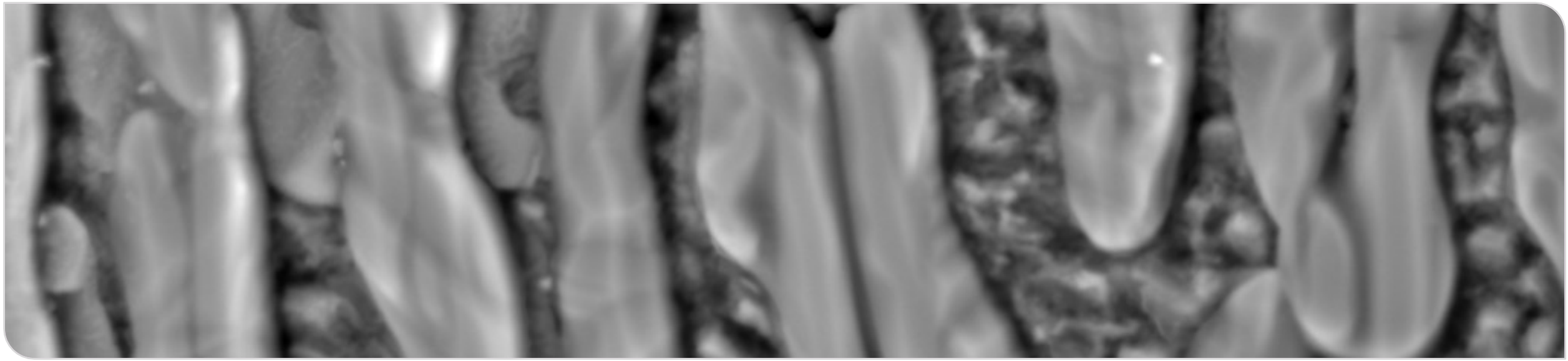
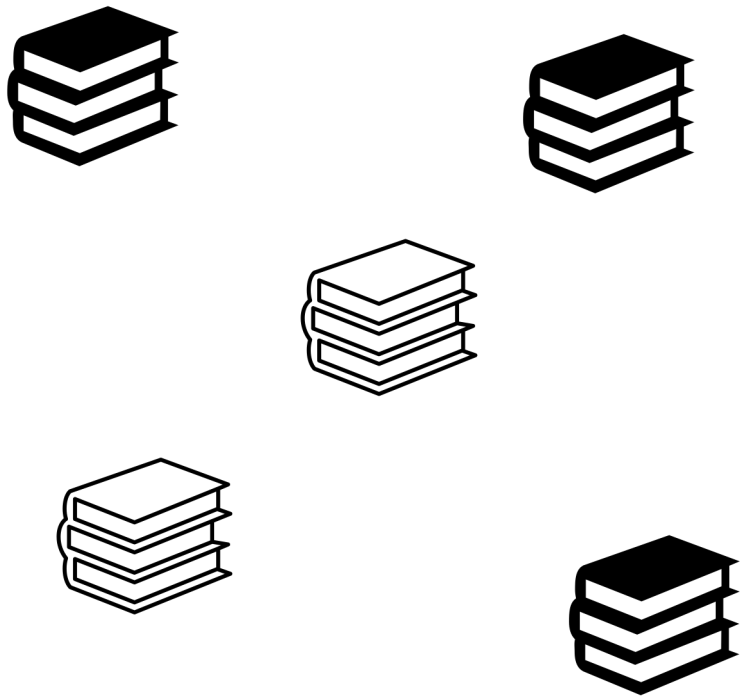
The Scheme for a Metadata Schema

Unlocking the Power of Schemas

Reetu Elza Joseph, Rossella Aversa et al. (Metadata WG of MDMC)



The Reality that We Live in



- Lab books with hand written notes
- No standard languages
- No common vocabularies
- Different measurement techniques do not correlate
- Different instruments for the same measurement technique use different terminologies
- Most ELNs act as stand-alone localised systems with very little use of standards or common practices

