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Supplementary information

to

A technique-driven materials categorisation scheme to support regulatory identification of nanomaterials

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Particles embedded in a matrix

The materials categorisation system can also be applied, in a slightly extended form, to nanoparticles embedded in an article or in a formulation. In the example shown in Figure S1, this is done for a sunscreen lotion which contains titanium dioxide nanoparticles. In that case, the categorisation system is extended by two main criteria: (i) type of matrix and (ii) removal of non-particulate components. 'Removal' includes all means of separating the particulate components from the matrix, including filtering, digestion and ashing.

Type of matrix

The type of matrixes in which particles are embedded or suspended is also a necessary criterion to be taken into account in order to know which techniques can be applied. Three cases can be selected:

- Particles are embedded in a solid matrix
- Particles are embedded in a liquid/gel matrix
- Particles are suspended in a gas

If the particles cannot be removed from the matrix, the analysis must be performed directly on the embedded particles.

Removal of the non-particulate components and particle extraction

If the matrix can be separated without altering the particulate components, the techniques used to measure the latter can be the same as those used for materials with monotype and multiple types of particles. For instance, if the matrix of a sunscreen which contains particles of titanium dioxide can be removed, the techniques to analyse the remaining particles would be the same as for pristine titanium dioxide. A variety of procedures to separate the matrix in order to extract nanoparticles are described in the literature [1,2], including digestion methods to remove food matrices. However, such procedures must be compatible with the particles to extract them without modifying the particles during the extraction process.

The criterion of matrix removal can then be selected as follows:

- the non-particulate components can be separated (or alternatively the particles can be extracted). In that case, the conditions should also be specified.
- the non-particulate components cannot be separated (or the feasibility is unknown)

An example of the categorisation of a sunscreen containing coated titanium dioxide particles is presented in Figure S2. The non-particulate components can be removed and the type of matrix is a gel/liquid. The particulate material is a composite of the core-shell type, has three small dimensions and the exact shape is unknown. Due to the latter condition, the option 'unknown' has been chosen instead of '3 (spherical, equiaxial)'. Further, it is expected that the size range is between 20 and 120 nm and it is known that the particles are of only one type. A known specific property is size-dependent photon absorption, whereas others are also unknown, so that the corresponding boxes remain unfilled. Matching these characteristics with the technique performance table leads to EM and AFM as applicable techniques. The main limiting condition for this recommendation is the fact that the shape of the particles is not known.

