

Minutes of the WG4 meeting - 2016-02-16

Present: Freddie Ehrhart, Johannes Pelzer, Richard Marchese Robinson, Markus Hegi

Regrets: Peter Ritchie, Egon Willighagen, Nina Jeliazkova, Sara Tataro, Hugues Crutzen

Next meeting: March 8, 15 CET

Agenda

- Announcements
- NSC Sustainability Meeting
- eNanoMapper updates
- Linked Data Task proposal
- Nanoinformatics Book Chapter

Announcements

- [Minutes of 2016-01-12](#)
- [Updated WG4 page on NSC website](#) (per NSC request: all WGs pages in the same structure)
- NSC Steering Committee meeting has not taken place yet
- Egon Willighagen, Nina Jeliazkova, Sara Tataro, Hugues Crutzen are attending the 3rd ProSafe project meeting in Dessau today

NSC Sustainability Meeting 2016-01-25/26

- NSC Sustainability WG to be set up (to cover not just ontology and databases, but the full NSC infrastructure)
- There is a need for building a community for the eNanoMapper ontology
 - Maybe as a task of this WG4?
- Feedback from others?
 - How to fund, say, eNanoMapper database on an ongoing basis?
 - Cost depends very much on required functionality and Openness of the data (Open Data is a lot cheaper)
 - Could commercialisation support?
 - Yes, commercial support is being actively explored, e.g. the Freemium model.
 - Could projects be asked to pay for access to, say, eNanoMapper database? Possible concern raised: Would this be contradictory to the long term aims of the database as maybe projects have different, specific, short term goals?
 - Yes, the eNanoMapper solutions *can* be used for private data with access control. Mind you, from an eNanoMapper perspective there will not need be a single database to collect all data.
 - How to deal with specific needs of single projects when these are in conflict with the existing database setup?

- Various options exist' the architecture is flexible. Contract development may be needed, depending on the exact needs (and how different they are).

eNanoMapper updates

- Basel Workshop Feb 10th ([program with materials](#))
 - First [developers demo of a read-across tool](#)
 - [Example](#) of data integration over data sources
- Upcoming workshops
 - March 3rd: ontology workshop/hackathon with NECID
 - April/May: modelling/descriptor hackathon with NTUA
- New [experimental search interface](#)
- The EMBL-EBI released the [Ontology Lookup Service beta with the ENM ontology](#) (courtesy [spot-team](#))

Linked Data Task proposal

- See the email archived [here](#) (and see the below Appendix)
 - already discussion on the mailing list
- [Example Linked Data “bundles”](#) via new NanoWiki version: ArrayExpress, SigmaAldrich, Crystallography Open Database, JRC Representative Materials (will be used to explore and develop the Linked Data features in the API)
 - synergy with WG4 sought
- This Task Proposal was accepted, with no objections.

Nanoinformatics Book Chapter

WG4 has been invited to write a book chapter for the nanoinformatics book being developed in the USA NanoWG (coordinated by Mark Hoover): “Nanoinformatics: Principles and Practices”. (Further information can be found [here](#), after registering with the NCIPhub, or via contacting Mark Hoover.) We can write about the past work done, including the discussions we’ve had and things we discussed.

Are ‘we’ in? Please discuss and see if there is critical mass.

Richard Marchese Robinson - interested to assist, say, Egon W with work on this although cannot make a firm commitment at this stage.

Appendix: Linked Data Task proposal

From the email archived [here](#):

The proposed objective of this WG4 task is to create link sets that map identifiers using the ["lens" approaches](#) developed in the [Open PHACTS project](#). These allow explicit, semantic description of the level of similarity between two linked materials via their two identifiers. This approach allows expressing that two entries in two different databases are identical (e.g. same material from the same paper), similar (e.g. identical physchem properties), or relates (e.g. similar physchem properties). Specific tasks would be:

- define the levels of similarity we want to use in the NSC (and perhaps NanoWG too)
- identify the key databases we want to link (that have online presence, provide deep linked, etc; the SigmaAldrich/COD database are good examples that allow that) (as input we will take the output of Task 2013-1)
- make mappings between those databases (these mapping should be CCZero to allow wide adoption; they do *not* include data, and just are the ID-ID mappings)
- create a Linked Data graph for NanoSafety
- (optionally: embed our graph in the big [Linked Data Cloud](#))