

## **Post-Processing and making electron microprobe data FAIR with a new, open web-interface that is connected to an electronic lab notebook**

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Making data FAIR (Findable, Accessible, Interoperable, Reusable) has become increasingly important over the past years, and mandatory for publication in a growing number of journals. The major bottleneck of making data FAIR is during their transfer from the instrument output file to a repository or database that requires certain metadata, standard formats, or vocabularies. There is no common workflow established for this ‘data-pipeline’, and each researcher proceeds differently, which unsurprisingly results in mostly Excel-sheets of unstandardised and unstructured tables. This result is triggered by an instrument’s output file, which either does not follow any specific guideline or tries to satisfy too many needs.

We developed a web-interface that solves this bottleneck with a simple work-flow, and at the same time adds much more structure to data files by using an electronic lab notebook (ELN) in the background. Further, this web-interface allows post-processing of the data such as data clean-up, formula calculation, or data visualisation, and is built to be easily expandable with additional tools.

The procedure after data acquisition works as follows: (i) a specified set of data files from the electron microprobe is produced and uploaded as a new record to an ELN. Such an ELN entry allows for simple, semi-automated meta-data additions that might serve as a starting part of making the data FAIR. We use Kadi4Mat (<https://kadi.iam-cms.kit.edu>), as it has a Python API, through which our web-interface connects to this ELN. (ii) On the web-interface (on [geoplatform.de](http://geoplatform.de) go to ‘Microprobe’ and then to ‘Data Processing’), each ELN record can be directly accessed through its unique identifier. Only this needs to be provided, after which the microprobe data are automatically converted into a standardised, FAIR output file. A highly formalised method section is automatically produced that can directly be copied into a publication, but also provides additional details.

Built-in tools on the web-interface can then be used for further post-processing such as data clean-up, formula calculation, visualisations, etc.

This workflow is quick, simple and currently developed for the JEOL software for MS Windows, but can be easily expanded to other microprobe software.