Knowledge transfer and data sharing through the H2020 NanoCommons transnational access services: User cases and lessons learned

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Introduction

The Environmental Nanosciences Group at the University of Birmingham (UoB), through the Horizon 2020 e-infrastructure project NanoCommons, is designing, testing and implementing nanosafety data management processes and tools applicable from the beginning of the data lifecycle; i.e. the experimental or computation design phase to facilitate knowledge transfer and data sharing for the further advancement of nanosafety and novel and advanced materials (NAMs) research and nanoinformatics. Currently a substantial amount of nanosafety data remains inaccessible or if available non-interoperable due to the lack of sufficient metadata, semantic annotation or a structured way to present the data. This inhibits the maximisation of data exploitation and data driven innovation. Here, we present selected case studies from the Transnational Access projects offered by UoB, and show how these approaches can maximise data exploitation and the transferability and reusability of certain tools under different contexts.

Aims & Objectives

- To maximise nanosafety data exploitation and added value and promote data driven innovation
- To make metadata capturing and recording (Figure 1) and data annotation part of everyday scientific practice in nanosafety
- To use metadata to promote data quality, interoperability and transferability
- To promote Open and FAIR data through provision of data management tools
- To offer a range of analytical and modelling tools to the scientific community
- To demonstrate the transferability of tools between the different fields of materials science, and especially to complex and advanced materials.

