

From Ontologies to Knowledge Graphs

with the ELN Herbie

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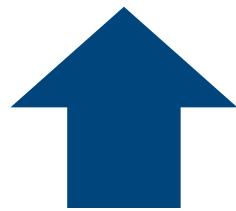
Heron, Institute of Metallic Biomaterials

Martin Held martin.held@hereon.de

Heron, Institute of Membrane Research



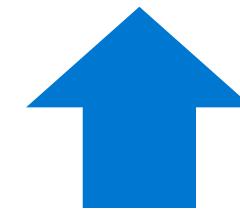
Knowledge Graph¹



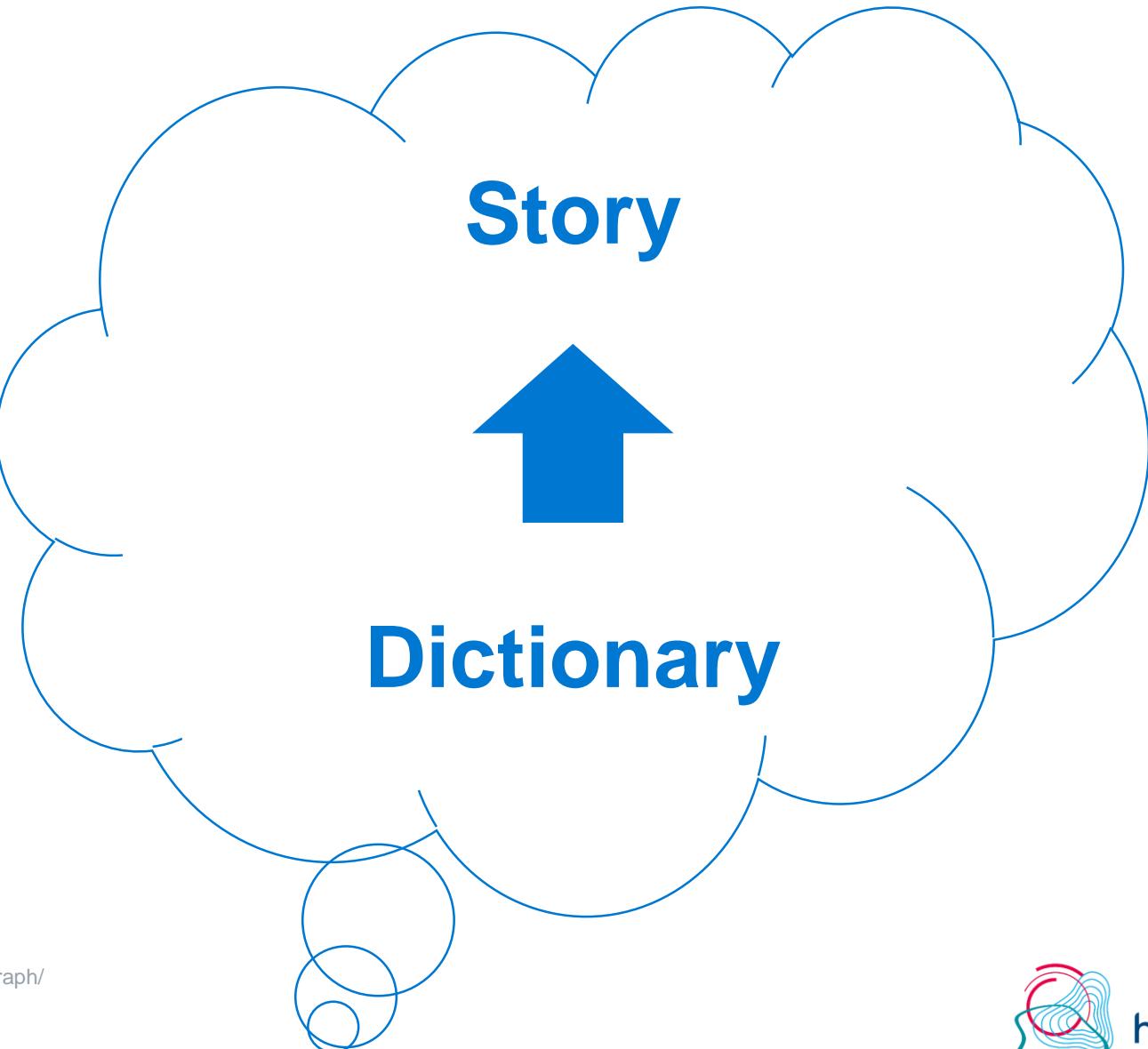
Ontology

Mental model

Story

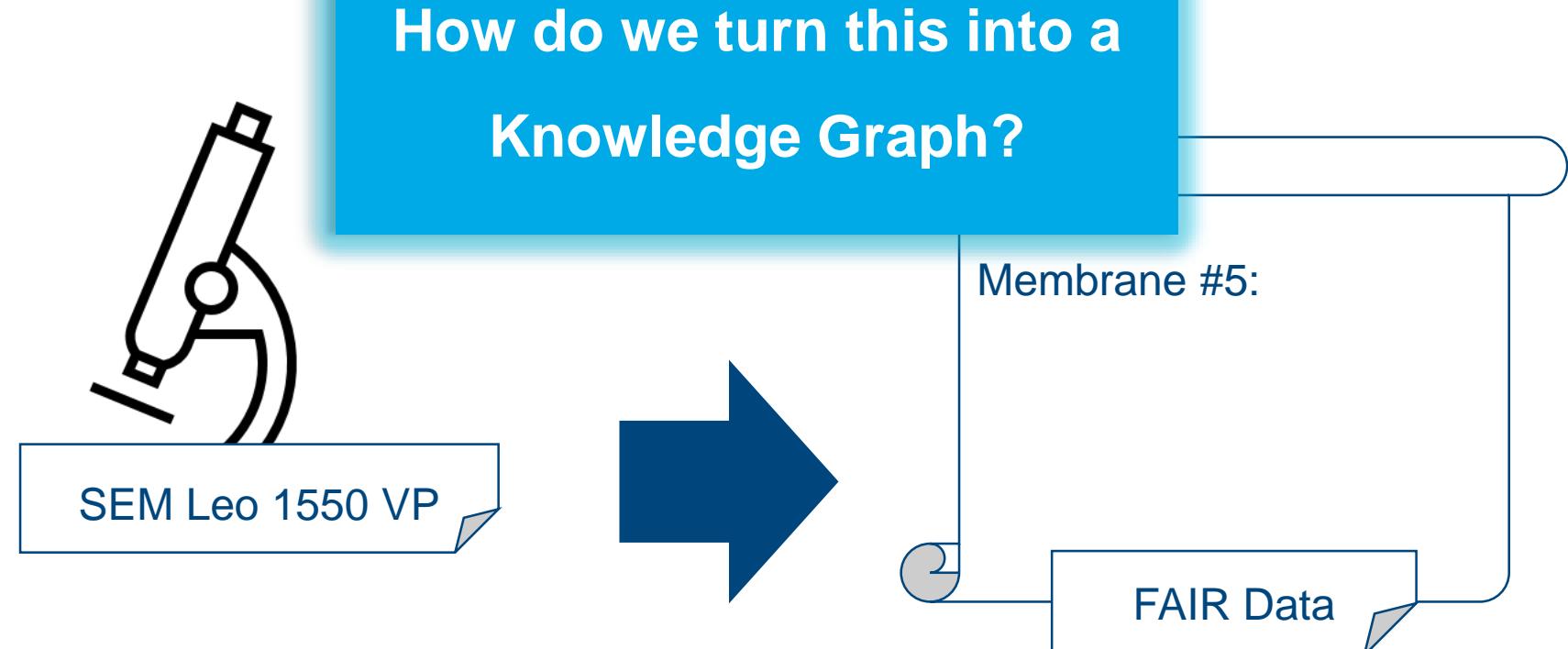


Dictionary



[1] <https://www.ontotext.com/knowledgehub/fundamentals/what-is-a-knowledge-graph/>

