FutureNanoNeeds

Nanomaterial identification and classification

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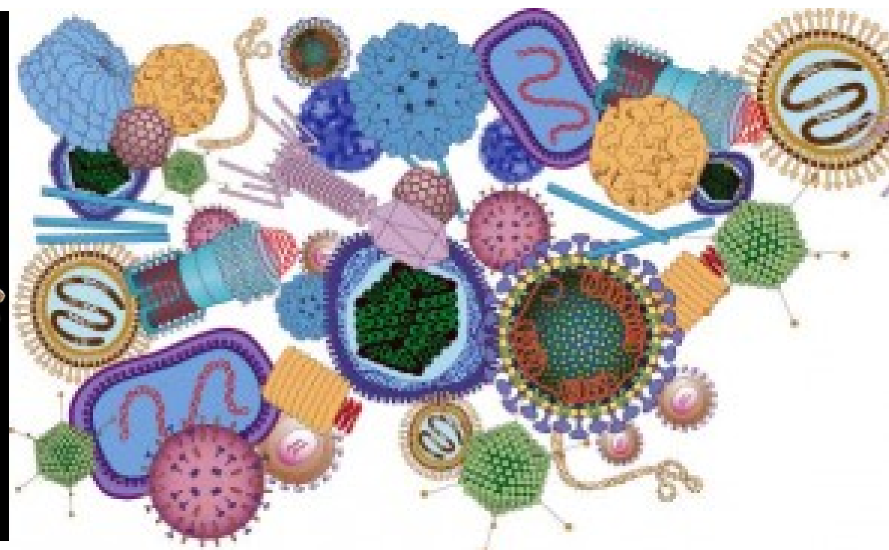
Introduction-*TECHNOLOGY*

RADICAL CONCEPTUAL CHANGE

In the coming decade, humans will create more novel material structures than at any time in human history. Within decades, there will be more diverse material structures than those occurring naturally since beginning of time.



SOME STRUCTURES WILL MIMIC NATURAL OBJECTS

SOME WILL BE ENTIRELY NEW

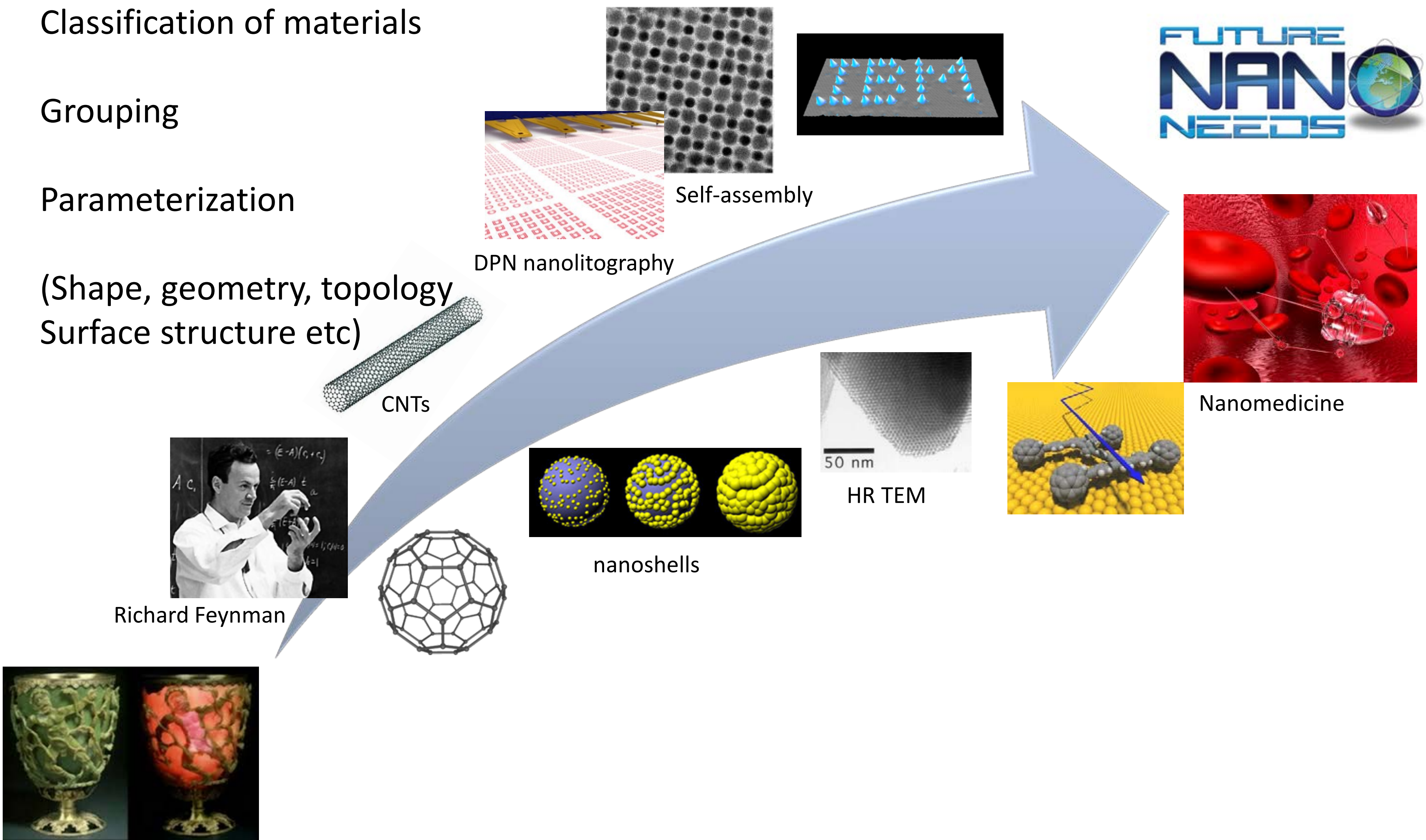
‘Identity’ of Ever More Complex Nanomaterials