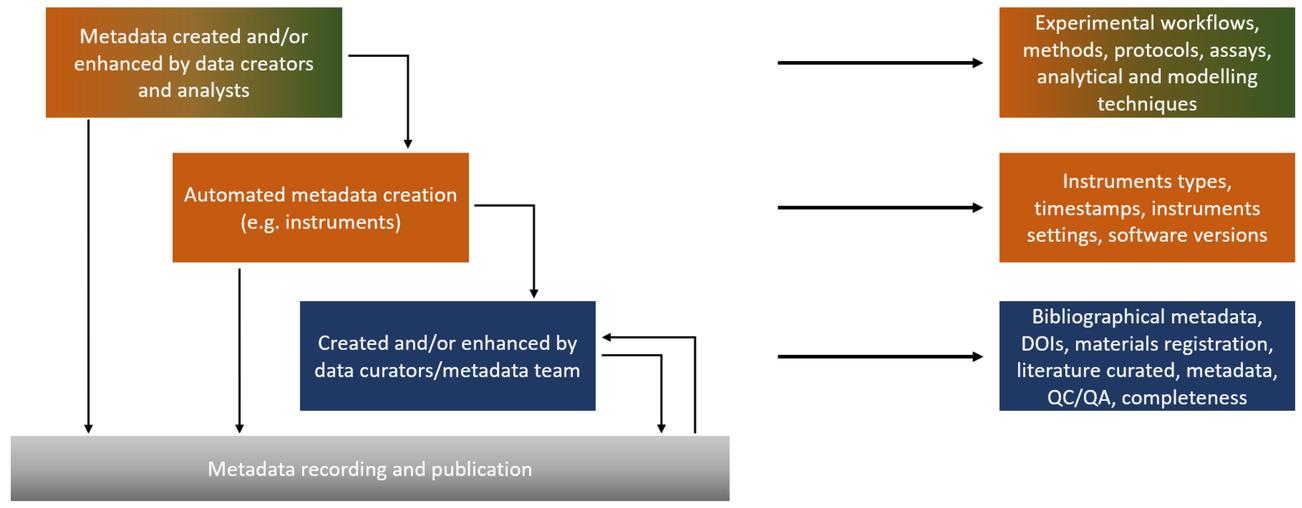
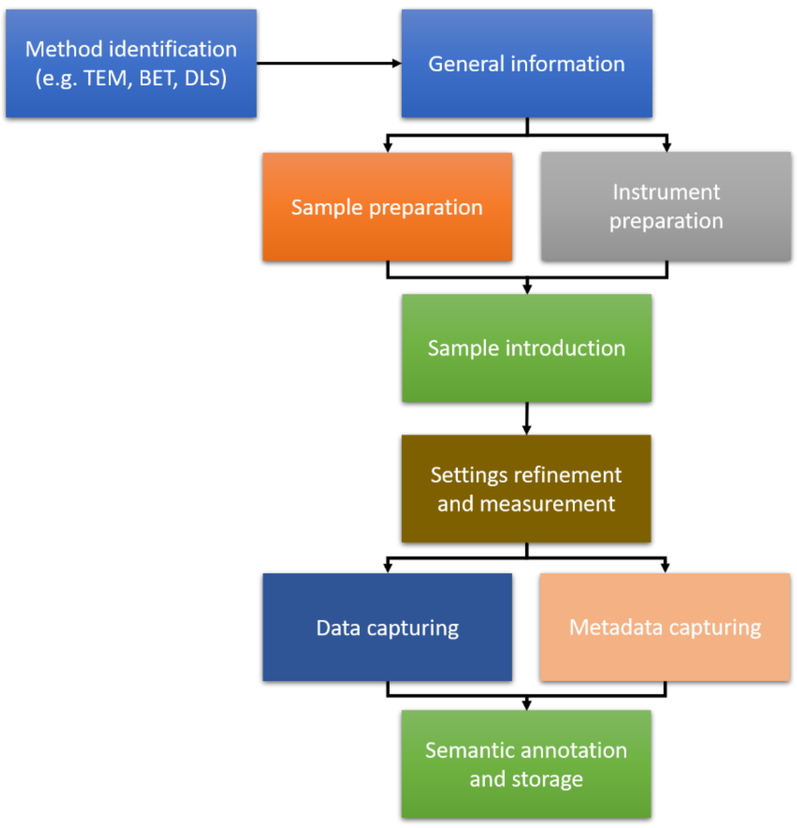
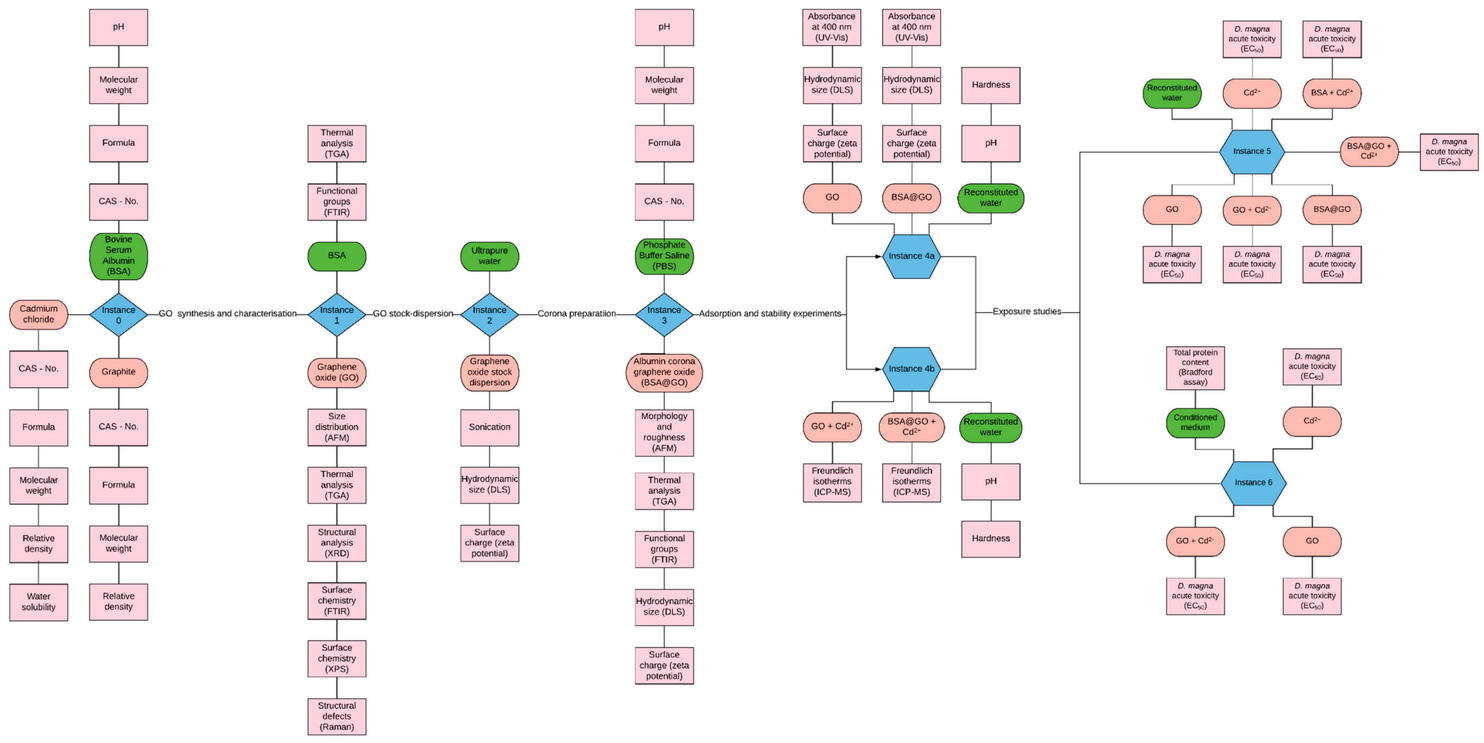


Figure 1: The metadata capture workflow and the respective metadata. Note that the colours in the metadata boxes correspond to the stages of the data life cycle, with orange representing descriptive metadata associated with the planning and acquisition stages, green representing technical metadata from the processing and analysis stages, and navy blue representing bibliographic metadata from the storing and sharing stages.