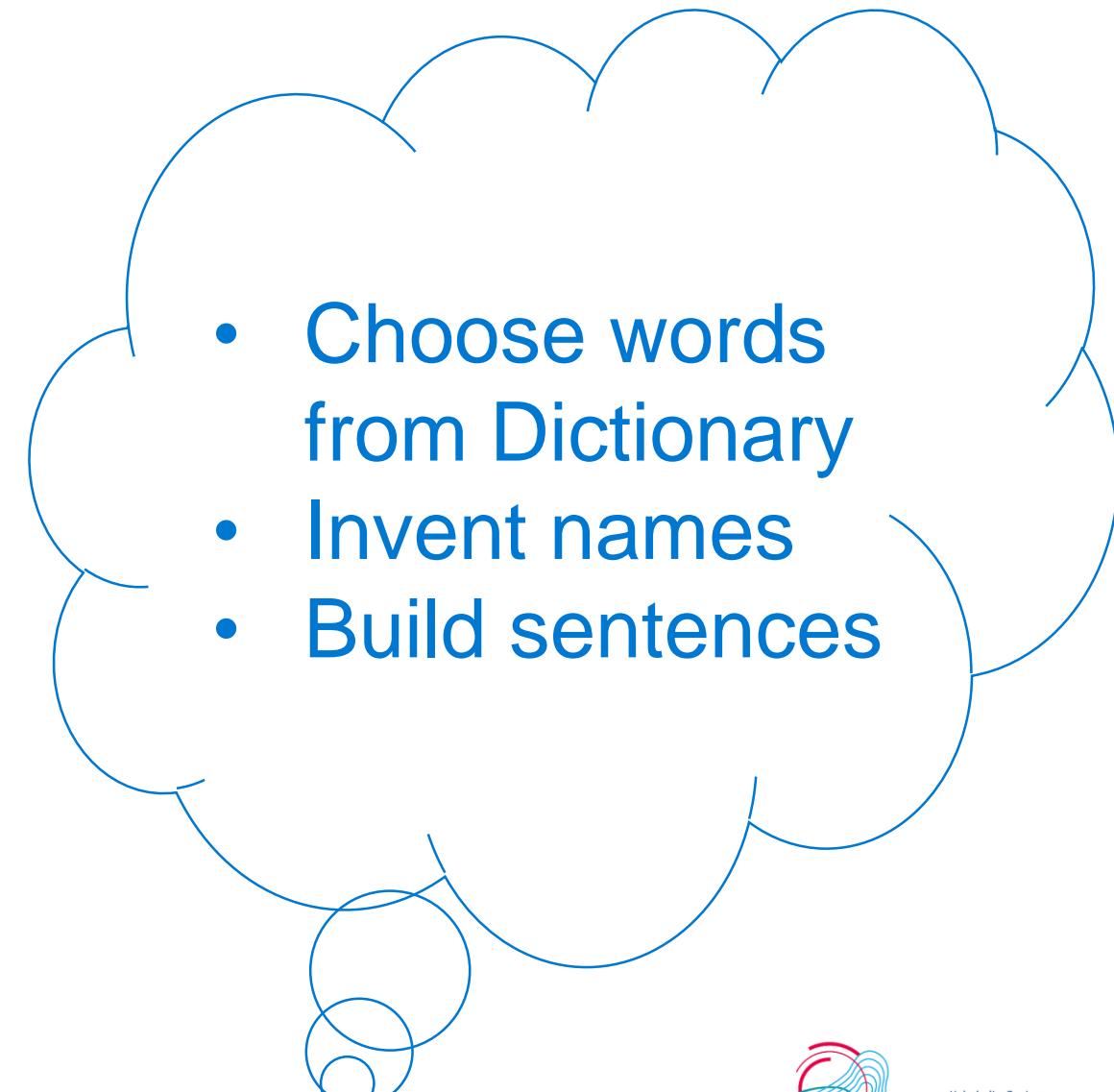
Example scenario



Alice performed an SEM measurement of the PTFE Membrane #5. She prepared the sample by applying a coating of 500 nm thickness. She then used the SEM Leo 1550 VP to perform an imaging analysis and determined a mean pore diameter of 20 nm of the sample.