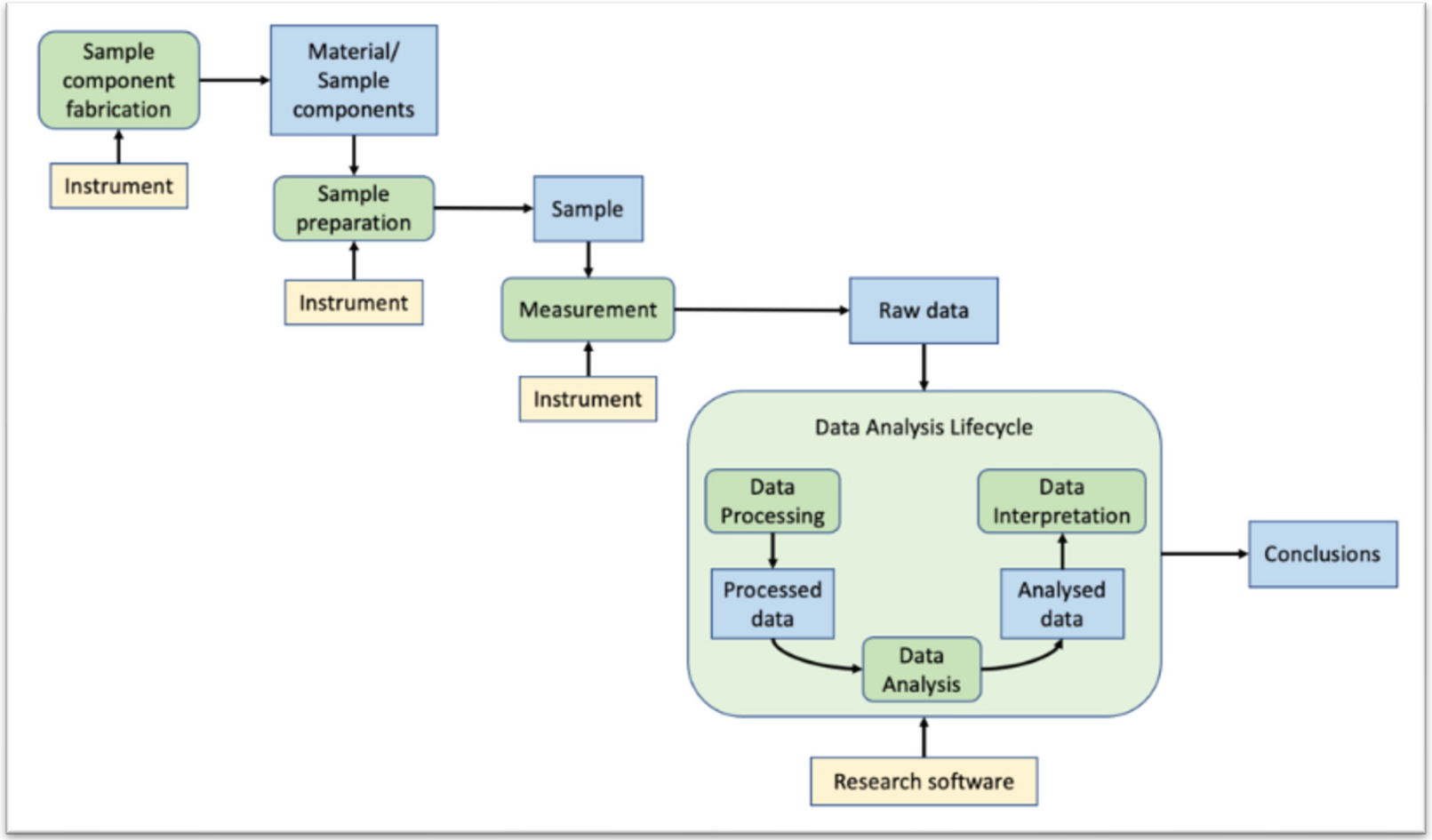
We need Schemas and Standards!