Classification of materials

Grouping

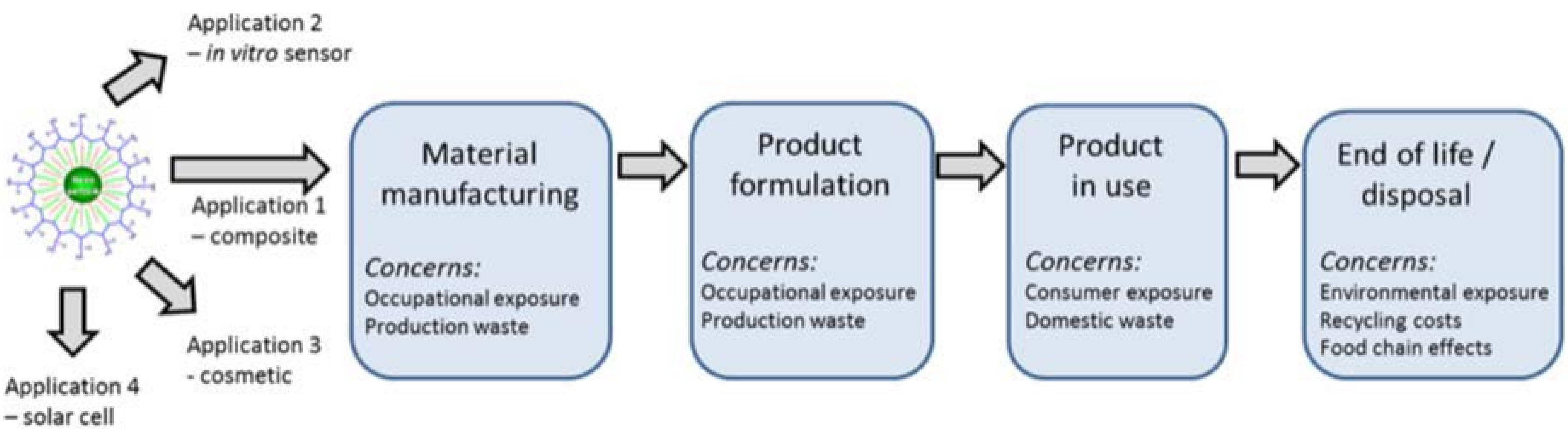
Parameterization

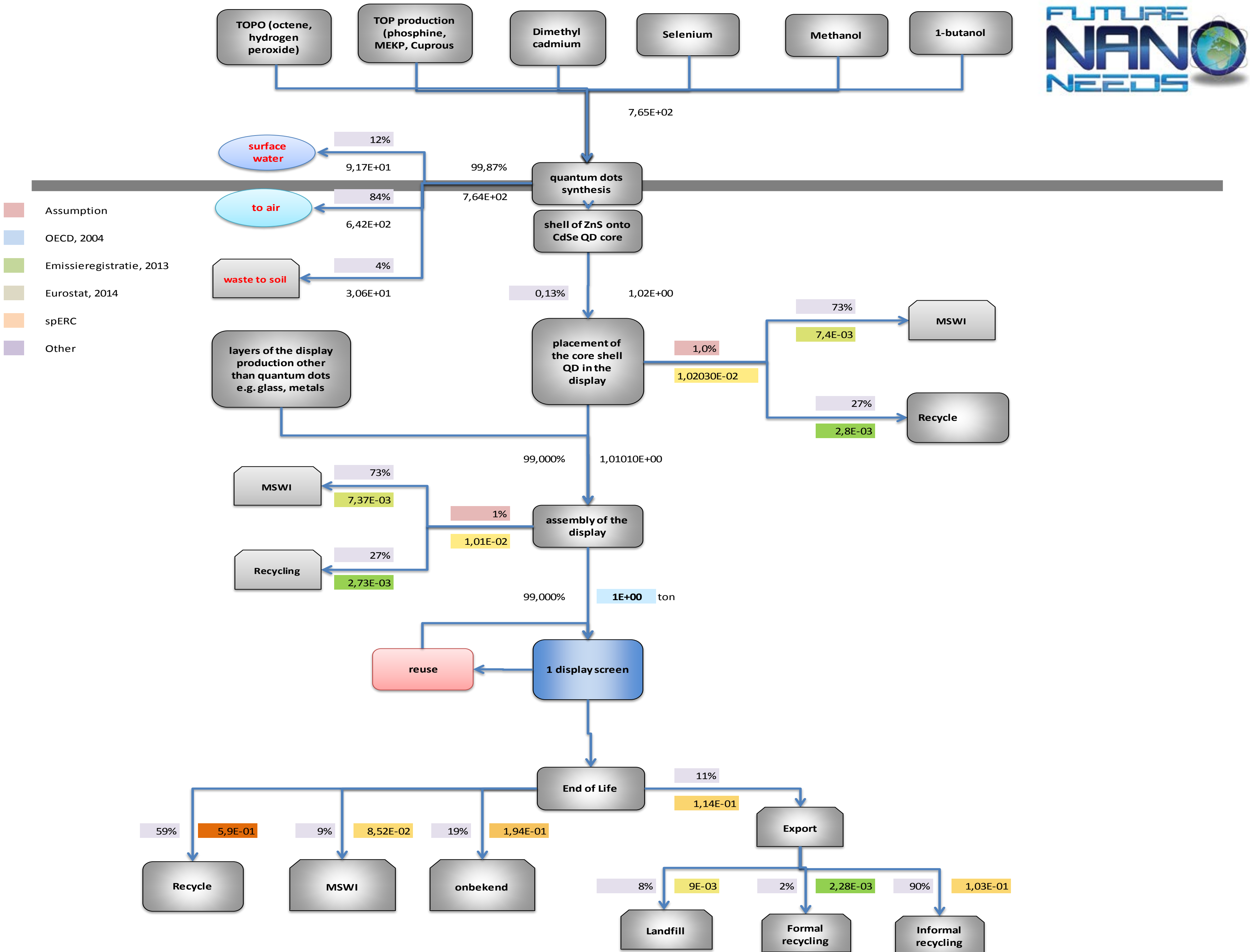
(Shape, geometry, topology
Surface structure etc)



Prioritizing Studies via Value Chains?

