

The eNanoMapper Ontology

Harnessing ontologies to enable data integration for nanomaterial risk assessment

Javier Millán Acosta

BiGCaT - Maastricht University

September 19, 2022



Overview

1 Introduction

- eNanoMapper
- What is an ontology?
- What is an ontology?

2 The eNanoMapper Ontology

- Development and QC
- Composition of the eNanoMapper ontology
- Uses of the eNM ontology

3 Future plans and challenges

- What is still needed
- Migrating the ontology development?



Overview

① Introduction

- eNanoMapper
- What is an ontology?
- What is an ontology?

② The eNanoMapper Ontology

③ Future plans and challenges



eNanoMapper

- ▶ **eNanoMapper** is a broader European project which aims to address data and model interoperability challenges for data management for engineered nanomaterial safety.
- ▶ **The eNanoMapper ontology** is an application ontology and reuses parts of several ontologies to describe the full domain of nanomaterial safety assessment.

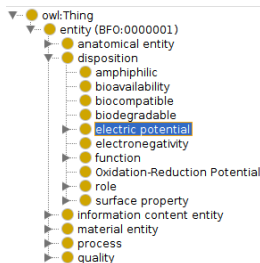
Figure 1: The eNanoMapper logo



What is an ontology?

- ▶ A formal description of a domain (a means to capture knowledge about things) ?
- ▶ It consists of three syntactical categories: **Entities**, **Expressions** and **Axioms**, which can be given annotations for further description.
- ▶ All entities (classes, object properties, named individuals...) are uniquely identified by a sequence of characters called IRI.

Figure 2: A class (highlighted in blue) in the hierarchy view of the ontology it is contained in.



What is an ontology?

Figure 3: A class in an ontology text file (the ontology document). IRIs in blue.

```

<!-- http://purl.obolibrary.org/obo/PATO_0001464 -->

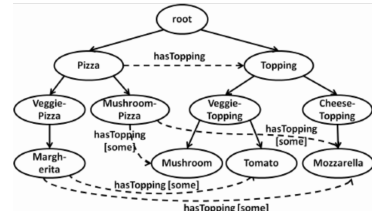
<owl:Class rdf:about="http://purl.obolibrary.org/obo/PATO_0001464">
  <rdfs:subClassOf rdf:resource="http://purl.obolibrary.org/obo/PATO_0001018"/>
  <rdfs:subClassOf rdf:resource="http://purl.obolibrary.org/obo/BFO_0000016"/>
  <obo:IAO_0000115
    rdf:datatype="http://www.w3.org/2001/XMLSchema#string">
    A quality that is equal to the potential energy per unit charge associated with a
    static (time-invariant) electric field, also called the electrostatic potential.
  </obo:IAO_0000115>
  <oboInOwl:hasOBONamespace
    rdf:datatype="http://www.w3.org/2001/XMLSchema#string">quality</oboInOwl:
    hasOBONamespace>
  <oboInOwl:id
    rdf:datatype="http://www.w3.org/2001/XMLSchema#string">PATO:0001464</
    oboInOwl:id>
  <oboInOwl:inSubset
    rdf:resource="http://purl.obolibrary.org/obo/pato#attribute_slim"/>
  <oboInOwl:inSubset
    rdf:resource="http://purl.obolibrary.org/obo/pato#scalar_slim"/>
  <rdfs:label rdf:datatype="http://www.w3.org/2001/XMLSchema#string">electric
    potential</rdfs:label>
</owl:Class>

```

What is an ontology?

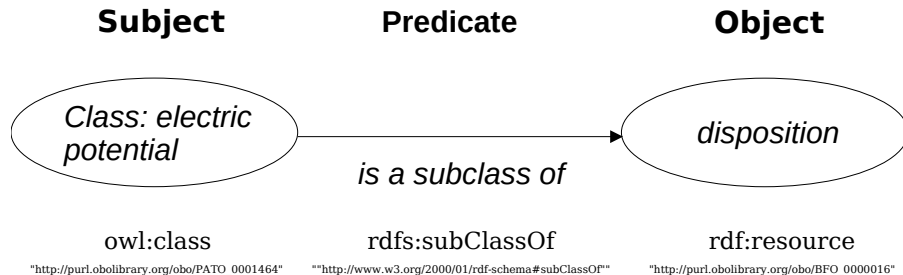
- ▶ Most ontologies use the W3C standard language for ontologies, Web Ontology Language **OWL**.
- ▶ OWL ontologies are mainly stored in `.owl` files, which are a sort of **RDF** document.
- ▶ **RDF** (Resource Description Framework) is a standard for data exchange. It defines **triples of (subject, predicate, object)**.
- ▶ These triples form labeled graphs where the edge (predicate) represents the link between two resources (subject and object)

Figure 4: The pizza ontology, visualized as a graph (add source)



What is an ontology?

Figure 5: A graph with two nodes (Subject and Object) and a triple connecting them (Predicate)



What is an ontology?

Figure 6: The triple in the previous figure as included in the .owl document file of the ontology it is contained in.

```
<!-- http://purl.obolibrary.org/obo/PATO_0001464 -->  
  
<owl:Class rdf:about="http://purl.obolibrary.org/obo/PATO_0001464">  
<rdfs:subClassOf rdf:resource="http://purl.obolibrary.org/obo/BFO_0000016"/>  
  
(...)  
</owl:Class>
```

What is an ontology?

- ▶ **Foundation ontologies:** they provide the most abstract or general classes, i.e., the top-level classes we see in a hierarchy view of our ontology.
- ▶ **Application ontologies:**
- ▶ **Domain ontologies**

Overview

- ① Introduction
- ② The eNanoMapper Ontology
 - Development and QC
 - Composition of the eNanoMapper ontology
 - Uses of the eNM ontology
- ③ Future plans and challenges

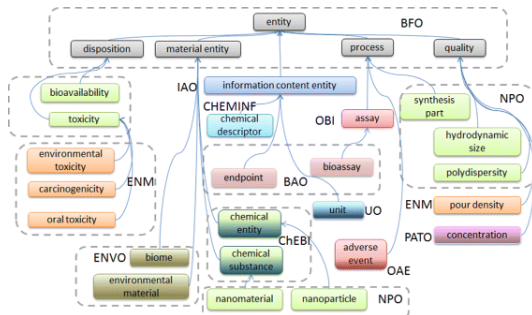
Development and QC

Pointers about this...



Composition of the eNanoMapper ontology

Figure 7: eNM ontology yadda quote



Uses of the eNM ontology

Pointers about this...



Overview

- 1 Introduction
- 2 The eNanoMapper Ontology
- 3 Future plans and challenges
 - What is still needed
 - Migrating the ontology development?

What is still needed

- ▶ OWL is not the best at modularity, but the eNM ontology heavily relies on importing modules. This leads to complications in class hierarchies, duplicate imports, etc.
- ▶ This peculiarity

Migrating the ontology development?

... ODK for automation, standardisation, interoperability... is it convenient for enm?

References I