Practical Steps by the Metadata WG

Experimental Workflow of a Study

We defined an
ideal workflow*
using the MDMC Glossary

available on the
MDMC website



* First published in 2021 in https://ceur-ws.org/Vol-3036/paper21.pdf

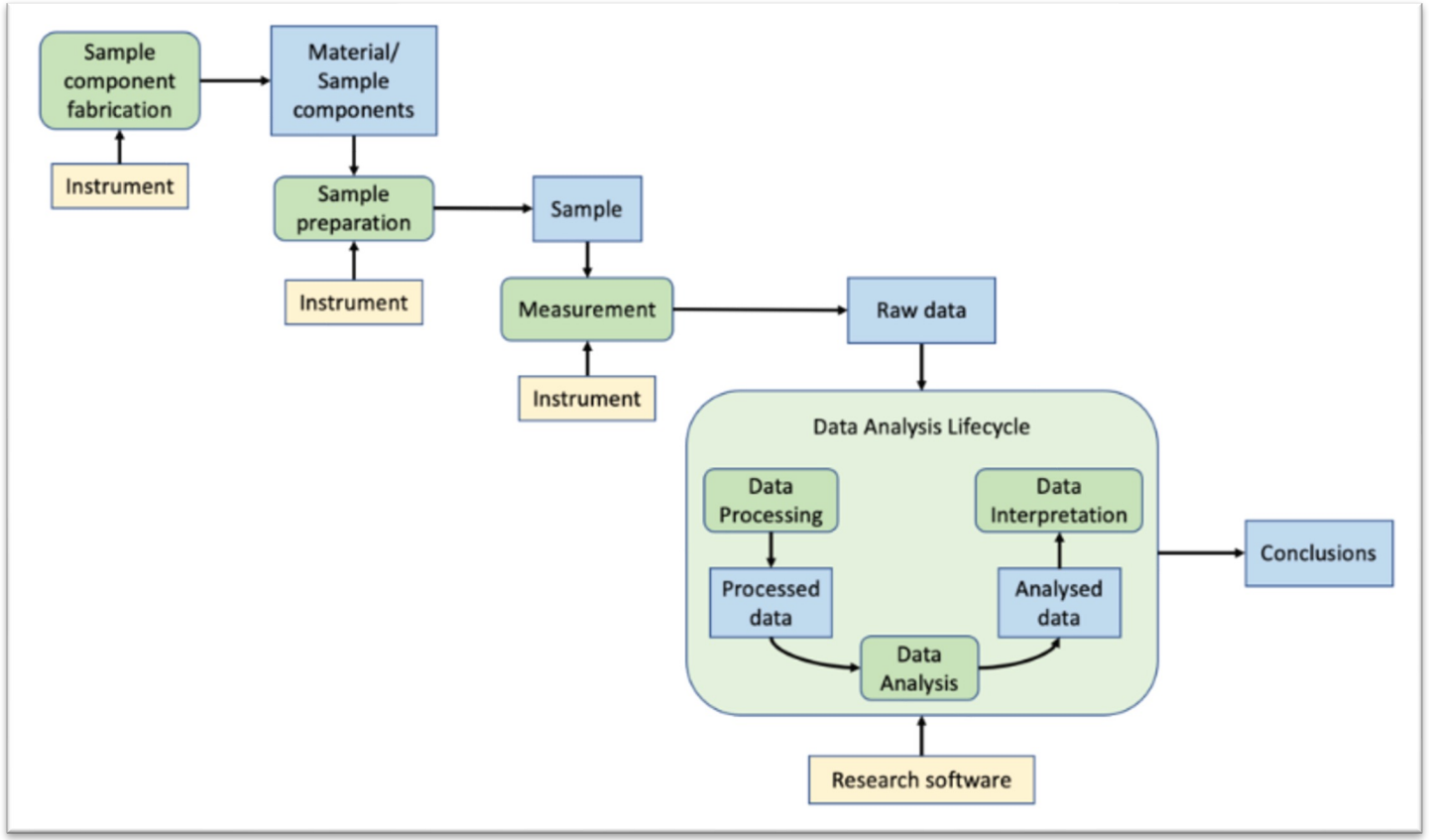
PRIMA Ontology (PRovenance Information for MAterials Science)

