Table S1. Physicochemical parameters to be determined for different hierarchical tiers with the corresponding characterization techniques [1]. For NM size measurements, readers are referred also to the NanoDefine methods manual [2].

Level/tier	Physicochemical parameter	Suitable characterization techniques
Chemical substance information (Tier 1)	Elemental-chemical composition	XRD, XPS, ICP-MS, ICP-OES, SEM-EDX, NMR, MFM, LEIS
	Crystal structure	XRD, EXAFS, HRTEM, electron diffraction, STEM
	Structural defects	HRTEM, EBSD
	Density	DCS, RMM-MEMS, He-pycnometry
	Optical properties	UV-Vis-NIR, PL, EELS-STEM
	Magnetic properties	SQUID, VSM, Mössbauer, MFM, FMR, XMCD, magnetic susceptibility
Morphology of NM (Tier 2)	Size (structural properties)	TEM, XRD, DLS, NTA, SAXS, HRTEM, SEM, AFM, EXAFS, FMR, DCS, ICP-MS, UV-Vis, MALDI, NMR, TRPS, EPLS, magnetic susceptibility
	Size distribution	DCS, DLS, SAXS, NTA, ICP-MS, FMR, superparamagnetic relaxometry, DTA, TRPS, SEM
	Shape	TEM, HRTEM, AFM, EPLS, FMR, 3D-tomography
Surface characteristics (Tiers 3–5)	Surface composition	XPS, FTIR, NMR, SIMS, FMR, TGA, SANS
	Surface area, specific surface area	BET, liquid NMR
	Chemical state–oxidation state	XAS, EELS, XPS, Mössbauer
	Surface charge	Zeta potential, EPM
	Concentration of surface atoms/ligands/impurities etc.	ICP-MS, UV-Vis, RMM-MEMS, PTA, DCS, TRPS
	Single particle properties	Sp-ICP-MS, MFM, HRTEM, liquid TEM
	Agglomeration state[1]	Zeta potential, DLS, DCS, UV-Vis, SEM, Cryo-TEM, TEM
	Ligand binding/arrangement	XPS, FTIR, NMR, SIMS, FMR, TGA, SANS
	Dispersion of NP in matrices/supports	SEM, AFM, TEM

[1] Although this is an extrinsic property that depends on the surrounding medium, we have kept it in this table of characterization needs as it is an essential parameter for toxicity assessment and is very closely linked with the surface properties of the nanomaterial (NM): "...The surface properties of nanoparticles determine the agglomeration state and the size of the particles under physiological conditions" and "...a comprehensive and accurate characterization of the material under physiological conditions is crucial to correlate the observed biological impact with defined colloidal properties..."[3]

Table S2. Proposal by Gentleman and Chan (2009) for a classification protocol for describing NMs. Reproduced with permission from [4]; Copyright John Wiley and Sons, 2009.

Table 1. Codification protocols for the nanomaterial classification system.

Chemical Class	Size and Shape	Core Chemistry	Ligand Chemistry	Solubility
XT_1T_2	$r(r_e)M_1M_{1b}(m_2)M_3M_4M_5$	$(Z_1,Z_2,\ldots,Z_n)$	$[(f_i,f_e)_1;(f_i,f_e)_2;\ldots;(f_i,f_e)_n]$	S[log D(pH)]
X 1 if organic/ fullerene (contains no metals)	r = smallest defining dimension in nm r_e = other defining size (if applicable)	0 if no core	0 if no ligands	**S** **O** if log D > 1 **W** if log D < −1 **OW** if −1 < log D < 1
2 if inorganic/ organometallic	M_1 **B** = ball **H** = polyhedron/faceted **R** = rod/wire **P** = plate/disc/well	list core elements in conventional chemical order; dopants can be included if known	f_i (see Table 2) functional group on inside/ adsorbed to core f_e (see Table 2) outer functional group	indicate log D and pH measurement (if know
T_1 outermost chemistry **D** = dendrimer **F** = fullerene **L** = liposome **P** = polymer	M_{1b} (M_1 value not nec.) **A** = astral (not after B) **I** = irregular			
	m_2 (omit if unknown) **B(b)**, b = # radii: 1 = spheroid; 2 = ellipsoid **H(h)**, h = # faces **R(r)**, r = # barrel faces, 0 = cylinder **P(p)**, p = # sides, 0 = circle **A(a)**, a = # arms	/ indicates inter–core boundary, for example (Cd,Se/Zn,S) is a core/shell	/ indicates multilayer structures, for example $[(f_i,f_e)/(f_i,f_e)]$ is a bilayer for nested structures, only indicate outermost shell	
	M_3 **L** if elongated		bioconjugation $[(f_i,f_e/Bio)]$ or $[(f_i,Bio)]$	
T_2 **N** = nested	M_4 **T** if teethed/ jagged edges		sheet structure, list twice, for example CNT [(Ful,Ful)]	
	M_5 **C** if coiled/helical/ twisted			

