

Minutes of the WG4 meeting - 2016-05-10

Present: Egon Willighagen, Lucian Farcas, Rob Reedijk, Jan Kirrbach, someone from Gdansk, Camille de Garidel-Thoron, Nina Jeliazkova, Freddie Ehrhart, Shahzad Rashid

Regrets: Johannes Pelzer, Peter Ritchie, Axel Mustad (*could not connect*)

Time: 15 CEST

Next meeting: Tuesday June 14, 15 CEST

Announcements

- Updated [participant](#) and representation lists
 - Egon will add Camille to the list (Prosafe and the Labex Serenade)
- Updated Compendium contribution WG4
- [Minutes of 2016-04-12](#)
- [NanoSafety Cluster Newsletter is out](#)
- New paper(s)
 - Marchese Robinson et al. **How should the completeness and quality of curated nanomaterial data be evaluated?** Nanoscale, 2016, [10.1039/C5NR08944A](https://doi.org/10.1039/C5NR08944A)

Project updates

- eNanoMapper
 - Nikolay Kochev et al. (2016). nmdataparser: nmparser-1.0.2. Zenodo. [10.5281/zenodo.49605](https://doi.org/10.5281/zenodo.49605)
 - new paper: Drakakis et al. **Decision Trees for Continuous Data and Conditional Mutual Information as a Criterion for Splitting Instances**, Combinatorial Chemistry & High Throughput Screening, 2016, [10.2174/1386207319666160414105217](https://doi.org/10.2174/1386207319666160414105217)
 - 2nd NanoSafety Forum for Young Scientist. Abstract submission deadline 30th May, <http://trippus.net/nanosafetyforum2016>
 - New outline of the eNM database: <https://data.enanomapper.net/>
- NanoMILE:
 - There is still no experimental data in the database.
 - We try to get minimal physicochemical information about nanomaterials in.
 - Cross-links between Jan-Iseult and Iseult-Freddie

ISA-TAB and ISA-JSON

- Nina reports good progress in her eNanoMapper work on ISA-JSON export from the database
- ISA-TAB and ISA-JSON can be interconverted <https://github.com/ISA-tools/isa-api>
- ISA-JSON has an extension mechanism.
 - Nina is reworking the Nano extension into this JSON mechanism

- https://github.com/enanomapper/isa-api/tree/master/isatools/schemas/isa_model_version_1_0_schemas/material material extension [example json](#)
- Aligned with the NanoWG/USA work on ISA-TAB-Nano
- Working on command line converter that takes spreadsheets (based on nmdataparser?) into ISA-JSON directly
<https://github.com/enanomapper/nmdataparser>
- Projects planning on using ISA: eNanoMapper, NanoMILE
 - Camille: Serenade database project will consider also the ISA-Tab format

Linked Data Task

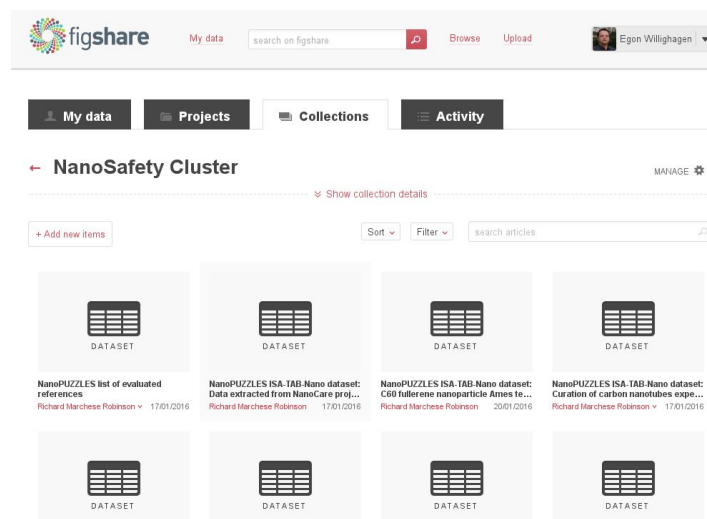
- Egon will work out some ideas related to the matching eNanoMapper task
- All: invited to join the discussion, shows needs, etc

Brussels 28 April

- Meeting was canceled
- NSC Steering Group telcon
 - WG reorganisation not covered (so, no news on the Sustainability WG brought up in the January NSC meeting in Brussels)
 - No discussion on EU data infrastructure (Elixir, Open Data pilot, ...)
 - Various roadmaps, including one on nanoinformatics

FigShare Collections

- See proposal on the mailing list
 - And <https://figshare.com/blog/>
- Demo: <https://figshare.com/account/home#/collections/2860960>
 - Private, currently. Egon will open it, shared screen, and here's the screenshot:



- Go or No-Go? Go forward.

- Egon will pick it up with WG7 and send feedback to the WG4 mailing list

Meeting schedule in the summer months

- We continue meetings over the summer holiday
 - Also in July and August
- Egon and Lucian will plan the chairing and hosting