Formalize all information into a Knowledge Graph

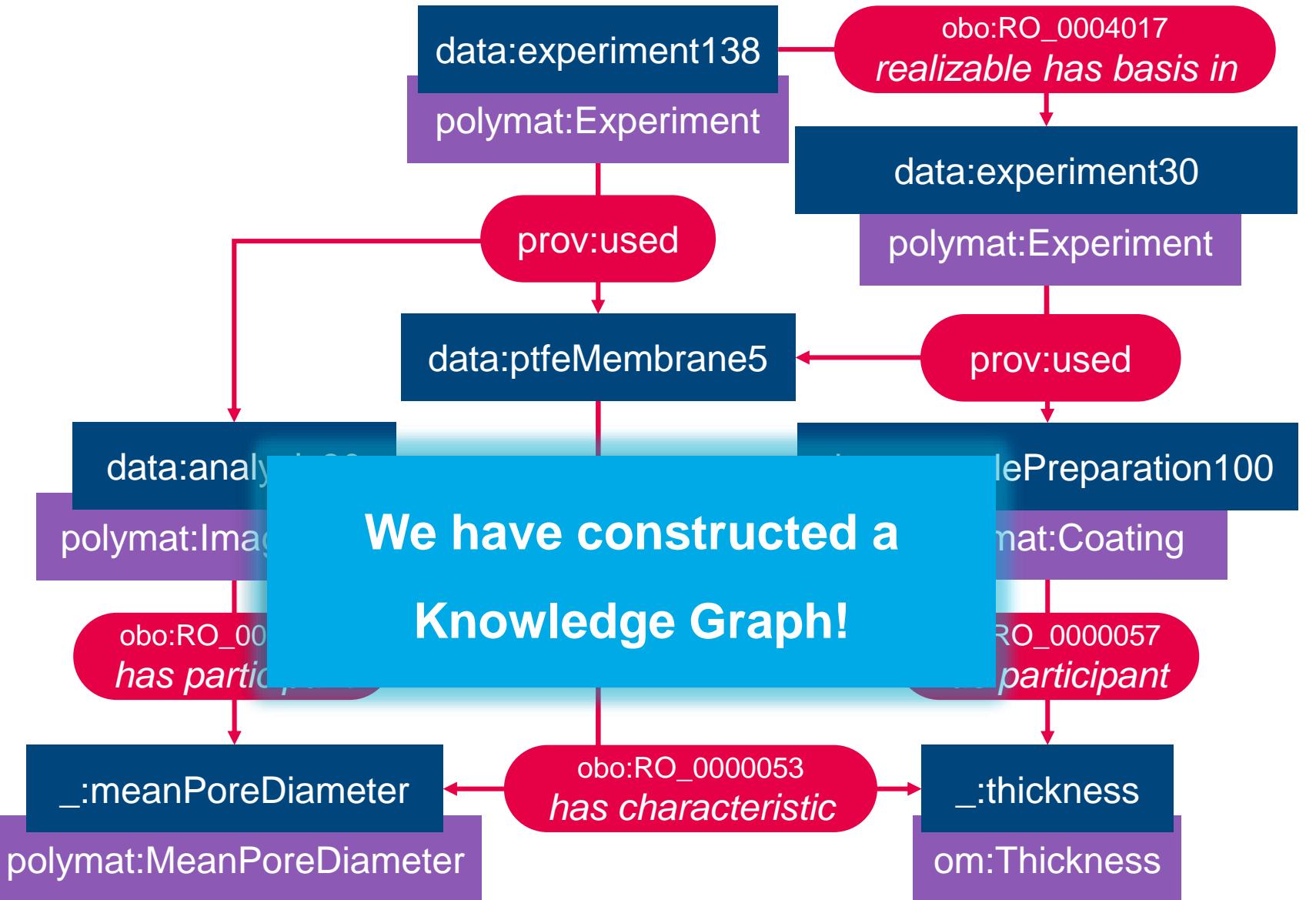
- Choose classes and properties from Ontology
- Invent identifiers (IRIs²)
- Build RDF triples³



[2] <https://datatracker.ietf.org/doc/html/rfc3987>

[3] <https://www.w3.org/TR/rdf11-concepts/>

Knowledge Graph



Alice performed an SEM measurement of the PTFE Membrane #5.

She prepared the sample by applying a coating of 500 nm thickness.

She then used the SEM Leo 1550 VP to perform an imaging analysis

and determined a mean pore diameter of 20 nm of the sample.

Legend

Instance

Class

Property

Knowledge Graph

RDF Turtle⁴

[4] <https://www.w3.org/TR/turtle/>

data:experiment138

relatesTo

data:analysis30

Publish file to Gitlab/Zenodo/
including Ontology files

data:analysis30

polymat:Imaging

obo:RO_0000057
has participant

_:meanPoreDiameter

obo:RO_0000053
has characteristic

FAIR

data

*sem_experiment_data.ttl - Notepad

File Edit Format View Help

```
data:experiment138 a polymat:Experiment ;
  prov:used data:ptfeMembrane5 ;
  obo:RO_0004017 data:experiment30 ; # "realizable has basis in"
  prov:used data:analysis30 .

data:experiment30 a polymat:experiment138 ;
  prov:used data:samplePreparation100 ;
  prov:used data:ptfeMembrane5 .

data:samplePreparation100 a polymat:Coating ;
  obo:RO_0000057 _:thickness . # "has participant"

_:thickness a om:Thickness ;
  om:hasValue [
    om:hasNumericalValue 500 ;
    om:hasUnit om:nanometre ] .

data:analysis30 a polymat:ImagingSEM ;
  obo:RO_0000057 _:meanPoreDiameter . # "has participant"

_:meanPoreDiameter a polymat:MeanPoreDiameter ;
  om:hasValue [
    om:hasNumericalValue 20 ;
    om:hasUnit om:nanometre ] .

data:ptfeMembrane5
  obo:RO_0000053 _:thickness ; # "has characteristic"
  obo:RO_0000053 _:meanPoreDiameter . # "has characteristic"
```

Ln 37, Col 1

100%

Windows (CRLF)

UTF-8

Pros

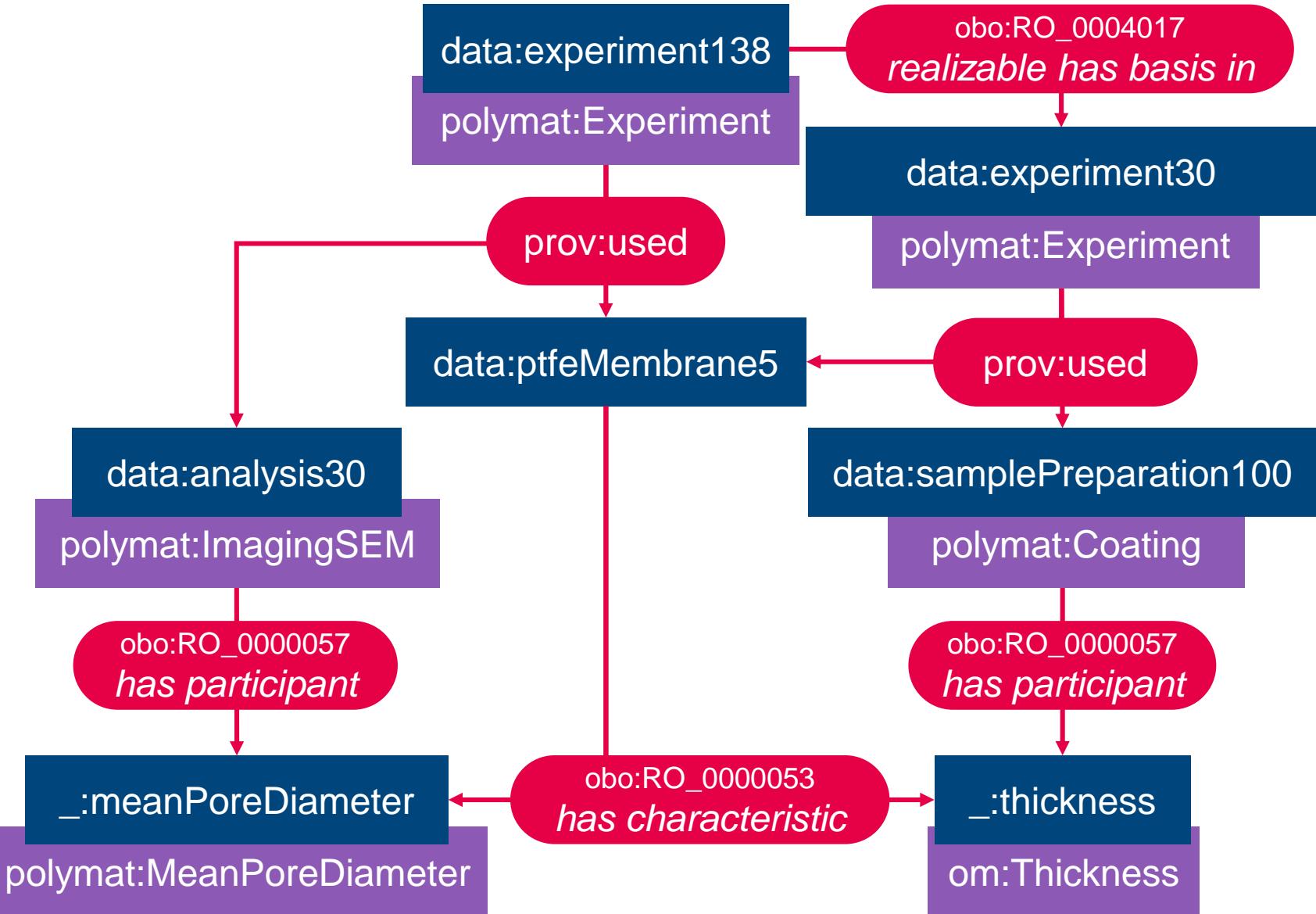
- Structured knowledge
- No extra tools required
- Very flexible