- Energy Materials
- Display Materials (QDs)
- Battery Materials
- Thermoelectric Materials
- 3D Printing Materials





TOPO (octene, hydrogen peroxide)
TOP production (phosphine, MEKP, Cuprous
Dimethyl cadmium
Selenium
Methanol
1-butanol
FUTURE NANO NEEDS
7,65E+02
surface water
12%
9,17E+01
99,87%
quantum dots synthesis
to air
84%
7,64E+02
6,42E+02
shell of ZnS onto CdSe QD core
waste to soil
4%
3,06E+01
0,13%
1,02E+00
Assumption
OECD, 2004
Emissieregistratie, 2013
Eurostat, 2014
spERC
Other
73%
MSWI
7,4E-03
placement of the core shell QD in the display
1,0%
1,02030E-02
layers of the display production other than quantum dots e.g. glass, metals
27%
Recycle
2,8E-03
99,000%
1,01010E+00
MSWI
73%
7,37E-03
1%
assembly of the display
1,01E-02
Recycling
27%
2,73E-03
99,000%
1E+00
ton
reuse
1 display screen
End of Life
11%
1,14E-01
Export
59%
5,9E-01
9%
8,52E-02
19%
1,94E-01
Recycle
MSWI
onbekend
8%
9E-03
2%
2,28E-03
90%
1,03E-01
Landfill
Formal recycling
Informal recycling

Life Cycle Analysis – release and exposure

Sustainable Nanotechnologies Project

- Aging and transformation
  - during incorporation into products as well as weathering when NPs are released into the environment
- Categorization/grouping to enable read-across
  - need to investigate innovative parameters in different systems (e.g. alteration of MNs' interfacial and physical characteristics when come in contact with heterogeneities of in dispersions)
- Establish structure-reactivity relationships
  - hypothesise modes of action of MNs
  - develop screening methods to identify "concerning" properties, nano-bio interactions and specific lifecycle stages.
  - Support Safe by Design surface engineering strategies

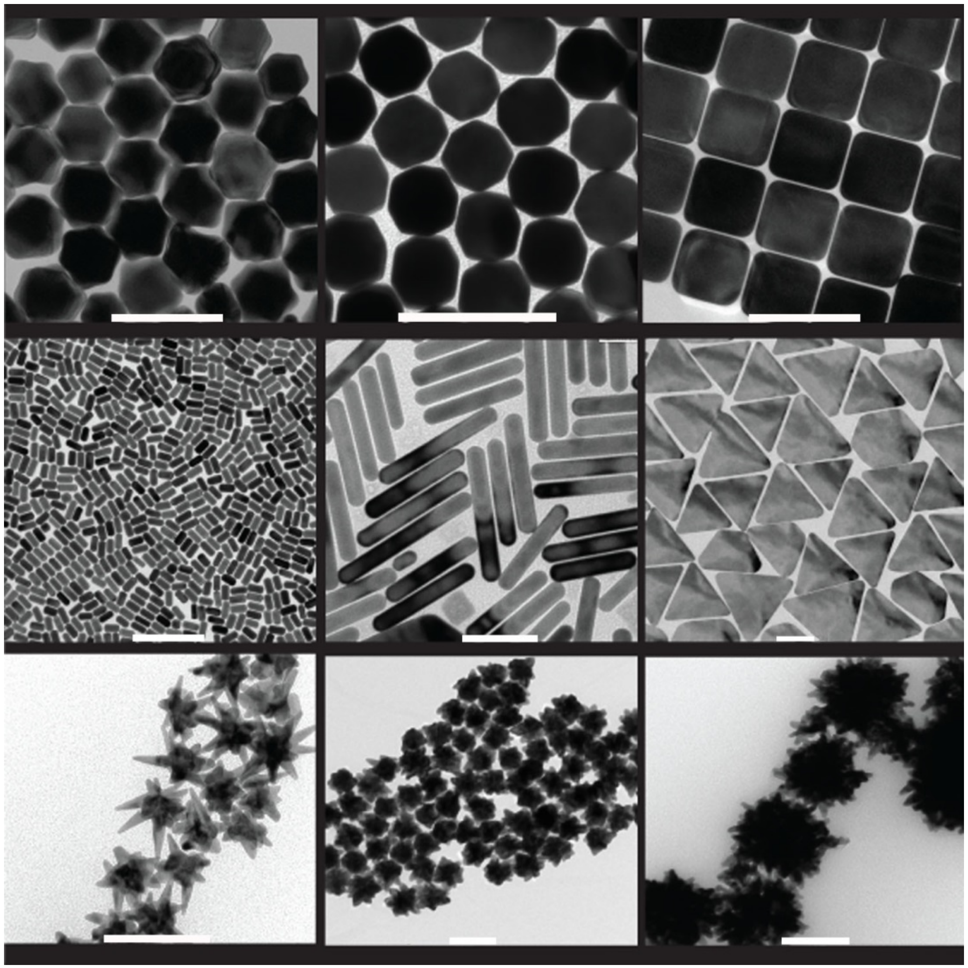
THE PROCESS

RESOURCE BUILDING

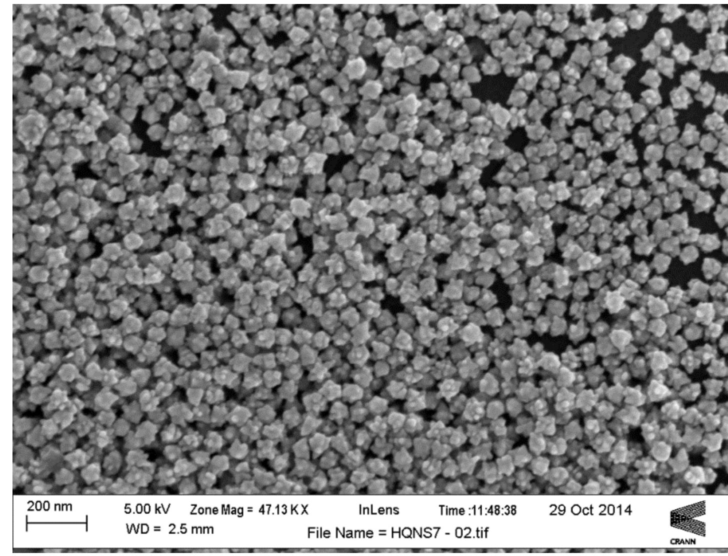
REFERENCE LIBRARIES FOR
IDENTITY OF ALL FUTURE STRUCTURES

Library of Gold Nanoparticles

WP4 – Synthesis (UCD)