Table S3. Overview on safety assessment studies on different morphologies, sizes, and functionalizations of Au NMs (Reproduced with permission from [5,6]; Copyright Royal Society of Chemistry, 2011; Copyright Springer Nature, 2013).

NM Type	Size	Functionalization	Reference
Colloidal Gold (Au nanosphere)	(2 nm)	Quaternary amines	Goodman et al., 2004 [7]
Colloidal Gold (Au nanosphere)	(3 nm)	Tiopronin, TAT-peptides	de la Fuente et al., 2005 [8]
Colloidal Gold (Au nanosphere)	(3.5 nm)	Lysine & poly-L-lysine	Shukla et al., 2005 [9]
Colloidal Gold (Au nanosphere)	(4, 12, 18 nm)	Biotin & CTAB	Conner et al., 2005 [10]
Colloidal Gold (Au nanosphere)	(14 nm)	-	Pernodet et al., 2006 [11]
Colloidal Gold (Au nanosphere)	(15 nm)	Coumarin-PEG-SH	Shenoy et al., 2006 [12]
Colloidal Gold (Au nanosphere)	(20 nm)	BSA & peptides	Tkachenko et al., 2004 [13]
Gold nanorod (GNR Au-Ni)	(200 × 100 nm)	DNA / transferrin	Salem et al., 2003 [14]
Gold nanorod (GNR-65 × 11)	(65 × 11 nm)	CTAB & PEG-SH	Niidome et al., 2006 [15]
Gold nanorod (GNR-65 × 11)	(65 × 11 nm)	CTAB & phosphatidylcholine	Takahashi et al., 2006 [16]
Gold nanoshell			Manju & Sreenivasan, 2010 [17]

An example of the power of identifiers for searching and organising nanosafety data

A simple example of the power of identifiers for NMs are the JRC representative industrial nanomaterial identifiers. A quick overview of these identifiers and ontology mapping is found in a NanoCommons guidance document (https://nanocommons.github.io/specifications/jrc/). Section 3 of this document shows an overview of literature that uses these JRC identifiers in the text, making it easy to find articles about a particular JRC NM. Here, the indexing service is Wikidata [18] allowing us to use Scholia [19,20] to list the information about the JRC NMs (unpublished). For example, on https://scholia.toolforge.org/topic/Q47462008 we can find the literature in which JRCNM01101a is discussed. The guidance also provides the eNanoMapper ontology [21] mappings, allowing to list all TiO_2 JRC nanomaterials. Of course, the list of JRC identifiers is quite limited and not a general solution.

If you want to index identifiers, it must be easy to recognize them. The new JRCNM-based identifiers are therefore better than the older NM-based JRC identifiers. Even then, it can require text mining to extract them. Alternatively, semantic web approaches can be used. The schema.org-based Bioschemas (bioschemas.org) is an ELIXIR-supported open standard that allows providing metadata about the things discussed on webpages [22]. Like schema.org itself, Bioschemas has various topic types it can represent, and *ChemicalSubstance* is most suited for NMs (https://bioschemas.org/profiles/ChemicalSubstance/0.4-RELEASE/, unpublished). The content is commonly added to webpages as a snippet of JSON-LD, and may look like the script shown in Figure S1, which specifies the chemistry of the NM only as ZnO and the size as 152 nm. Thus, it has minimal support for the chemical composition, and a *NInChI* identifier would provide a lot more detail than the above Bioschemas ChemicalSubstance example.

```
{
  "@context" : "https://schema.org",
  "@type" : "ChemicalSubstance" ,
  "name" : "ZnO-152nm" ,
  "identifier" : "JRCNM01101a" ,
  "chemicalComposition" : "ZnO" ,
  "url" : "https://scholia.toolforge.org/topic/Q47462008"
}
```

Figure S1. *ChemicalSubstance* is most suitable Bioschemas format for representing NMs, and adding this text to webpages provides the relevant NM metadata (composition = ZnO; size = 152 nm; Identifier = JRCNM01101a) allowing indexing.

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