Cons

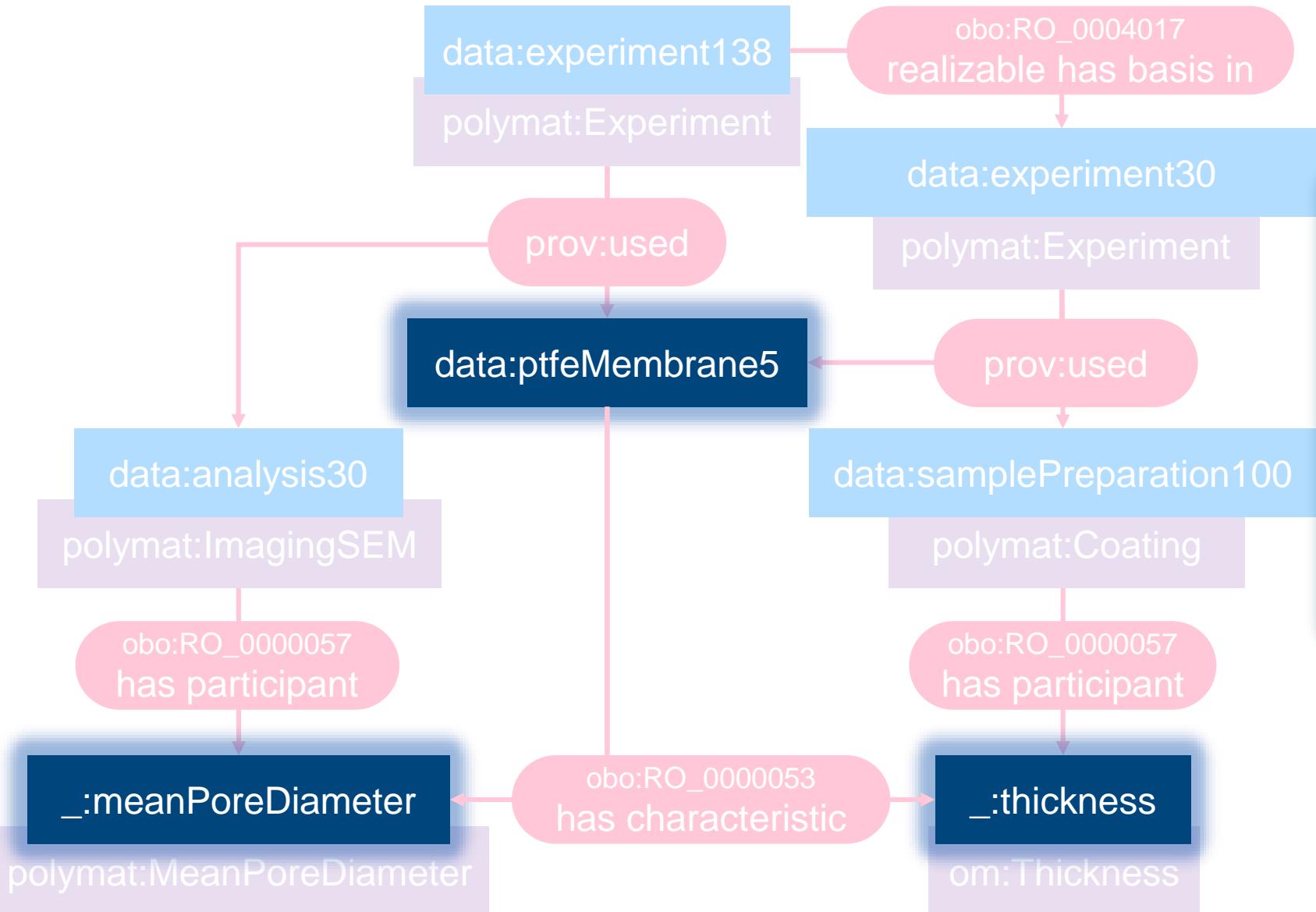
- Text editor
- Very flexible
- No validation
- FAIRness not guaranteed
- Complicated
- Tedium
- Repetitive

Can we do better?