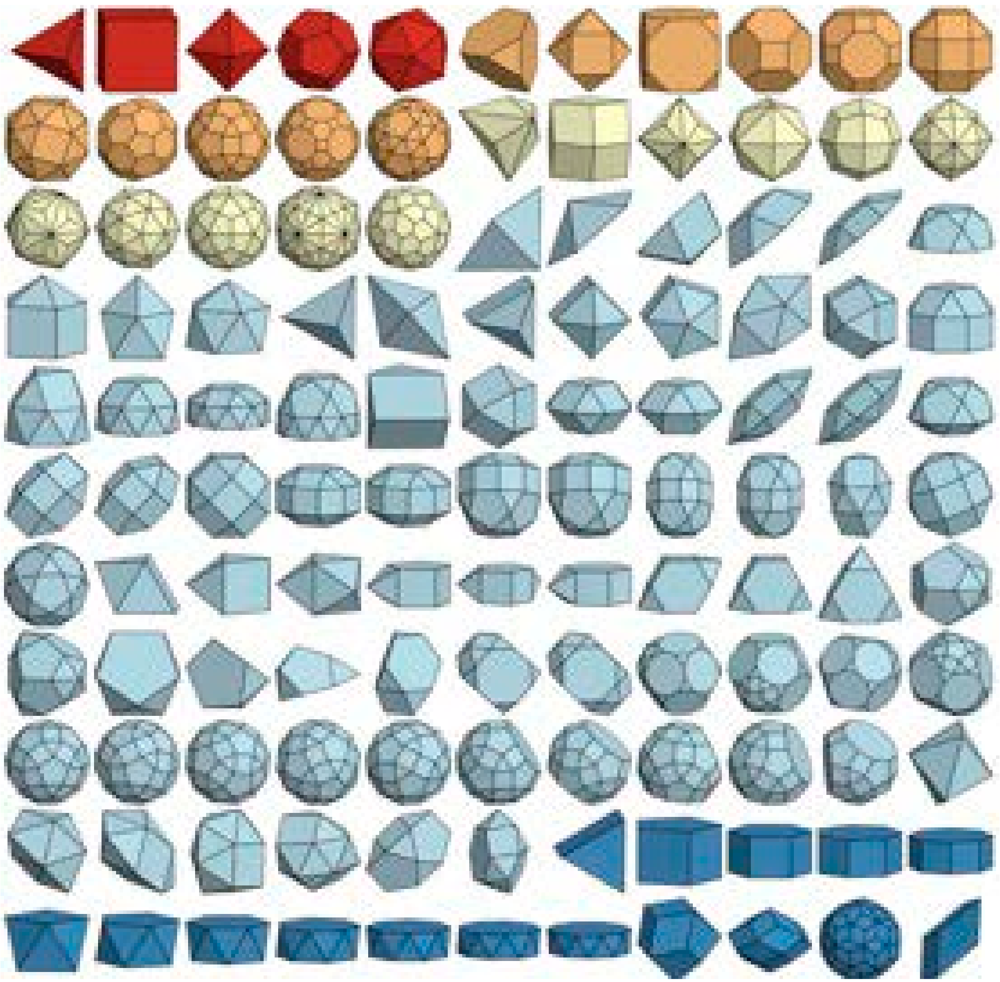


Library of anisotropic gold nanoparticles: Transmission Electron Microscopy (TEM) micrographs by Dr Željka Krpetić, Qi Cai and Jennifer Cookman (CBNI, UCD). From the top left: nano-trisoctahedra, faceted gold nanorods (top view), nanocubes, nanorods, nanoprisms and nanostars. Scale bars are 100 nm.



Shape and size monodispersity

Libraries of Nanomaterials
Shaping out the Future



- FNN is aiming for **high quality reproducible NP synthesis**

- **Reference Libraries of Nanomaterials**

- **Excellent size & shape monodispers**ity

- **Impact on advanced NP characterisation** new challenges in analytical methods (shape, morphology, aspect ratio …)

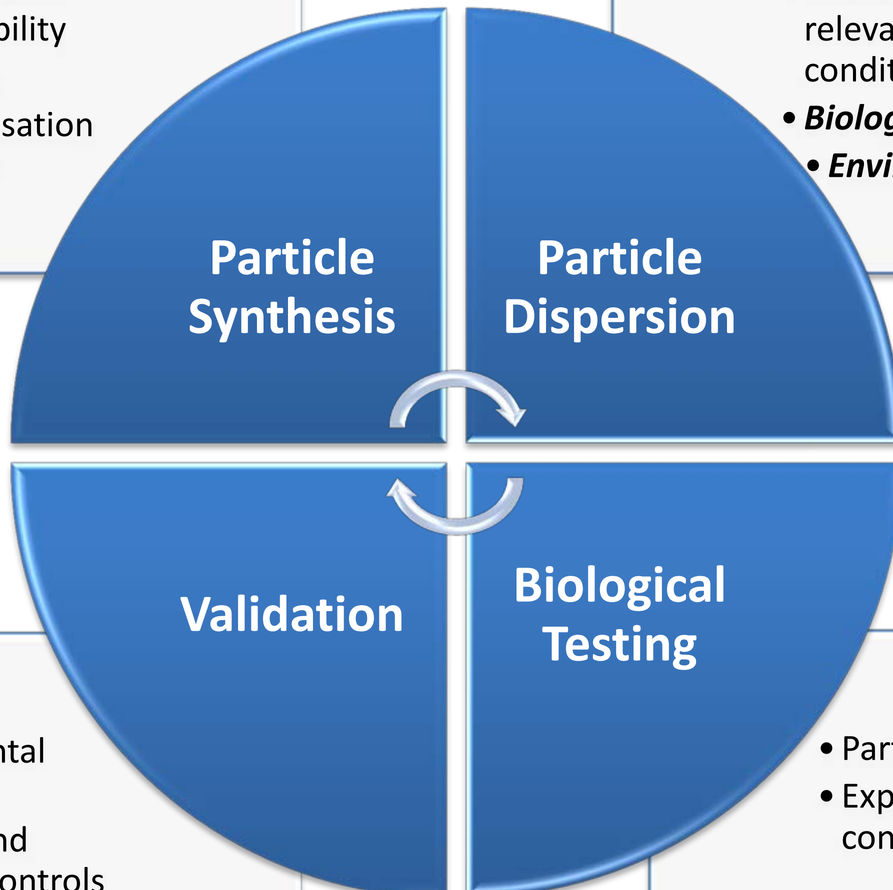
BENCHMARKING

WITHOUT STRESS ON QUALITY CONTROL THESE QUESTIONS ARE MEANINGLESS

Many challenges

- Batch to batch reproducibility
- Scaling up
- Characterisation of pristine surfaces

