

NFDI4Chem Consortium Meeting 3.0

10/11 October 2022 (Hannover)

General Discussion with the Advisory Boards

10 October: 16:30 – 17:00

Topics that have been discussed with the Advisory Boards:

Dissemination in Academia

- how to convince people and university to use the tools and services developed by NFDI4Chem (goal is to cover all Germany)?
- The community is interested in the topic, as could be observed at conferences
- Large visibility of <https://doi.org/10.1002/anie.201907260>
- In industry ELNs are broadly integrated, but rarely used in academia
- The pressure on scientists to use ELNs is rising and motivation will be pushed with further digitalisation
- ELNs enable submission of publications with a low barrier because data are already prepared; collaboration is also expedited with ELN
- To make tools appealing to chemists from all subdisciplines is challenging
- Comment: demonstrate use cases and showcases (usage as notebook as well as knowledge management and collaborations) to the community, invest more into outreach and communication
- Changing of name 'Chemotion' might be considered, if the target group should include biologists (e.g. 'LabIMotion')
- Wide usage is a critical mass problem: once seen in other labs or by other researchers it will become self-perpetuating
- Education of young students on ELN is already well established

Engagement with Publishers

- The existence of different business models for different journals is a challenge (most want to make it easy for the researchers to publish)
- Different approaches are needed for different journals to achieve as uniform as possible journal guidelines for data publication
- 13 publishers and 14 journals were represented at the last editors4chem Workshop
- ACS is interested in Chemotion ELN as it is open source

Cooperation with Industry

- industrial collaborations should be strengthened in terms of ontologies (broader ontology instead of more)
- cross-cutting activity on ontology: 3 working groups are in this section, but level of expertise is different
- There is the need to correlate molecular information with materials more
- Hackathon is a good way to involve people
- Comment: Chemotion was mentioned at IUPAC ELN adoption in Cornell
- Instrument facility vendors might be involved to increase 4Chem distribution
- Tech support for ELN deployment is limited because of funding. Commercial Chemotion support services (analogously to eLabFTW) in the future?