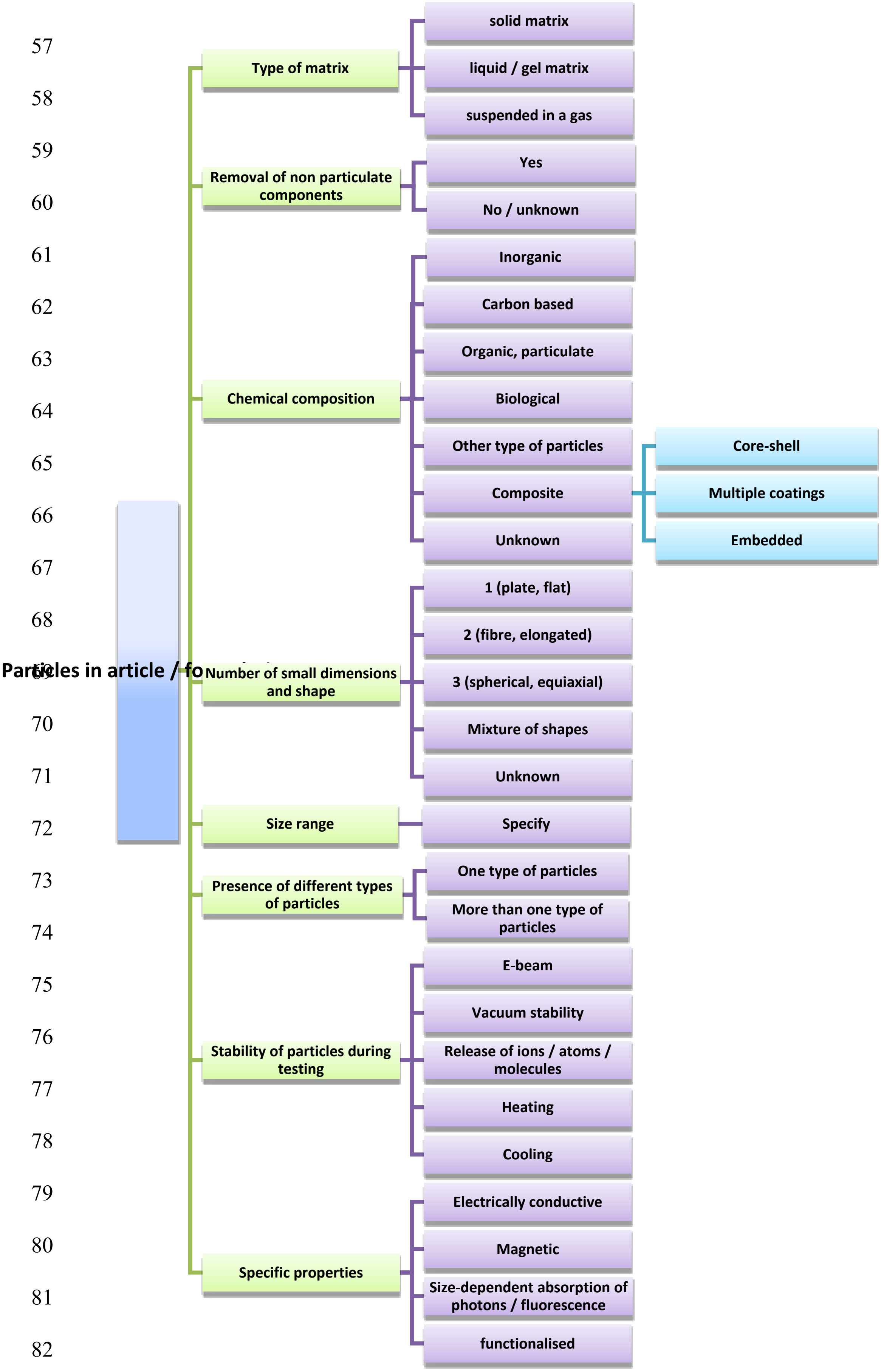

Figure S1: Scheme of the Material Categorisation System for an article / formulation that contains particles

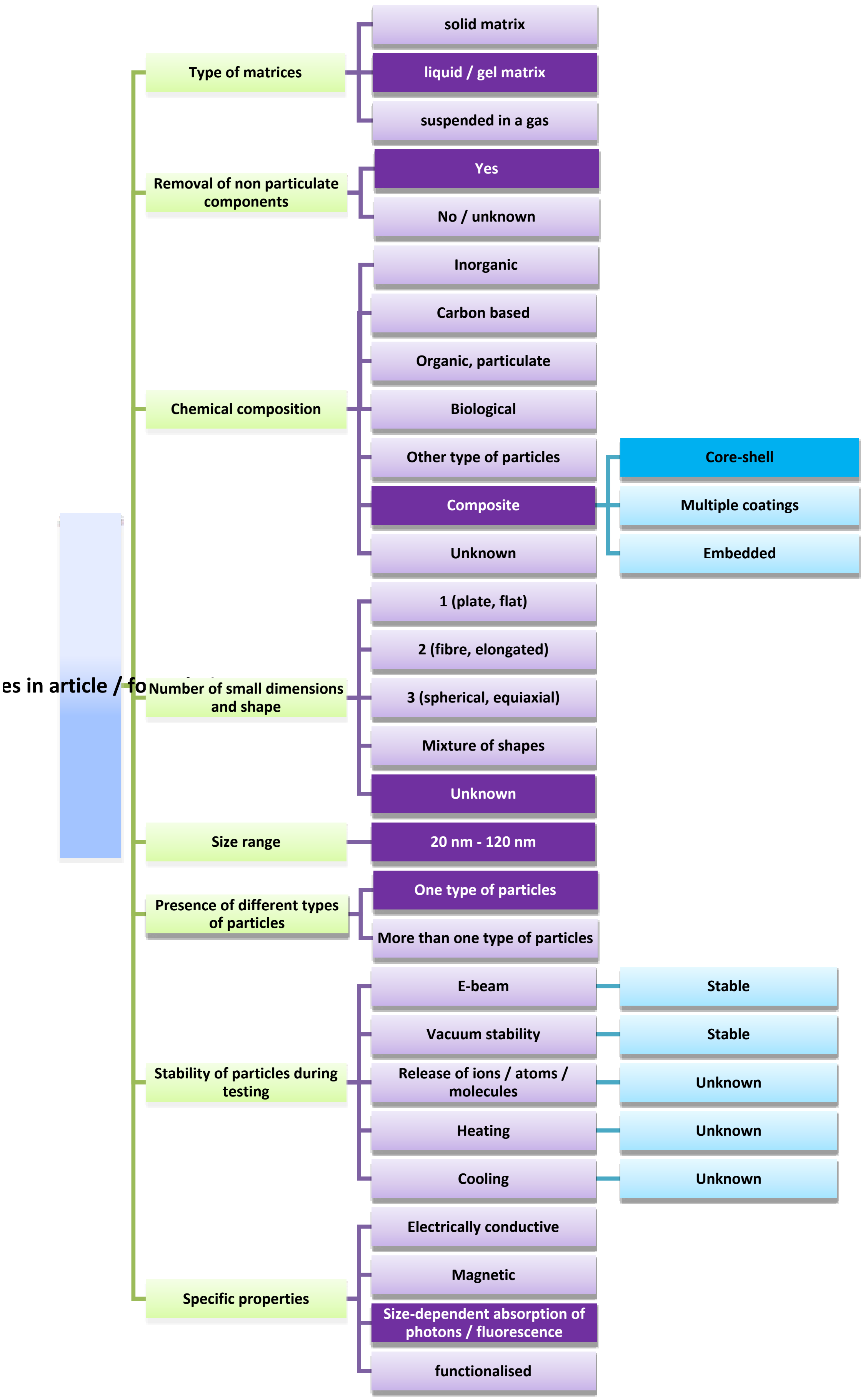

Figure S2: Scheme of the Material Categorisation System applied to coated titanium dioxide particles in a sunscreen formulation

References

[1] Singh, G., Stephan, C., Westerhoff, P., Carlander, D., Duncan, T. V., Measurement Methods to Detect, Characterize, and Quantify Engineered Nanomaterials in Foods, *Comprehensive Reviews in Food Science and Food Safety* **13**, 693–704 (2014).

[2] Peters, R., ten Dam, G., Bouwmeester, H., Helsper, H., Allmaier, G., von der Kammer, F., Ramsch, R., Solans, C., Tomaniov´a, M., Hajslova, J., Weigel, S., Identification and characterization of organic nanoparticles in food, *Trends Anal. Chem.* **30**, 100–112 (2011).