Classification and Reporting of Nanostructured Silica Materials

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There is currently no specific provision that correctly defines the information required for substance identification and reporting of manufactured nanomaterials (MNM) in REACH. Challenges (*Figure to the left*) arise as MNM increasingly become more and more advanced and move from first to higher generation materials that are mixtures with important fractions of different inorganic and organic compounds.

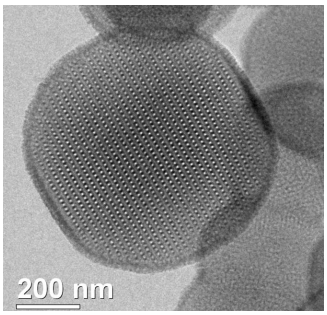
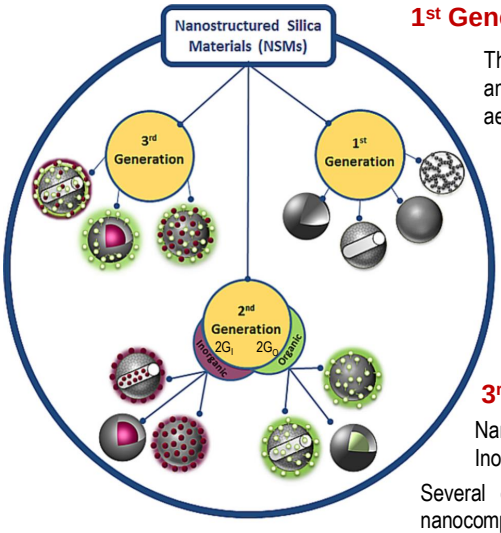


Figure: How to define and identify (Under REACH) a mesoporous silica particle whose internal pore structure is in the nanoscale and an external particle diameter is in micron size?

Classification

Using Nanostructured Silica Materials (NSMs) as an example, we established a classification system (*Scheme below*) based on their composition, extent and location of surface treating agents. The system enables systematic classification of a wide range of silica materials and can aid identification of potentially unknown MNM for further assessment of potential hazards and risks. The system could also be applicable to metal and oxide MNM in general.



1st Generation Nanostructured Silica materials (1G-NSMs):

The generation, includes only bare silica nanoparticles (SNPs) where the surface or in the internal structure of amorphous silica contains end groups such as silanols or siloxanes. Examples including aggregated SNPs (e.g., silica aerogels, fumed silica), monodispersed SNPs, and porous SNPs (e.g., mesoporous (*Figure*) and hollow).

2nd Generation Nanostructured Silica materials (2G-NSMs):

The composite of nanostructured silica contains: 1) One or more organics or 2) One or more Inorganic compounds as their secondary phase.

Depending on the composition of the surface treating agent, the 2G-NSMs are further divided into Nanocomposite of Silica-Organic ($2G_O$) and Nanocomposite of Silica-Inorganic ($2G_I$). The complexity is given by the location of the compounds which is either external (E) or as a core (C) of silica or combination of both,

3rd Generation Nanostructured Silica Materials (3G-NSMs):

Nanostructured silica comprises of surface treating agents in the form of one or more organics *and* one or more Inorganic compounds as their counter parts.

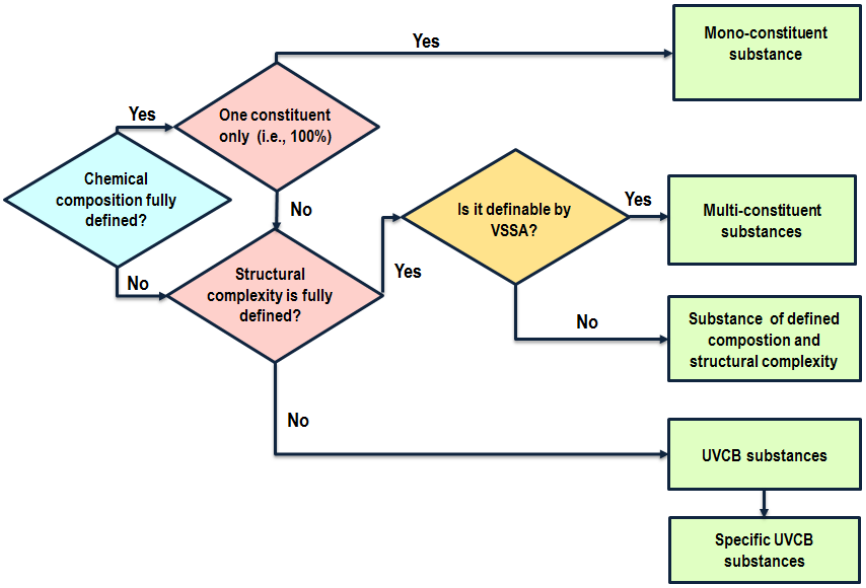
Several combinations can be derived such as Silica-Organic/Inorganic nanocomposite, Inorganic /Organic -Silica nanocomposite, and Organic/Inorganic- Silica-Inorganic/ Organic nanocomposite. Few examples are schematically shown in the Scheme.

Substance Identification and Reporting of Nanostructured Silica Materials

The volume specific surface area (VSSA) is proposed as an additional identifier for silica-based NM to enable their identification and information requirements for reporting. In line with the REACH guidance document to identify a substance by its chemical composition, we also propose a new *Scheme (left)* for identification of silica-based nanomaterials. In the scheme, the structural complexity of a nanocomposite is used as a cross check to define VSSA as an additional identifier.

Under this approach, bare silica nanoparticles are justified as mono-constituted substances; substances of known constituents are considered to be a multi-constituent substance and substances of unknown or complex composition as UVCB (Unknown or Variable Composition, Complex reaction products or Biological materials) substances.

Accordingly 1G, 2G and 3G-NSMs can be identified by their composition, structural complexity and VSSA.



Overall, a range of nanostructured silica materials could be classified by their composition and structural complexity associated by the surface treatment. The volume specific surface area (VSSA) is used as an additional identifier, to ease identification and reporting of silica-based MNM. Actual implementation of the proposed *scheme* would require more studies, in particular to define a threshold value for VSSA and must be validated. In our future work, we will evaluate the scheme with examples and validate the classification system.

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