciej Gromelski[9], Egon Willighagen[10], Blair D. Johnston[11], Mary Gulumian[8], Marianne Matzke[12], Amaia Green Etxabe[12], Nathan Bossa[13], Angela Serra[14], Irene Liampa[6], Stacey Harper[15], Kaido Tämm[16], Alexander CØ Jensen[17], Pekka Kohonen[18], Luke Slater[1], Haralambos Sarimveis[6], Georgia Melagraki[2*]

INITIAL RESPONSES FOR DISCUSSION BY NInChI WORKING GROUP

- Is a nanomaterial an extension of a molecule, or is a molecule a component of a nanomaterial? If it is the former, then an AuxInfo approach might be best.

  → Nanomaterials are materials, not molecules - multiple InChIs are currently used as part of the NInChI

- Is the nanomaterial InChI canonical? The RInChI achieves this by minimising the information in the main string, and using AuxInfo to hold anything with a floating point number

  → Not yet since properties can be quantified using different measures (e.g. radius or diameter for spherical NM)

  → Proposal of NInChI also as a group identifier makes canonicalization even more demanding

  → Transferring the values into AuxInfo should be tested

INITIAL RESPONSES FOR DISCUSSION BY NInChI WORKING GROUP

- Can developments of the core InChI, including improved descriptions of organometallics and inorganics, fit easily into the Nano InChI without requiring substantial reprogramming?

  → Existing descriptions should definitely be used - this is already done with mixture and polymer InChIs

  → Will need reprogramming, but the NovaMechanics team have the capability to do this

- Does the Nano InChI describe nanomaterials in a way which is globally accepted, or might take up in some regions be higher than in others?

  → Large efforts were taken to collect views from as many researches across the world to get consensus inside the nanosafety community - outreach has been started towards other communities and has resulted in immense interest

INITIAL RESPONSES FOR DISCUSSION BY NInChI WORKING GROUP

- How should the Nano InChI software interact with the core InChI software? Would the aim be to integrate it, or could it be an independent program which called the core software whenever an InChI needed to be generated?

  → NInChI software will need to provide specific functionality and being independent, at least at the beginning, will allow faster development of these

  → Core software already used for creating the InChI for the components

  → Mutual exchange of functionality between the core and the NInChI software might make merging beneficial later on

  → Currently we are extracting the InChIs for the elements from the core InChI software

ACKNOWLEDGEMENTS

Dr. Antreas Afantitis
Novamechanics Ltd.

Dr. Thomas Exner
Seven Past Nine

Dr. Georgia Melagraki
Novamechanics Ltd.

Dr. Martin Himly
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University of Salzberg

Dr. Andreas Tsoumanis
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to join the NInChI working group

NanoSolveIT

NanoCommons
Nano-Knowledge Community

European Commission
Horizon 2020
European Union funding
for Research & Innovation