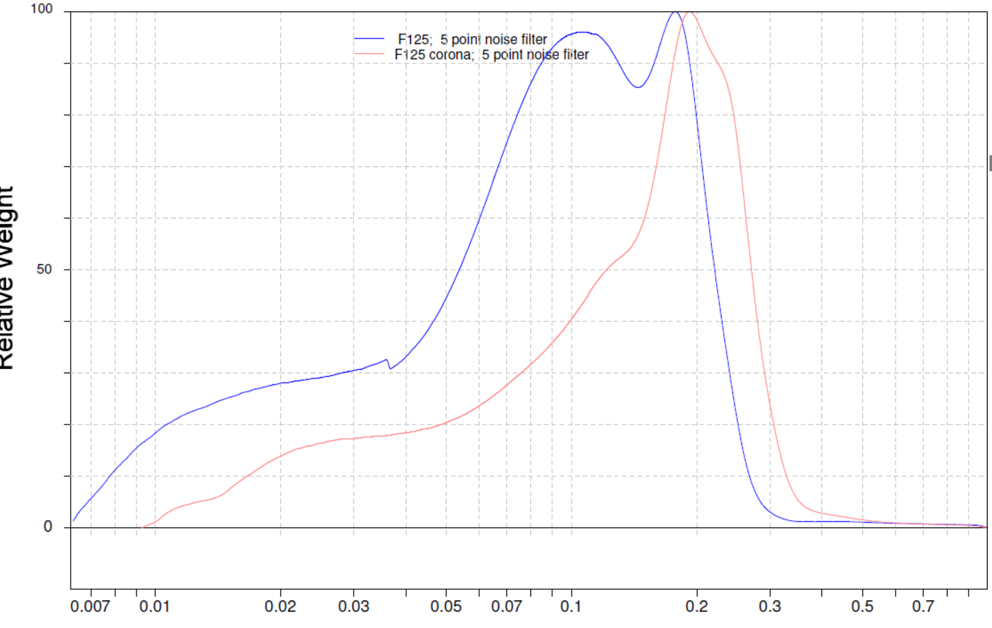
- Characterisation in relevant conditions
- ***Biological***
  - ***Environmental***