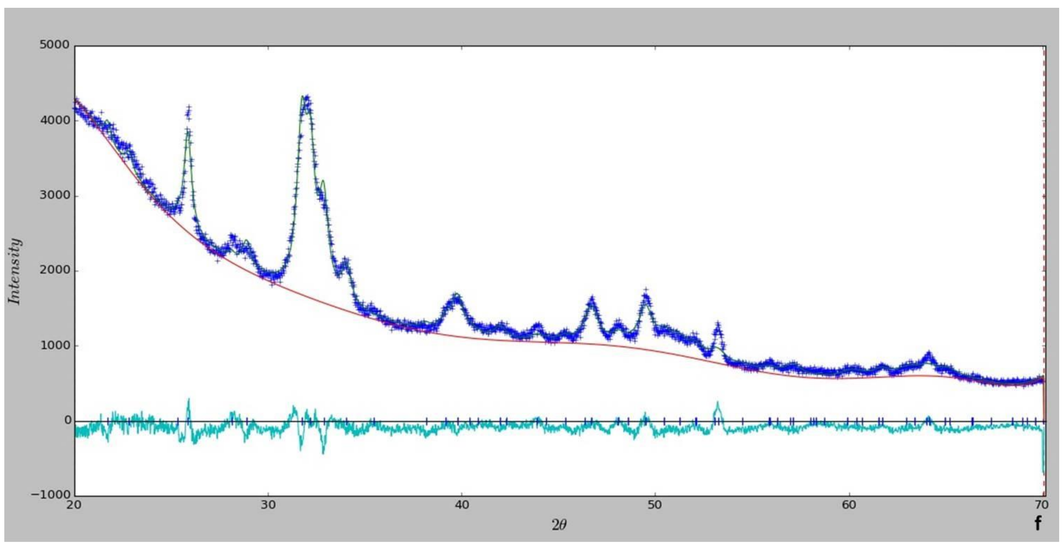
Selected Case Studies



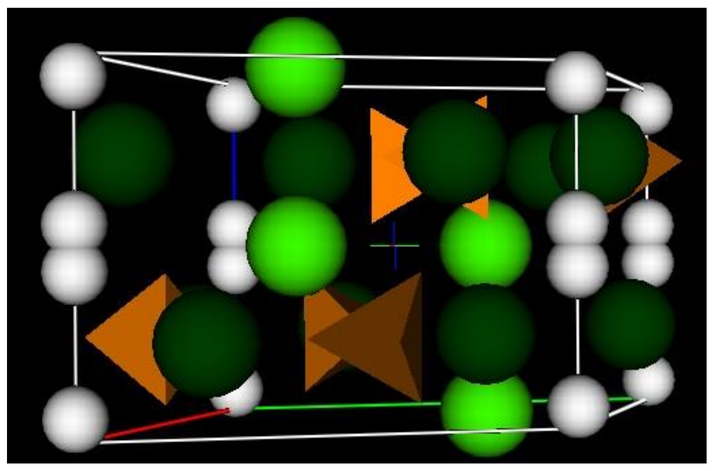
Case Study 1: The NanoCommons data integration workflow incorporating the capture of the optimum amount of data and metadata, along with respective ontological annotation.



Case study 1: Instance map implementation of experimental workflows, data capture, management and annotation for transfer to Electronic Laboratory Notebooks (ELN) for assessment of the toxicity of graphene oxide and cadmium mixtures to *D. magna*. The workflow included all steps from ENM synthesis, to toxicity studies, data management and uploading to the NanoCommons Knowledgebase. Collaboration with the Brazilian Nanotechnology National Laboratory (LNNano). Reference: Martinez et al. (2020), MDPI Nanomaterials, 10(10), 1936 DOI: https://doi.org/10.3390/nano10101936



Case Study 2: Rietveld refinement and crystal unit cell reconstruction from XRD data of biological hydroxylapatite from bones originating from ancient burial cites in Belgium. Rietveld refinement has been used to analyse the structure of complex nanomaterials (e.g. r-doped TiO_2) and structural modelling of the resulting unit cells. Collaboration with Vrije University, Brussels.



Case Study 2: Crystal unit cell reconstruction from XRD data of biological hydroxylapatite from bones originating from ancient burial cites in Belgium. Light and dark green spheres Ca^{2+}, yellow pyramids PO_4^{3-} and white spheres O^{2-}. Collaboration with Vrije University, Brussels.

Lessons learned

- Data management needs to start from the onset of a scientific project
- Visualising the clearly defined experimental workflows assists greatly with data and metadata capture
- Metadata capture and annotation needs to start prior to data capture to assist with the development of detailed and harmonised templates
- The tools developed for the study of (nano)materials can be adapted and used for the study of complex and advanced materials.

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