**Systematically varied nanoparticle libraries for nano-ecosafety assessment**

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*Project description*: In order to facilitate the commercialization of applications of nanotechnologies (so-called nano-enabled products) it is necessary to move beyond case-by-case safety assessment and towards predictive models based on quantitative structure-activity relationships (QSARs). The prerequisite for establishment of such relationships is availability of libraries of nanomaterials (NMs) in which single properties are systematically varied in order to correlate degree of a specific property with toxicity. Currently such libraries are not widely available, and the aim of this PhD project is to develop such a nanoparticle library, synthesizing multiple variations around an initial core. Variations to the *intrinsic* particle properties may include size, shape, redox activity and bandgap, surface charge, and to the *extrinsic* properties may include surface charge, surface coating, surface functionalisation etc. and the consequences of each on the nature of the resulting bio-nano interface. Potential core materials include cerium dioxide, zinc oxide and copper oxide as these are excellent candidates for assessing mechanisms of toxicity and the potential for tuning out toxicity by modifying specific physico-chemical parameters. While the focus of the project is on nanoparticle library synthesis, the candidate will also have the opportunity to perform some *in vitro* biological assays to assess the toxicity of their particle libraries, using a semi-high throughput format in order to construct QSARs.

The overarching hypothesis being assessed in this project is that there are specific NM physico-chemical properties (or combinations of properties) that correlate with specific toxicity mechanism(s), and that by developing libraries of NMs, made via identical synthesis routes and systematically varying only a single parameter, it will be possible to determine (a) which physic-chemical parameters are linked to which toxicity mechanism; (b) which physic-chemical parameters merely modulate the extent of toxicity induced by other physic-chemical parameters, and (c) what amount or degree of each parameter is required in order to induce the specific toxicity pathway in representative cell lines / sentinel organisms. Coupling this knowledge will facilitate the development of QSARs and from this enable the prediction of toxicity of new or unknown NMs on the basis of their combination of physico-chemical parameters. A key parameter for analysis of impacts of variation of physico-chemical parameters will be the resulting NMs interactions with biological and environmental macromolecules and the composition and nature of the coronas, as we believe that these interactions will be a very sensitive correlator with NM fate and behaviour, as well as being measureable in semi-high throughput manner, which is a pre-requisite for onward development as a screening tool for use in regulation and safety assessment.

The project combines NM synthesis, characterisation and assessment of macromolecule interactions as the basis of development of QSARs for prediction of NM (environmental) fate & behaviour. It will feed into the EU FP7 NanoMILE project, thereby providing a strong route for dissemination of findings to regulatory authorities and industry. Candidates should have a strong background in physical sciences and chemistry with mathematics being desirable.

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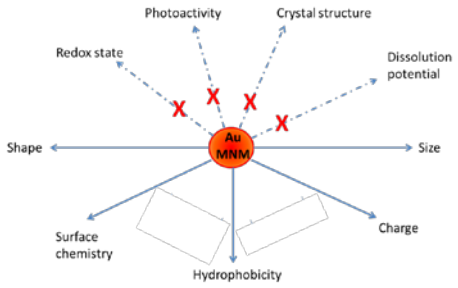


**Figure:** Schematic illustration of the approach to systematically varying available parameters for specific NMs. Note that not all parameters are available for all NMs, since, in the example given, Gold (Au) NMs cannot (easily) be made of varying solubility or photoactivity. It is also clear that not all parameters can be varied independently, and this project will map out the variable space and identify interlinked parameters

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