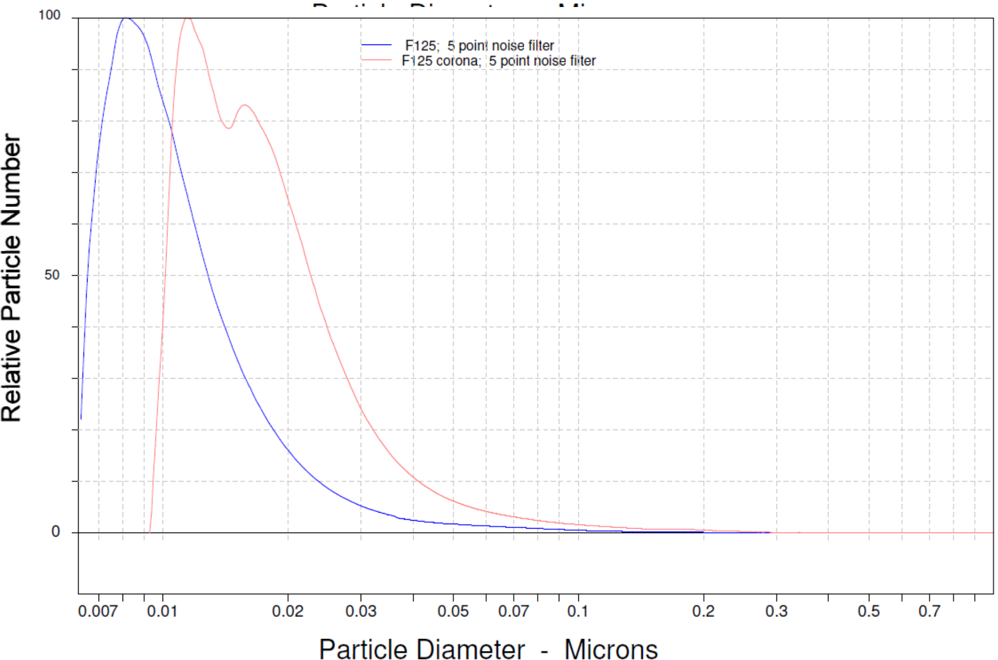


- Experimental protocols
- Positive and negative controls
- ILC

- Particle quality
- Experimental conditions

Typical NP supplied within FP 7 project

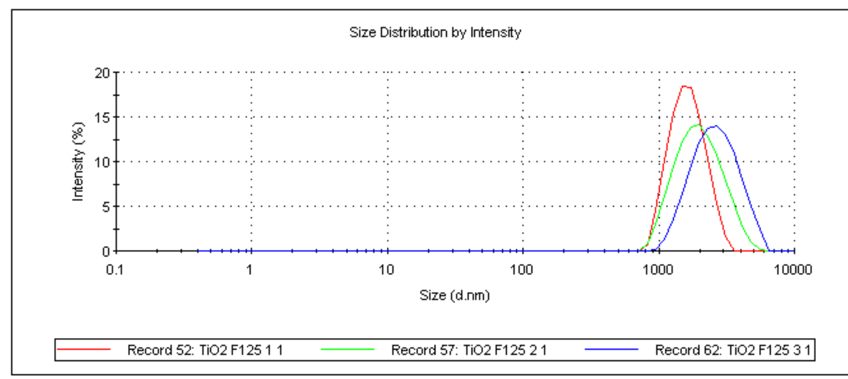




In water

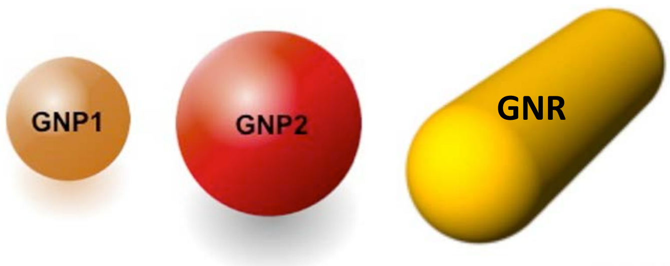
NP-Hard corona

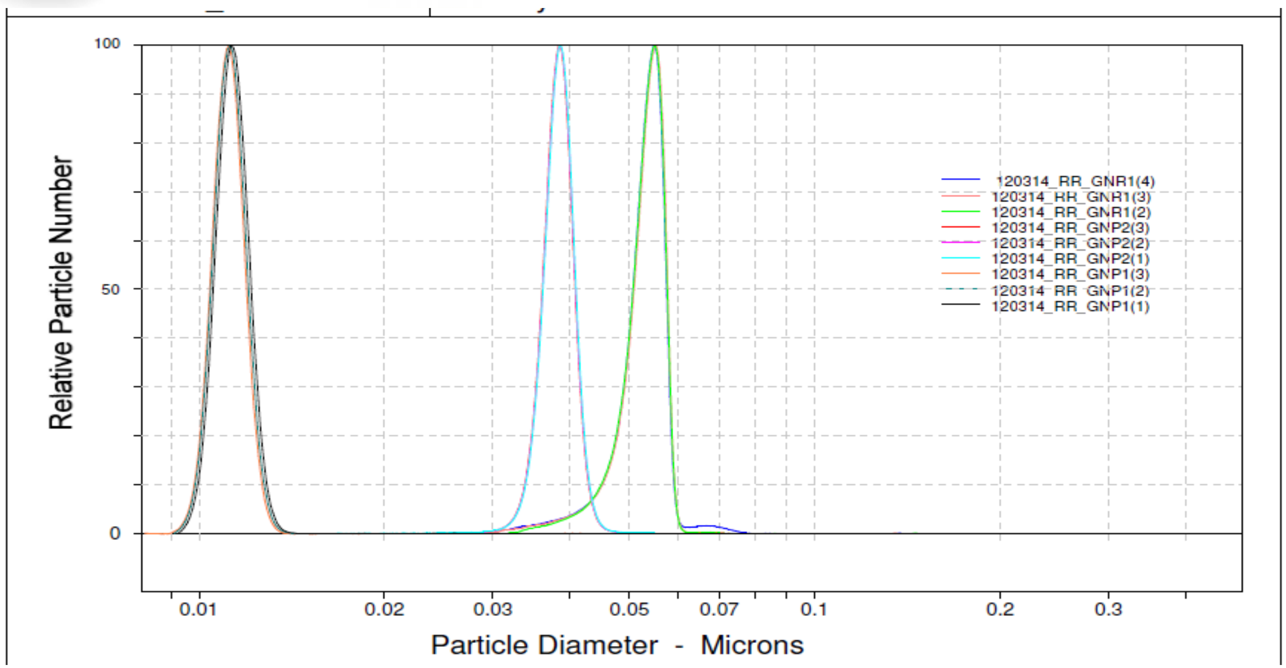
			Diam. (nm)	% Intensity	Width (nm)
Z-Average (d.nm):	2241	Peak 1:	2743	100.0	1033
PdI:	0.191	Peak 2:	0.000	0.0	0.000
Intercept:	0.943	Peak 3:	0.000	0.0	0.000
Result quality :	Good				



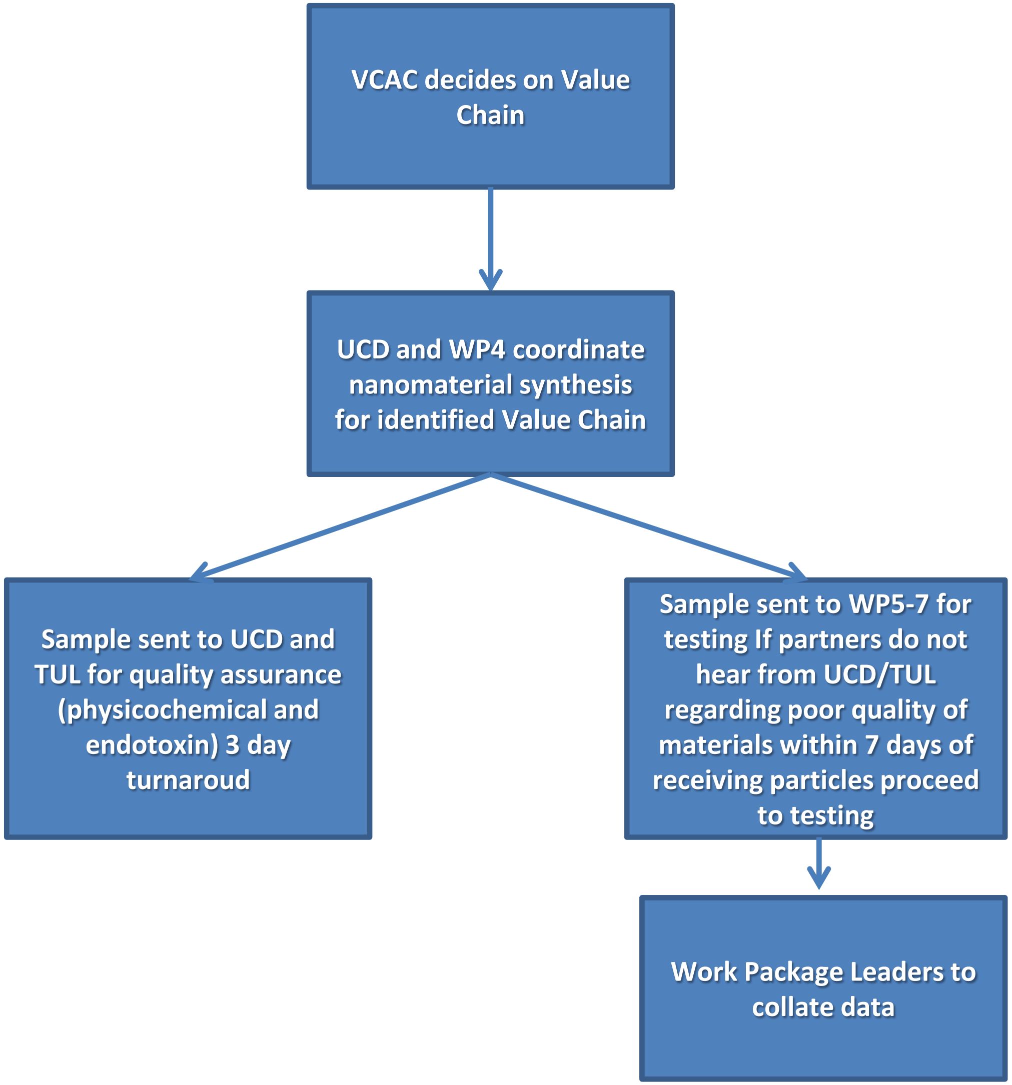
High quality Mono dispersed AuNP

HS-PEG-functionalised gold nanoparticles: spheres and gold nanorod





Materials Flow



Quality Assurance

- Regular MTA quality checks (UCD)