- contains high-level provenance information to describe or annotate the entire experimental workflow.
- Co-developed by the Metadata WG, the NFFA-Europe Pilot (NEP), EOSC-Pillar and the Helmholtz Metadata Collaboration (HMC)
- More on MDMC Website

GitHub page with implementation and competency questions →

Schemas

To be developed for each block of the experimental workflow, inputs and outputs



Schemas: Sample Description

- Under progress
- If interested to contribute, contact us

List of contributors:

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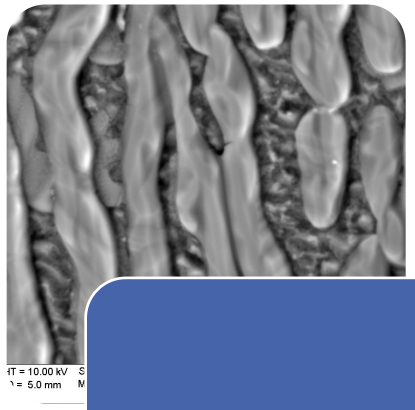
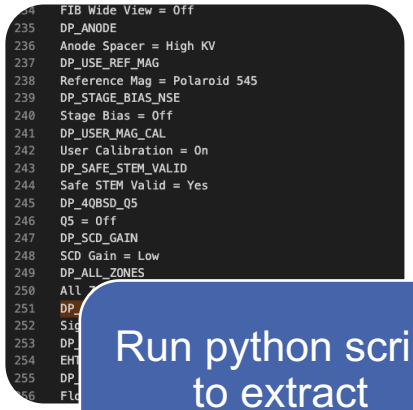
Schemas: Measurement Techniques

- Scanning Electron Microscopy (SEM) ☑
- Magnetic Resonance Imaging (MRI) ☑
- Atomic Force Microscopy (AFM)
- Vertical Scanning Interferometer
- Confocal Scanning Microscope
- Transmission Electron Microscope (TEM)
- Nano computed Tomography (nano CT)
- Scanning Tunneling Microscope (STM) ☑

SEM Metadata Extractor and Mapper

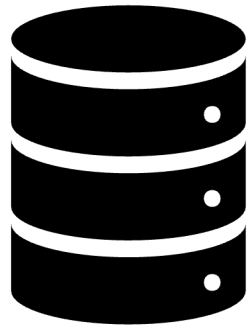


Load image



Run python script to extract metadata and convert it to JSON format according to the published schema*

Import metadata into Electronic Lab Notebook (ELN) or custom interface for editing/reviewing