Knowledge Graph



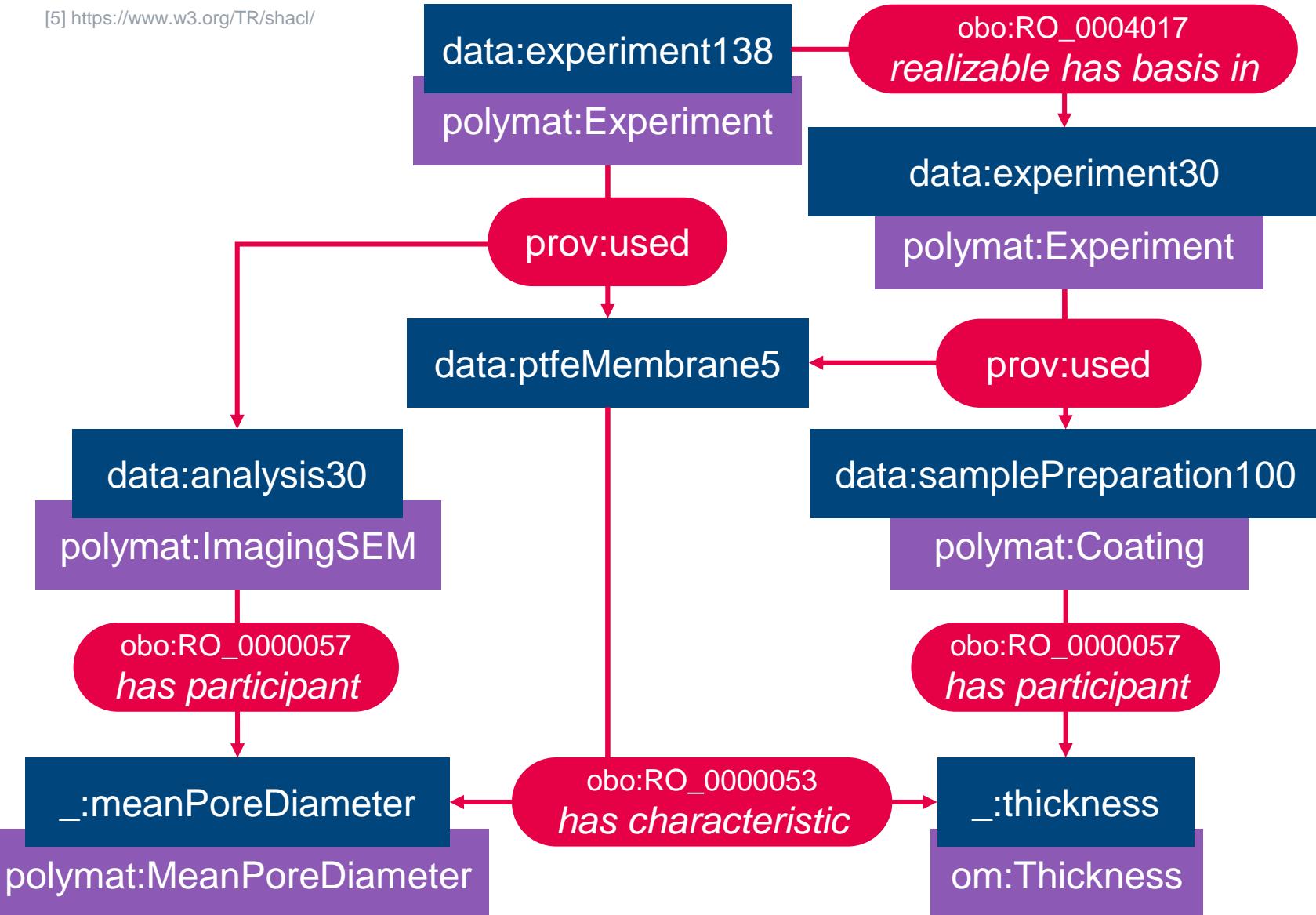
Knowledge Graph



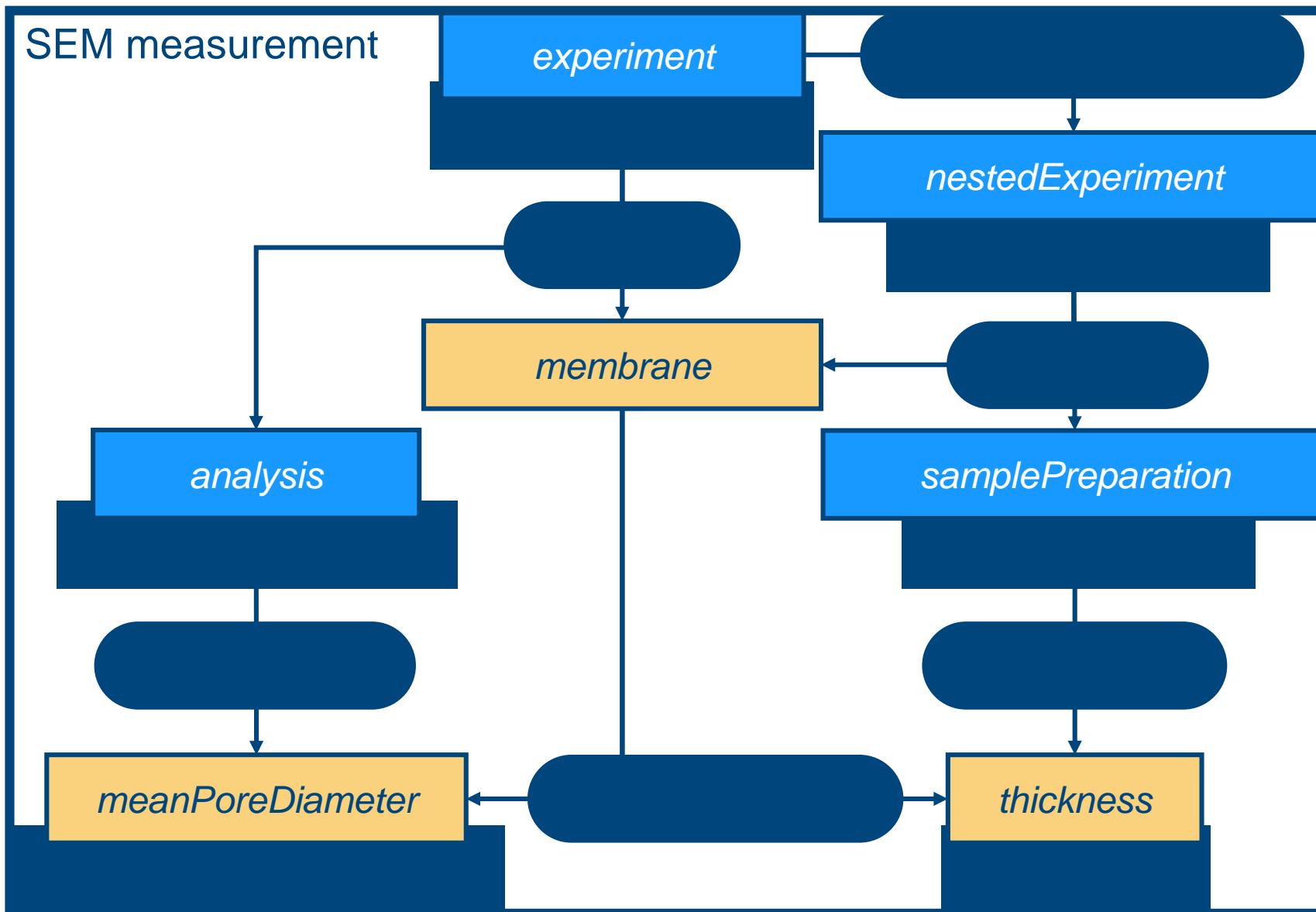
We only want to enter
these 3 values,
everything else should
be implicit!

Create a SHACL⁵ shape...