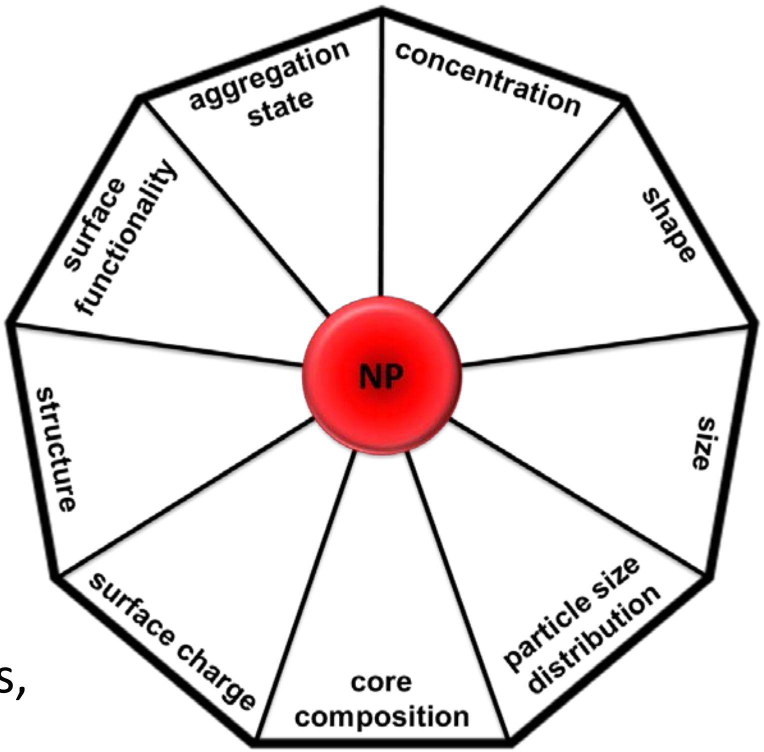
Full characterisation of nanomaterials – quality control of particles in dispersion in relevant media:

✓ UV-visible spectroscopy
✓ Nanoparticle Tracking Analysis (NTA)
✓ Differential Centrifugal Sedimentation (DCS)
✓ Dynamic Light Scattering (DLS)
✓ ζ-potential
✓ Transmission Electron Microscopy (TEM)

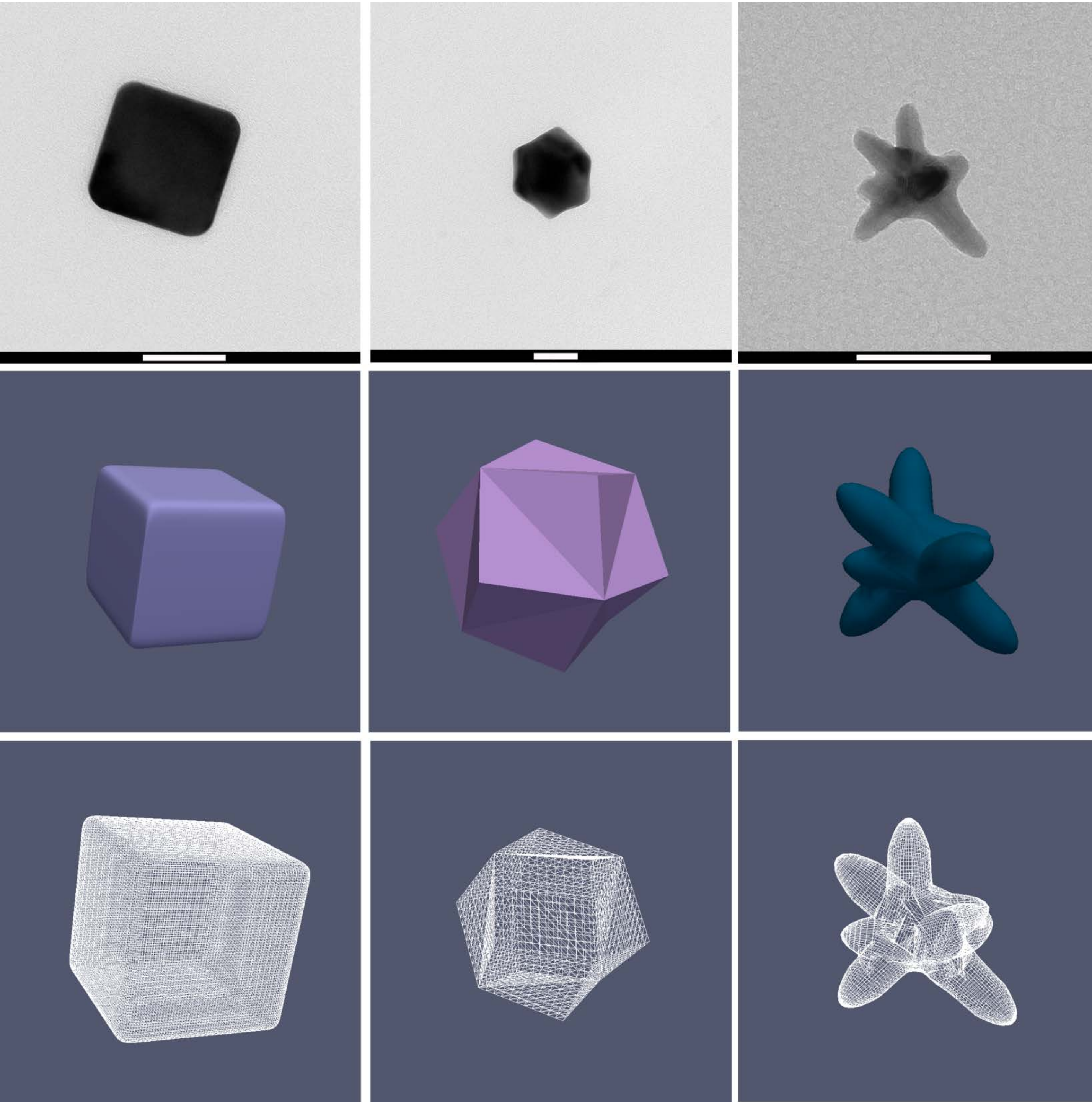
HINTS ABOUT ‘PROPERTIES AND CLASSIFYING

Minimum set of morphological descriptors for shaped nanoparticles

- Dimensions
- Curvatures
- Geometry
- Surface roughness / topography
- Porosity
- Aspect ratio
- Convexity
- Hybrid shapes (asymmetrical Janus, dot rods, core-shell, bio-hybrids)