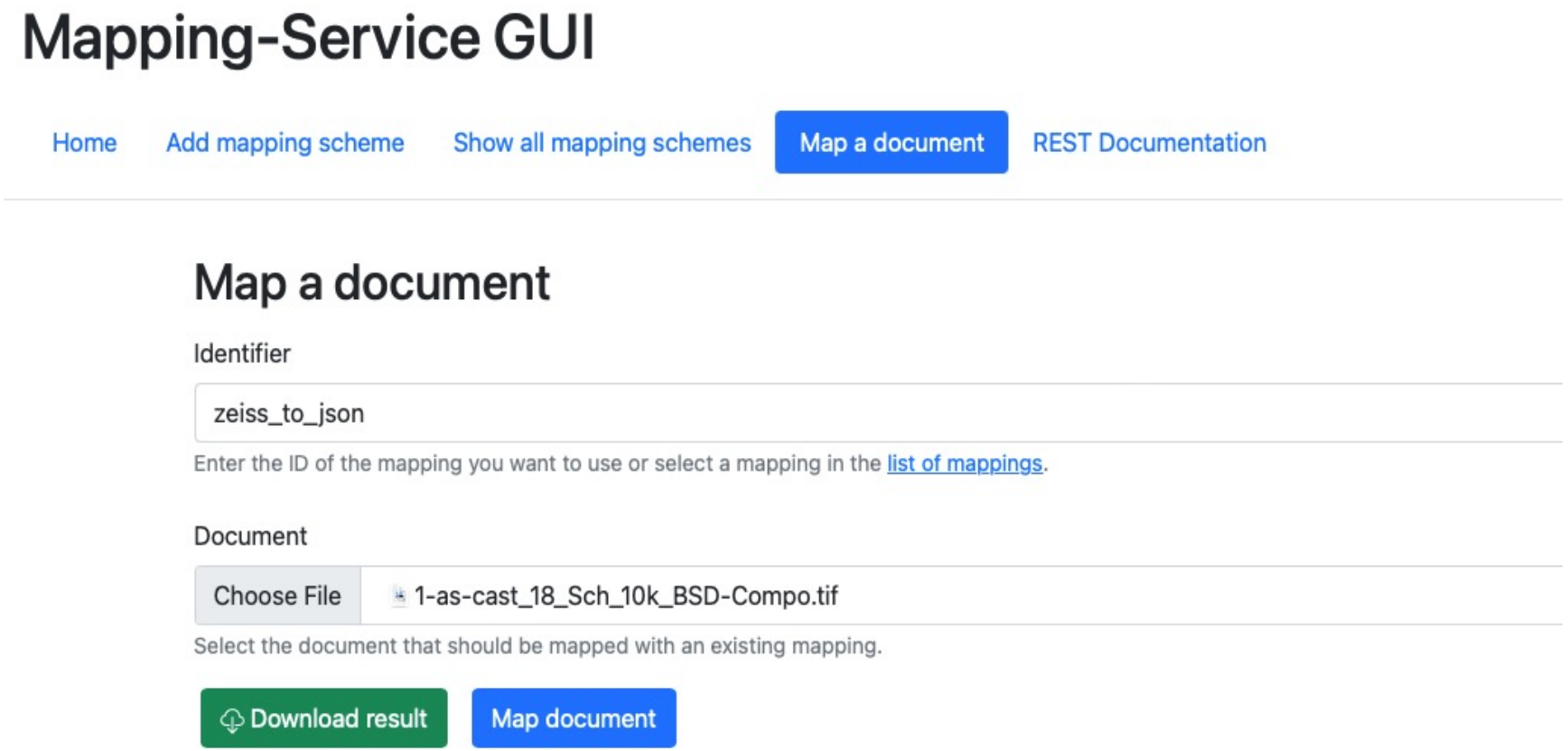


Upload metadata in a repository

* https://ceur-ws.org/Vol-3036/paper21.pdf

Contributors: Elias Vitali, Nicolas Blumenröhr (KIT)

Graphical User Interface

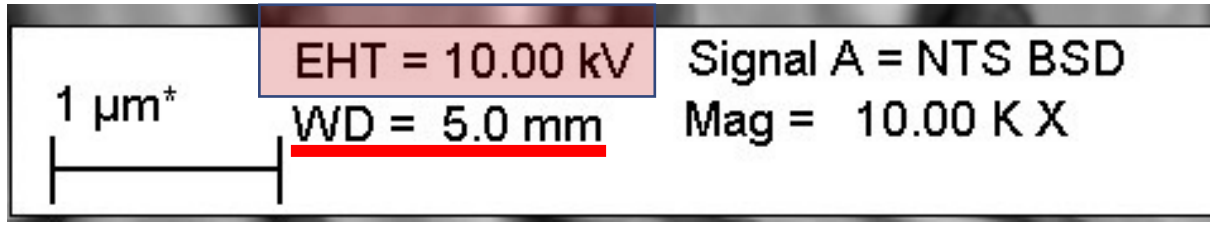


SEM Mapping Tool GUI:
https://metarepo.nffa.eu/mapping-service/mapDocument.html

Identifier: **zeiss_to_json**

- uses the python extractor located on GitHub
https://github.com/kit-data-manager/SEM-Mapping-Tool

Extracted metadata follows the Schema




```
"instrumentName": "Auriga 60",
"stage": {
  "eBeamWorkingDistance": {
    "unit": "mm",
    "value": 4.967
  },
  "stageAlignmentDone": true,
  "tiltAngle": {
    "unit": "degree",
    "value": 0
```