[5] <https://www.w3.org/TR/shacl/>



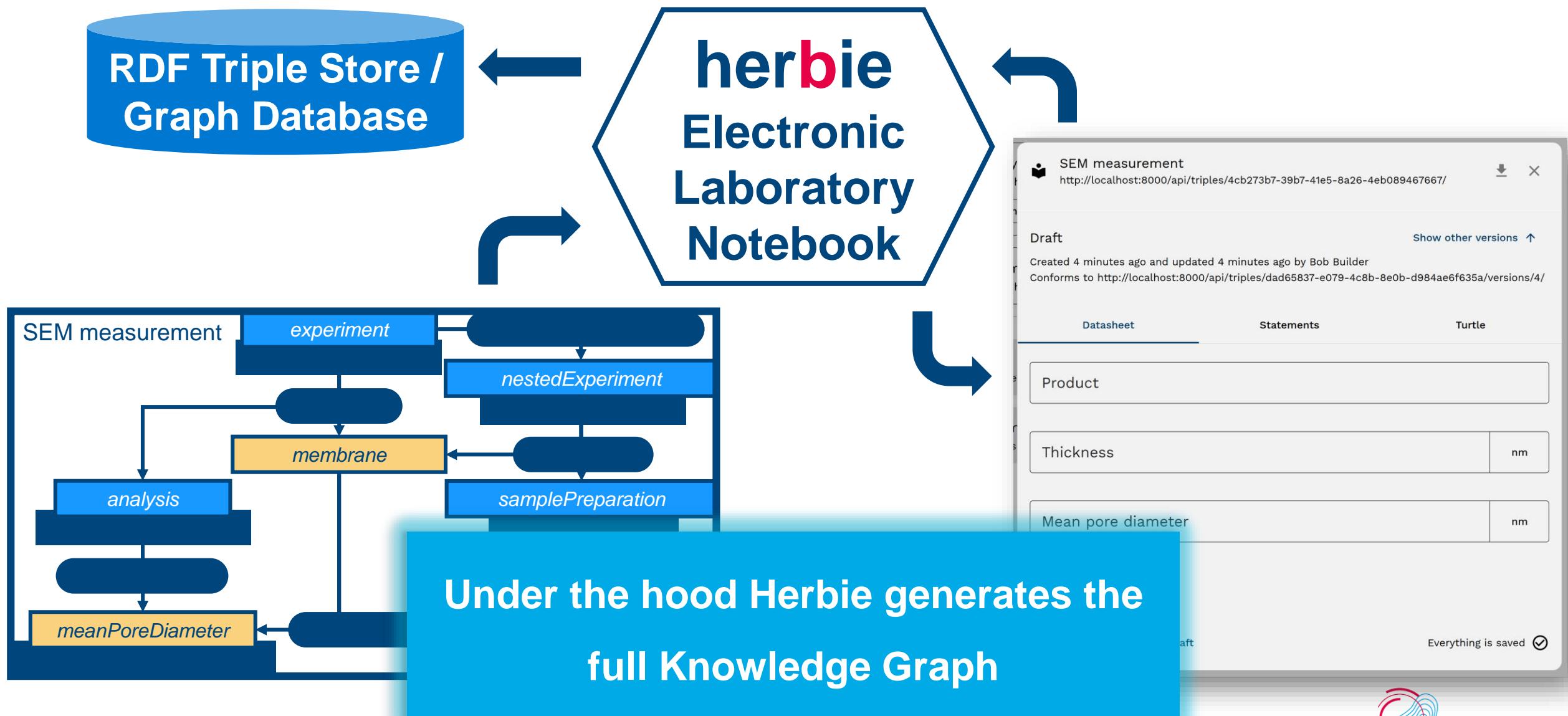
Create a SHACL⁵ shape...



Fill-in-the
-blanks text

Legend
fixed
will be generated
must be entered

... and Herbie provides an interface for data input



What does Herbie provide?

- **Easy data entry**
- **Flexible interface**
- **Reusability**
- **Customizability**
- **Validation**
- **Guaranteed FAIRness**
- **Versioning**

Planned

- **Access right management**
- **Advanced search and filter**

Summary

Storing data in a Knowledge Graph helps to make it FAIR

Manual approach:

- very tedious**
- prone to error**
- not reliably FAIR**

Using SHACL & Herbie:

- Structural work only required once**
- Data entry fast & easy**
- Offers a lot of other benefits**

Want to learn more?

Find Herbie at

codebase.helmholtz.cloud/hereon-mb/herbie

and reach out to us!

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Heron, Institute of Metallic Biomaterials

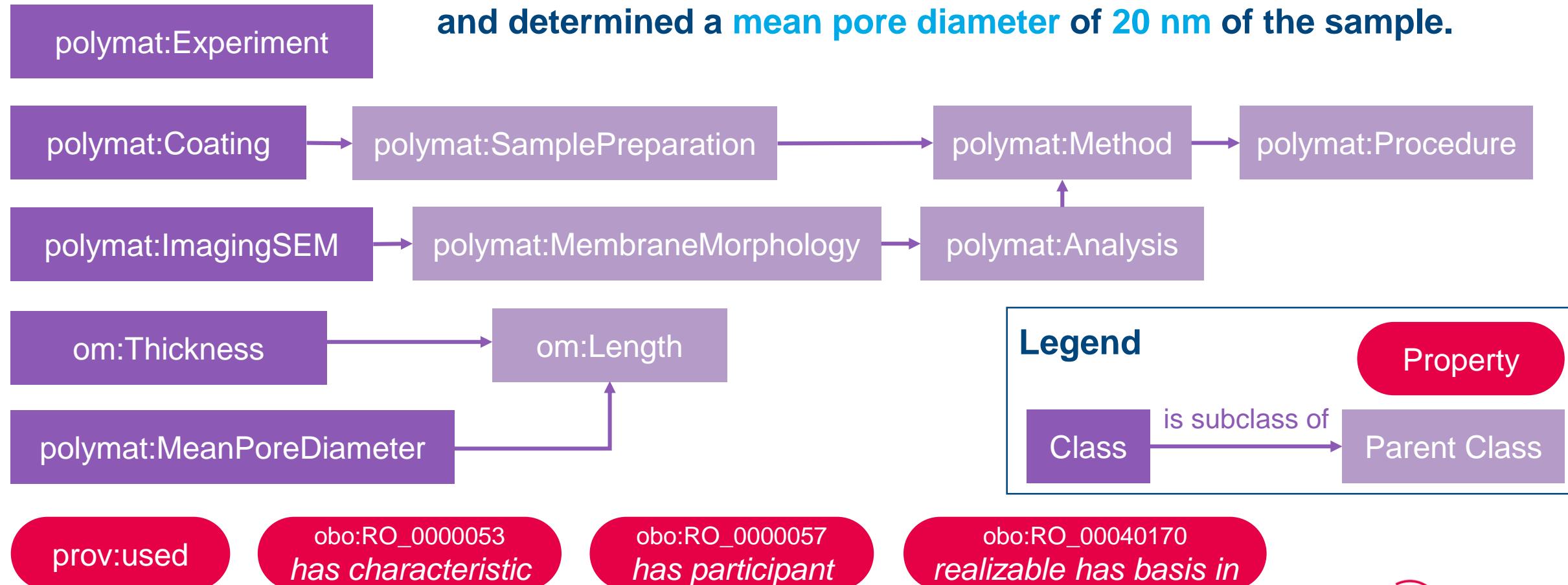
Martin Held martin.held@hereon.de

Heron, Institute of Membrane Research



Choose classes and properties

Alice performed an SEM measurement of the PTFE Membrane #5. She prepared the sample by applying a coating of 500 nm thickness. She then used the SEM Leo 1550 VP to perform an imaging analysis and determined a mean pore diameter of 20 nm of the sample.