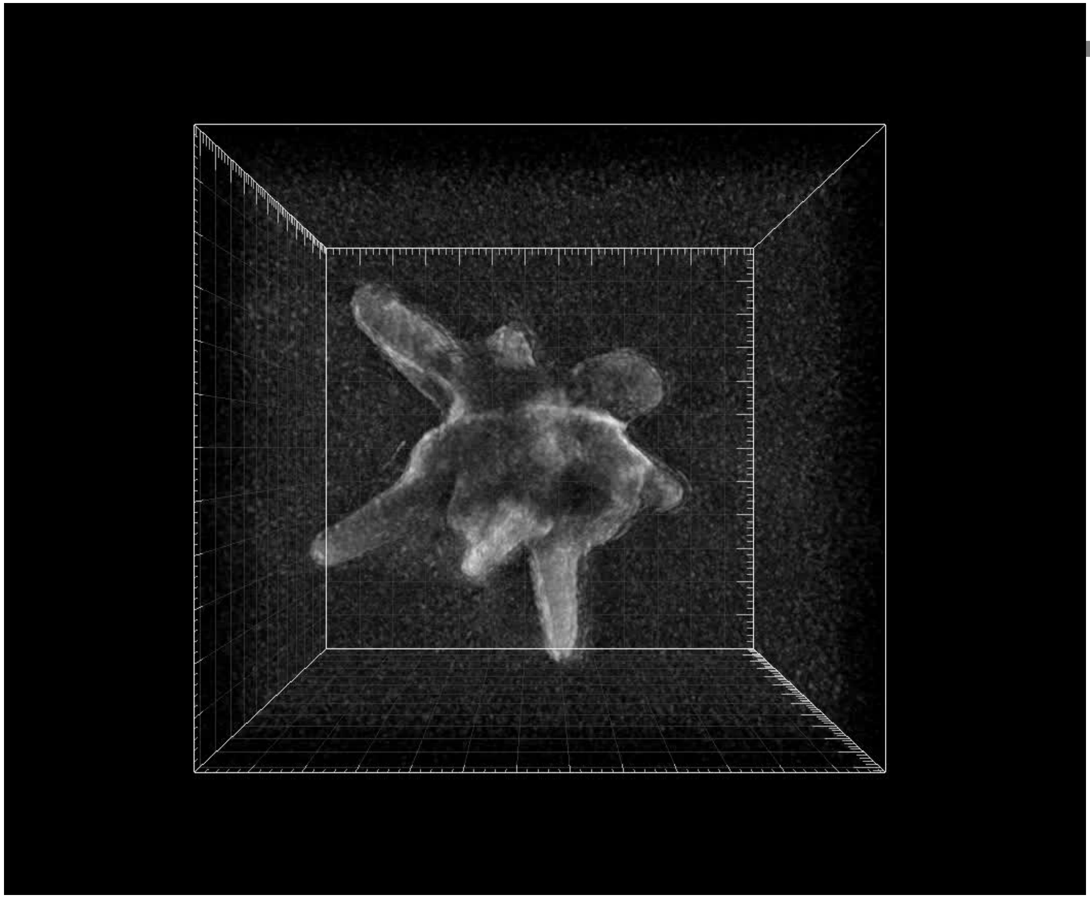


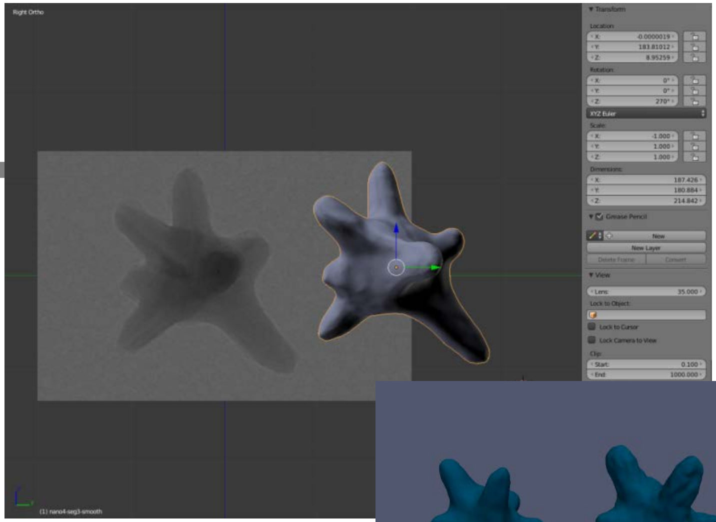
Dissemination to other projects and communities (workshop organization, international collaboration and Dissemination, public website, etc…)

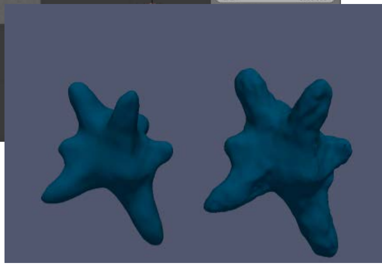


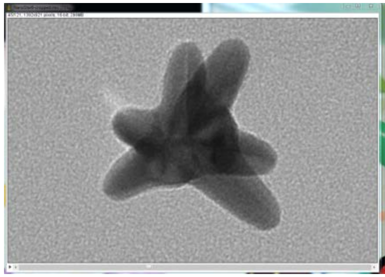
FUTURE NANO NEEDS

TEM Tomography & 3D reconstruction

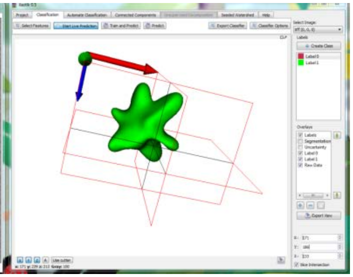








3dmod to visualise cropped sequence of Tiff images



Ilastik to segment the image sequence and reconstruct volume to make 3D model

EXPERIENCES

Successes:

- Moderately good process of deciding on priority materials

- Quite good Quality Process for making/sourcing and supplying material

- Some Workpackages work well (coherent vision with ‘us’)

- Libraries/References states, testing, validation central screening (all centrally accessible)

Difficulties;

- Materials as produced (synthetic chemists) produced are not always suitable for biological study, and consumes much energy to fix them

- Some success in biological arena might be easier than environmental area which requires more materials, harder to produce, different standards

- Possibly (still) too broad and ambitious, hard to control standards and quality across such diverse

- Too low budgets for key functions (eg materials control), leads to ‘bleed-through’ to other work

Uncertain Outcomes

- Will it produce a useful version of nanomaterial ‘identity’?

- Will the idea of ‘value chain’ be too restrictive to gain insight into key parameters?