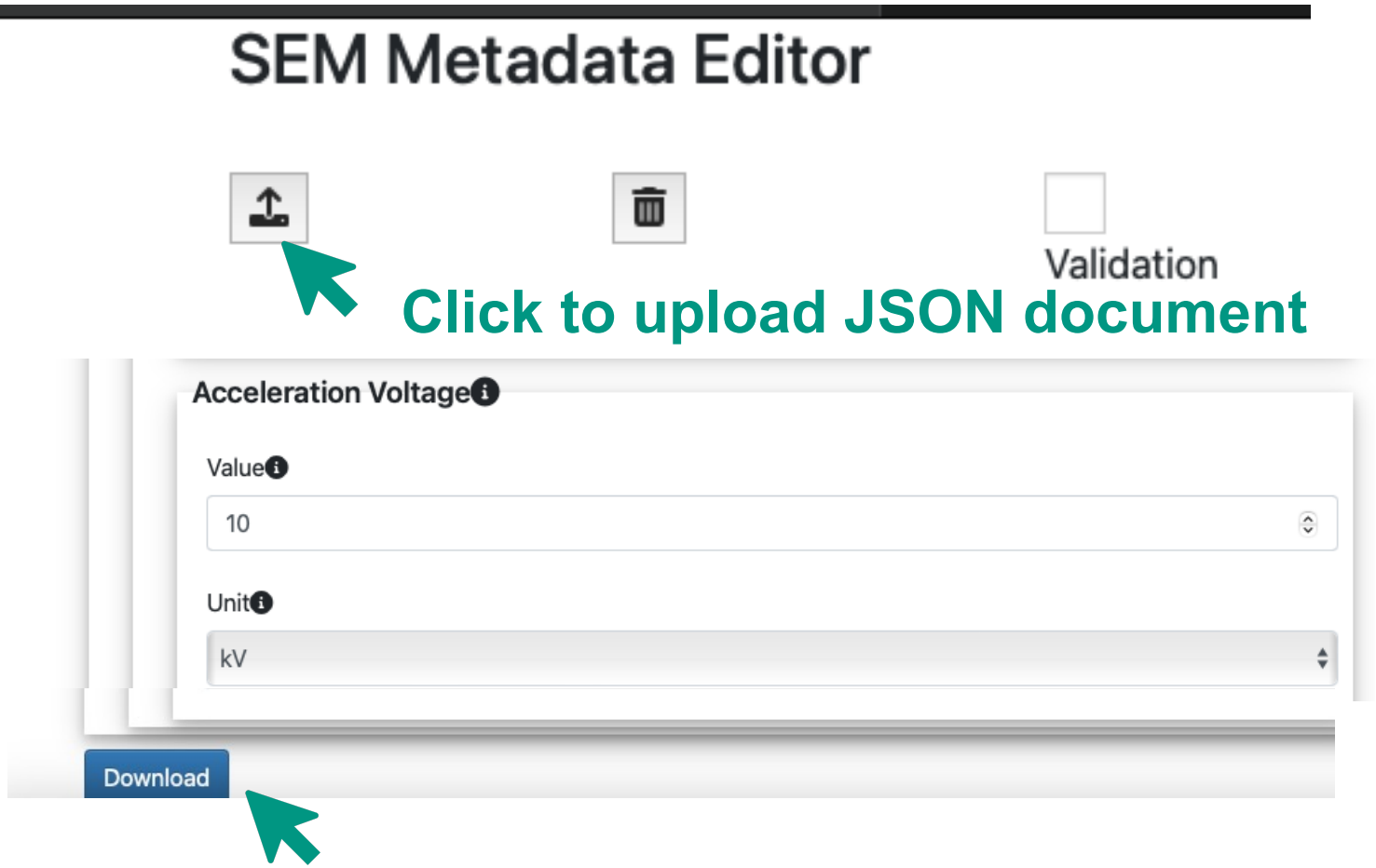
```
"eBeamSource": {
  "accelerationVoltage": {
    "unit": "kV",
    "value": 10
  },
  "beamCurrent": {
    "unit": "µA",
    "value": 80
  }
},
"imaging": {
  "apertureSetting": {
    "size": {
      "unit": "µm",
      "value": 120
    }
```

```
"sample": {
  "sampleHolder": "Carousel 8x6.5mm",
  "sampleSize": {
    "unit": "mm",
    "value": 10
```