Upload a SHACL Shape to Herbie

≡
+
☰
🔍
⚙️
➡️
❓
✉️

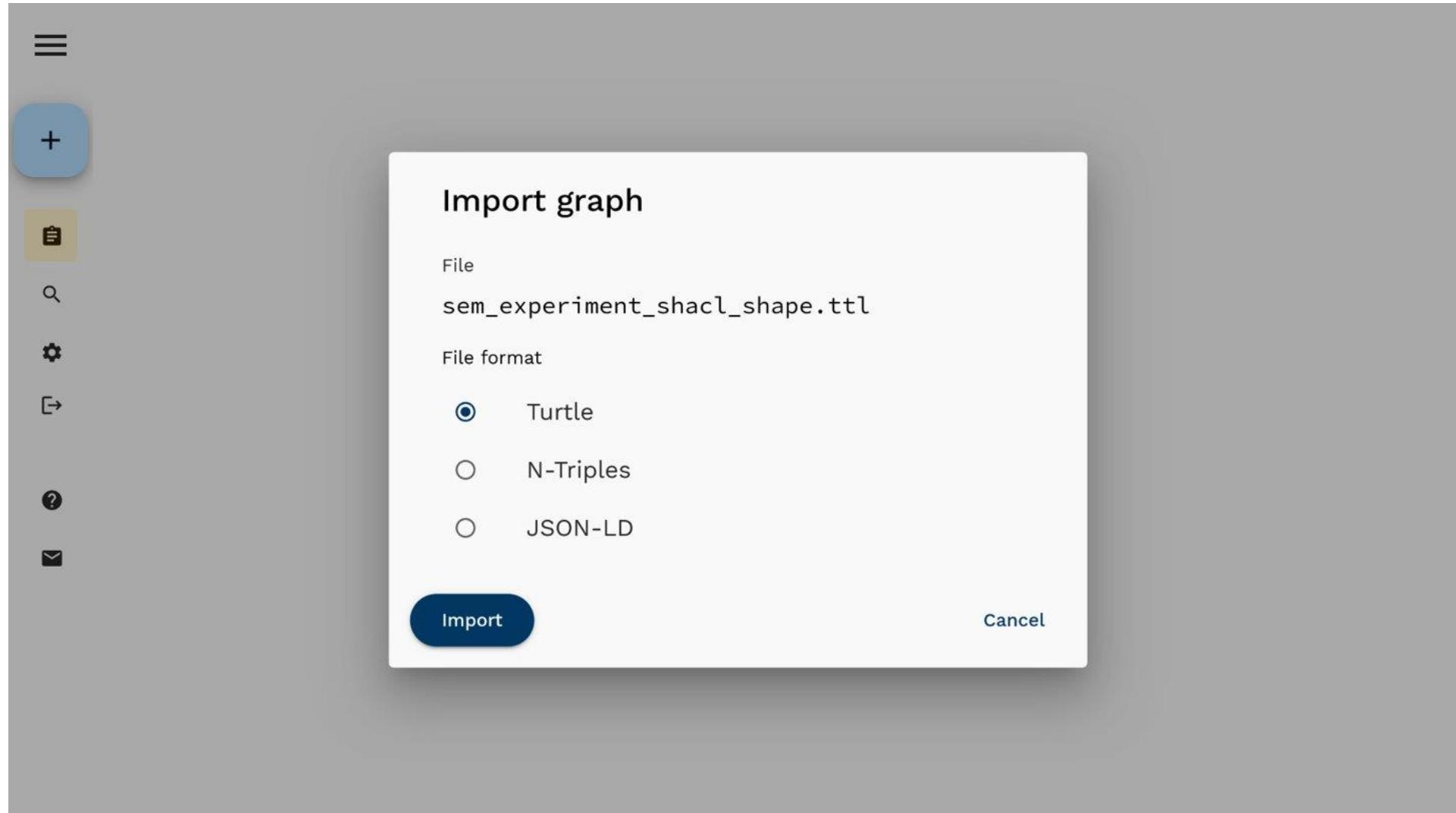
Upload a SHACL Shape to Herbie

The image shows the Herbie interface. On the left, there is a sidebar with the following icons and text:

- A menu icon (three horizontal lines) at the top.
- A blue button labeled "Document" with a pencil icon.
- A white button labeled "Import graph" with an upward arrow icon.
- A magnifying glass icon.
- A gear icon.
- A left arrow icon.
- A question mark icon.
- An envelope icon.

The main area of the interface is currently empty, awaiting a file upload.

Upload a SHACL Shape to Herbie



Upload a SHACL Shape to Herbie

The screenshot shows the Herbie interface for managing SHACL shapes. On the left, there's a sidebar with icons for navigation: three horizontal lines (menu), a plus sign (create), a document (drafts), a magnifying glass (search), a gear (settings), a left arrow (back), a question mark (help), and a right arrow (forward). The main area is titled "Drafts" and contains a list of drafts. One draft is selected: "The vocabulary for adding a SEM measurement" (modified half a minute ago). A "Create SEM measurement" button is visible. Below the list, the title "Draft" is shown, along with the creation and update information ("Created half a minute ago and updated half a minute ago by Alice Wonderland"). There are two tabs: "Statements" (selected) and "Turtle". Under "Statements", it says "Classes (1)" and lists "SEM measurement". At the bottom, there are buttons for "Submit" (highlighted in blue), "Delete draft", and a message "Everything is saved" with a checkmark.

Upload a SHACL Shape to Herbie

The screenshot shows the Herbie interface with a modal dialog open. The modal title is "The vocabulary for adding a SEM measurement" and the URL is "http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/". A "Create SEM measurement" button is visible. Below the modal, the sidebar menu includes icons for navigation, search, settings, and help. At the bottom of the screen are "Edit" and "Upload new version" buttons.

Upload a SHACL Shape to Herbie

≡

 The vocabulary for adding a SEM measurement
Published half a minute ago by Alice Wonderland

 Create SEM measurement



🔍

⚙️

➡️

❓

✉️

Create data from a SHACL Shape



The vocabulary for adding a SEM measurement

Published half a minute ago by Alice Wonderland



Create SEM measurement



Create data from a SHACL Shape

The vocabulary for adding a SEM measurement
Published less than 10 seconds ago by Alice Wonderland

Document

Import graph

☰

🔍

⚙️

➡️

❓

✉️

Create data from a SHACL Shape

The screenshot shows a user interface for creating documents. On the left, there is a sidebar with various icons: three horizontal lines (menu), a person icon (The voice), a plus sign (Create SEM), a document icon (Create document, highlighted in blue), a magnifying glass (Search), a gear (Settings), an arrow (Email), a question mark (Help), and an envelope (Feedback). The main content area has a title 'Create document' and a sub-instruction 'Create a new document by selecting a class.' Below this is a 'Filter' input field. The main content area lists several examples:

- Multi-select combobox example
<http://localhost:8000/api/ont/example/input-dropdown-multiselect/1.0.0/#Root>
- Grid example
<http://localhost:8000/api/ont/example/grid/1.0.0/#Root>
- Extrusion
[http://localhost:8000/api/ont\(mb/extrusion/1.0.0/#Extrusion](http://localhost:8000/api/ont(mb/extrusion/1.0.0/#Extrusion)
- Read-only/generated/persisted field example
<http://localhost:8000/api/ont/example/readonly-generated-persisted/1.0.0/#Root>
- File upload field example
<http://localhost:8000/api/ont/example/file-upload/1.0.0/#Root>
- Single-select combobox example

Create data from a SHACL Shape

The screenshot shows a user interface for creating documents. On the left, there is a vertical sidebar with various icons: a menu icon (three horizontal lines), a person icon with the text "The voice Published", a plus sign icon labeled "Create SEM", a document icon, a magnifying glass icon, a gear icon, an arrow icon, a question mark icon, and an envelope icon.

