



Event: WorldFAIR Chemistry Webinar: “ What is a Chemical? Handling Chemical Data Across Disciplines”. September 22, 2022. 12-1:30 pm EDT.

- ***This space is to share notes/comments and discuss the topic of the event above. This document is available to be downloaded and shared.***

- **Agenda:**
 - Flash Talks (Moderated by: Ian Bruno)**
 - 1. Environmental Cheminformatics: Emma Schymanski
 - Visualization of data is very important
 - Link to slides: <https://zenodo.org/record/7096404#.YyyNIXbMKUk>
 - 2. Environmental Nanoscience: Iseult Lynch
 - A notation of nanomaterials is being developed to be able to describe nanoparticles - based on the InChI so will be NInChI
 - Linking as-synthesized material to various transformed forms (during storage, upon dispersion, in the environment/body etc.) to correlate actual form with effect.
 - Same issues likely apply to geomaterials as once removed (sampled) is different / oxidizing etc.?
 - 3. Geoinformatics and Geoscience: Lesley Wyborn
 - In need of a single International Union -> we mainly have multiple geochemical societies and associations: few have data standards commissions or working groups.
 - Looking at the W3C/OGC [Sensor, Observation, Sampling and Actuation \(SOSA\) Ontology](#) as a structured way to exploit common patterns in science, chemistry and geoscience and to semantically describe the data/metadata.
 - Starting to think about whether InChI (or NInChI) could help with their materials representation - isotope ratios / crystal phases or domains etc. NInChI definitely includes crystal phases and proportions, and isotopes should be possible also.
 - Trying to leverage IUPAC and other standards to improve data reporting, as well as IUPAC's well established ways of developing, promulgating, governing and updating standards.
 - 4. Geoinformatics Data Management: Kerstin Lehnert

**WorldFAIR “Global cooperation on FAIR data policy and practice” is funded by the EC HORIZON-WIDERA-2021-ERA-01-41 Coordination and Support Action under Grant Agreement No. 101058393.*

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- ISGN (<https://www.igsn.org/>)
 - There are a variety of different cosmochemical sample types
 - Isotopes can be used to identify where material comes from
 - No discipline data standards across the testing sites for the Bennu samples
 - Spatial distribution of element concentrations is important
5. Astrophysics: Marie-Lise Dubernet
- XSAMS XML schema defined based on computational chemistry
 - Integration of a wide variety of databases into one system (VAMDC, <http://vamdc.org>) using InChI/InChiKey as the interoperability link on species ID
 - Needs (FAIR) identification of species, states, and reactions, machine actionable vocabularies
6. Material Development: Ken Kroenlein
- How do you engage with material science community with FAIR
 - Materials are heterogeneous,
 - Properties can vary substantially with small changes in structure
 - Materials history -> worry about where a sample has been exposed to over time
 - Terminologies are available but very different even for similar species
 - You have to relate identifiers from many different systems -> including historical...
 - Knowledge maps are very important
 - Very little computational expertise in the community
 - Need high quality data sources
7. Polymer Science and Materials: Dylan Walsh
- Cript <https://criptapp.herokuapp.com/>
 - How to represent stochasticity?
 - A lot of data is sourced via Google
 - Representation is a really big thing
 - Big SMILES
 - Properties to assemblies also needs

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- Most of data is present in papers - we don't know what has been done before of this

Panel Discussion

What are the big challenges?

- Being able to find data -> identifiers are needed and important for identify
- How to capture distributions -> real samples are not uniform
- This is a long tail ... its an issue
- How can we get together and help understand what the technology
- Modularity of things -> the sample space is incredibly complex
- Identify what are the core commonalities are in sample space
- High level controlled vocabulary/machine actionable for the chemical space
- Unify data models that can be broadly used
- There is a need for coordination of activities in enabling the community
- FAIR Cookbook! Reach the base communities at the bench level
- Chemical identifiers for a complex sample in different perspectives
- Interoperability based on sharing across the communities and representations

Announcement: the FAIR week events 24-26 October have now been announced and registration is open, including for the WorldFAIR workshop <https://codata.org/2nd-fair-convergence-symposium-24-26-october-2022-in-leiden-the-netherlands/>

Not a question for the panel but a reflection which *may* be useful to explore, or may not be! (SDH)

- Something we think about a lot in WorldFAIR work on Cross-Domain Interoperability Framework is what is the nature of the connectors used / needed when combining / comparing data from different / contiguous domains. For example place and time. Others widely used are in social sciences are particular classifications (age, social class,

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- etc). The challenge is that in the abstract these are almost infinite. Nevertheless, one can identify some priority issues and connectors, often related to specific use cases.
- Is it possible to list those connectors, beyond / in addition to the chemical represented by InChI. Some other things have been mentioned in the discussion. Structures, solutions etc have been mentioned, but not being an expert in the domain I'm not sure what the most important may be.

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