Import Metadata Document for Viewing/Editing

- Electronic Lab Notebooks
  - Schema can be imported as a template
  - Enable relevant fields for correlative characterisation
  - Metadata WG - ELN Developers
    - Catriona Eschke (Herbie)
    - Nicole Jung (Chemotion)
    - Michael Selzer (Kadi4Mat)
- Metadata should be uploaded in a repository like the MetaStore, which registers a schema, and then metadata can be validated against the schema fulfilling FAIR principles

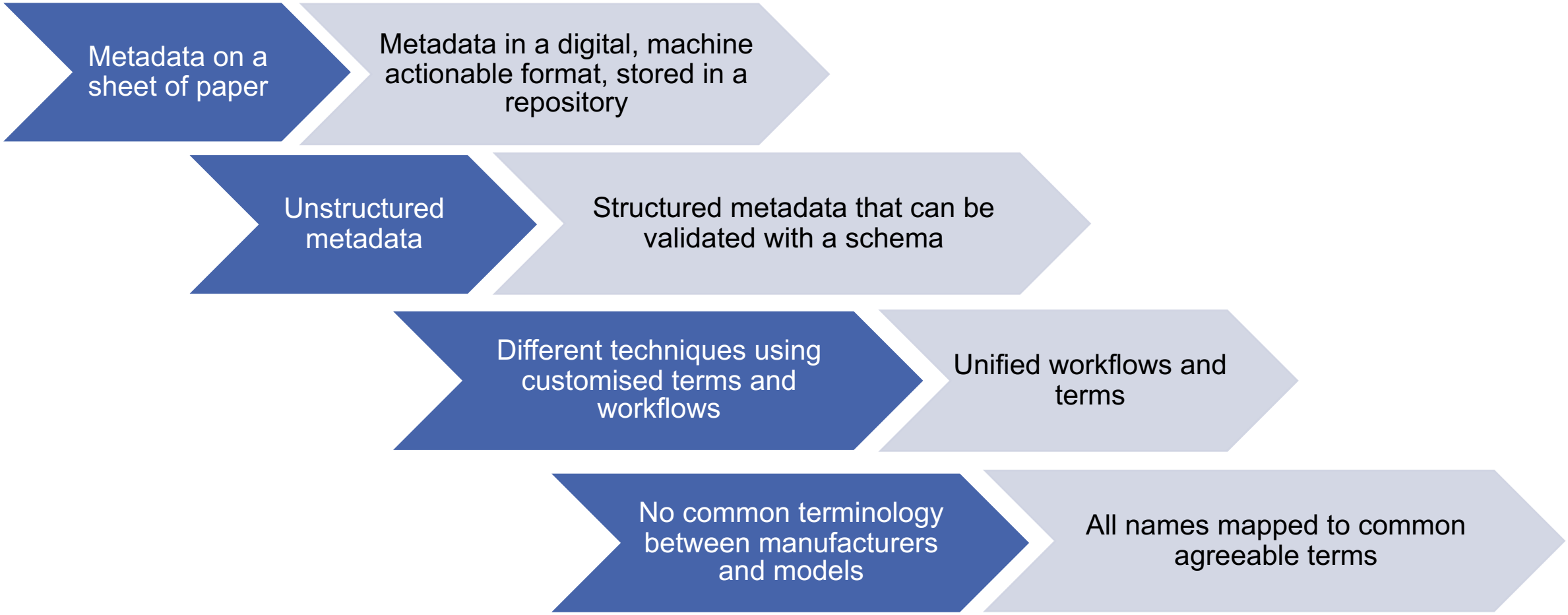
Custom Interface to Add, Review and Correct Metadata



- Based on the published schema
- With drop down menus
- Information on each field
- Integrated schema validation

Available at: https://kit-data-manager.github.io/Metadata-Schemas-for-Materials-Science/

Past vs Future with Schemas



Conclusions and Future Work

- Following schemas facilitates FAIR principles and eases correlative characterization
- Working with ELN developers for enabling schema or relevant fields import
- More Schemas in development

Call to action:
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