The main content area has a header "Create document" and a sub-instruction "Create a new document by selecting a class.". Below this is a "Filter" input field containing the text "sem measure".

Underneath the filter, there is a section titled "SEM measurement" with the URL "https://w3id.org/polymat/SemExperiment".

Create data from a SHACL Shape

The screenshot shows a user interface for creating data from a SHACL Shape. On the left, there's a sidebar with various icons: three horizontal lines, a plus sign, a document, a magnifying glass, a gear, a left arrow, a question mark, and an envelope. Below these are sections for 'Drafts' and a specific entry for 'SEM measurement'. The main area is a modal window titled 'SEM measurement' with a URL: <http://localhost:8000/api/triples/5ab629e8-65f7-4df2-88a7-3d561c5b3a8d/>. The modal has a 'Draft' status and a note about being created and updated recently by Alice Wonderland, conforming to a specific version of a schema. It contains tabs for 'Datasheet', 'Statements', and 'Turtle', with 'Datasheet' selected. The 'Datasheet' section contains three input fields: 'Product' (empty), 'Thickness' (with unit 'nm'), and 'Mean pore diameter' (with unit 'nm'). At the bottom are 'Submit', 'Delete draft', and a message 'Everything is saved' with a checked checkbox.

Create data from a SHACL Shape

The screenshot shows a user interface for creating data from a SHACL Shape. On the left, there's a sidebar with icons for navigation: three horizontal lines, a plus sign, a document, a magnifying glass, a gear, a left arrow, a question mark, and an envelope. Below these are sections for 'Drafts' and a specific 'SEM measurement' entry.

SEM measurement
http://localhost:8000/api/triples/5ab629e8-65f7-4df2-88a7-3d561c5b3a8d/
Published 3 minutes ago
Create SEM measurement

Draft
Created one minute ago and updated one minute ago by Alice Wonderland
Conforms to http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/versions/1/

Datasheet **Statements** **Turtle**

Product PTFE Membrane 5 (X)

Thickness 3.141 nm

Mean pore diameter 2.718 nm

Submit **Delete draft** Everything is saved ✓

Create data from a SHACL Shape

The screenshot shows a user interface for managing semantic triples. On the left, there's a sidebar with icons for navigation: three horizontal lines (menu), plus sign (create), document (read), magnifying glass (search), gear (settings), arrow (export/import), question mark (help), and envelope (mail).

The main area displays a list of triples. One triple is expanded into a detailed view:

SEM measurement
http://localhost:8000/api/triples/5ab629e8-65f7-4df2-88a7-3d561c5b3a8d/

Current version Show other versions ↑

Created 2 minutes ago and published less than 10 seconds ago by Alice Wonderland
Conforms to http://localhost:8000/api/triples/69e25917-6f1a-482b-9a49-d7d65a2f537c/versions/1/

Three tabs are available for viewing the data: **Datasheet**, **Statements**, and **Turtle**.

Datasheet table:

Product	Thickness	Mean pore diameter
PTFE Membrane 5	3.141 nm	2.718 nm

Statements and **Turtle** sections are currently empty.

At the bottom, there are two buttons: **Edit** and **Upload new version**.

Create data from a SHACL Shape



The vocabulary for adding a SEM measurement
Published 4 minutes ago by Alice Wonderland



[Create SEM measurement](#)



SEM measurement
Published less than 10 seconds ago by Alice Wonderland



This image displays a series of screenshots illustrating the creation and management of a Semantic Web Measurement (SEM) document using a specialized application interface.

Top Row:

- Screenshot 1:** Shows the main interface with a sidebar containing icons for search, filters, and navigation. A central panel has a "Document" tab selected, with a sub-menu showing "Import graph".
- Screenshot 2:** A modal window titled "Import graph" is open, showing the file path "sem_experiment_shacl_shape.ttl" and file format options: Turtle (selected), N-Triples, and JSON-LD. It includes "Import" and "Cancel" buttons.
- Screenshot 3:** A modal window titled "Drafts" shows a single draft entry for "The vocabulary for adding a SEM measurement" published by Alice Wonderland. It includes a "Create SEM measurement" button.
- Screenshot 4:** A modal window titled "Create document" shows a "Filter" input field and a list of examples: Multi-select combobox example, Grid example, Extrusion, Read-only/generated/persisted field example, File upload field example, and Single-select combobox example.
- Screenshot 5:** A modal window titled "Create document" shows a "Filter" input field containing "sem measure" and a result list with "SEM measurement" and its URL "https://w3id.org/polymat/SemExperiment".

Middle Row:

- Screenshot 6:** A modal window titled "The vocabulary for adding a SEM measurement" shows a "Draft" section with a "SEM measurement" entry. It includes tabs for "Datasheet", "Statements", and "Turtle". The "Datasheet" tab shows fields for "Product" (PTFE Membrane 5), "Thickness" (3.141 nm), and "Mean pore diameter" (2.718 nm). Buttons for "Submit", "Delete draft", and "Everything is saved" are at the bottom.
- Screenshot 7:** Similar to Screenshot 6, but the "Statements" tab is selected, showing the same data in a different format.
- Screenshot 8:** Similar to Screenshot 6, but the "Turtle" tab is selected, showing the same data in a triple-based format.
- Screenshot 9:** A modal window titled "The vocabulary for adding a SEM measurement" shows the "Current version" of the "SEM measurement" document. It includes tabs for "Datasheet", "Statements", and "Turtle". The "Datasheet" tab shows the updated data: Product PTFE Membrane 5, Thickness 3.141 nm, and Mean pore diameter 2.718 nm. Buttons for "Edit", "Upload new version", and "Everything is saved" are at the bottom.

Bottom Row:

- Screenshot 10:** A modal window titled "The vocabulary for adding a SEM measurement" shows the "Published" version of the "SEM measurement" document. It includes tabs for "Datasheet", "Statements", and "Turtle". The "Datasheet" tab shows the final data: Product PTFE Membrane 5, Thickness 3.141 nm, and Mean pore diameter 2.718 nm. Buttons for "Edit", "Upload new version", and "Everything is saved" are at the bottom.

Page Footer:

31 Titel der Präsentation, Z1, Arial Regular 9 pt