

MAMBO: the Materials And Molecules Basic Ontology

Fabio Le Piane, Matteo Baldoni, Francesco Mercuri - DAIMON Team - CNR-ISMN Bologna, Italy
Mauro Gaspari - Alma Mater Studiorum - University of Bologna

Email: fabio.lepiane@ismn.cnr.it

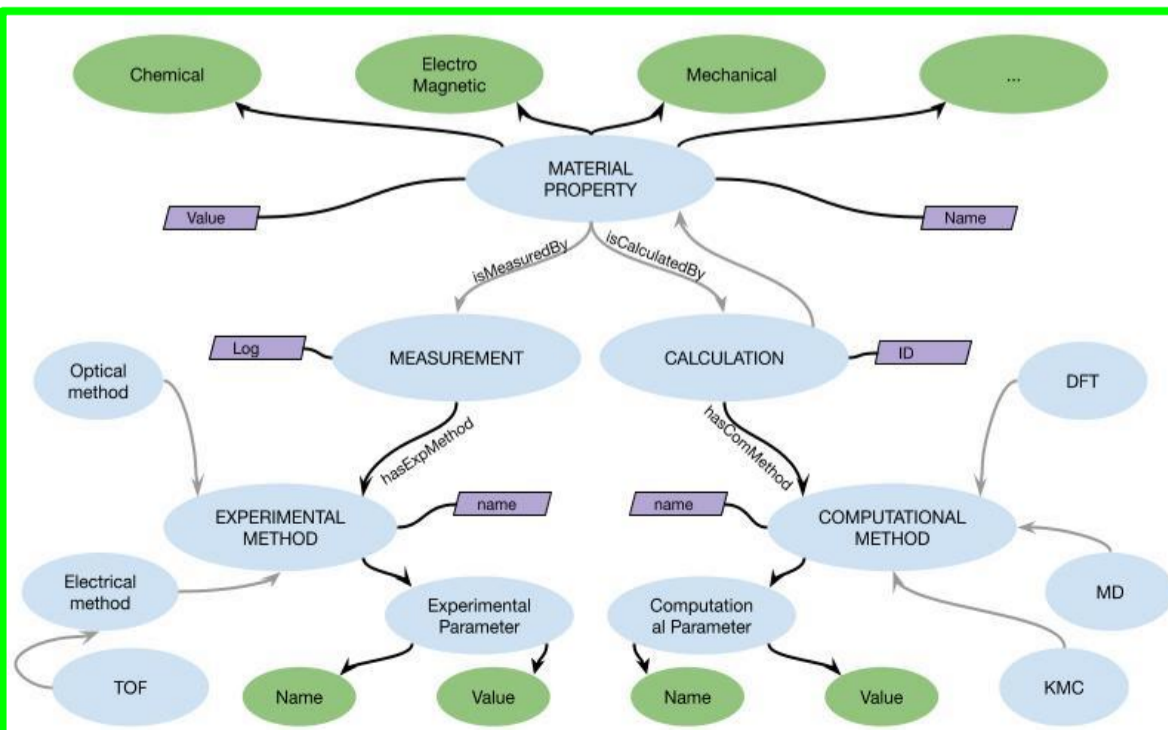
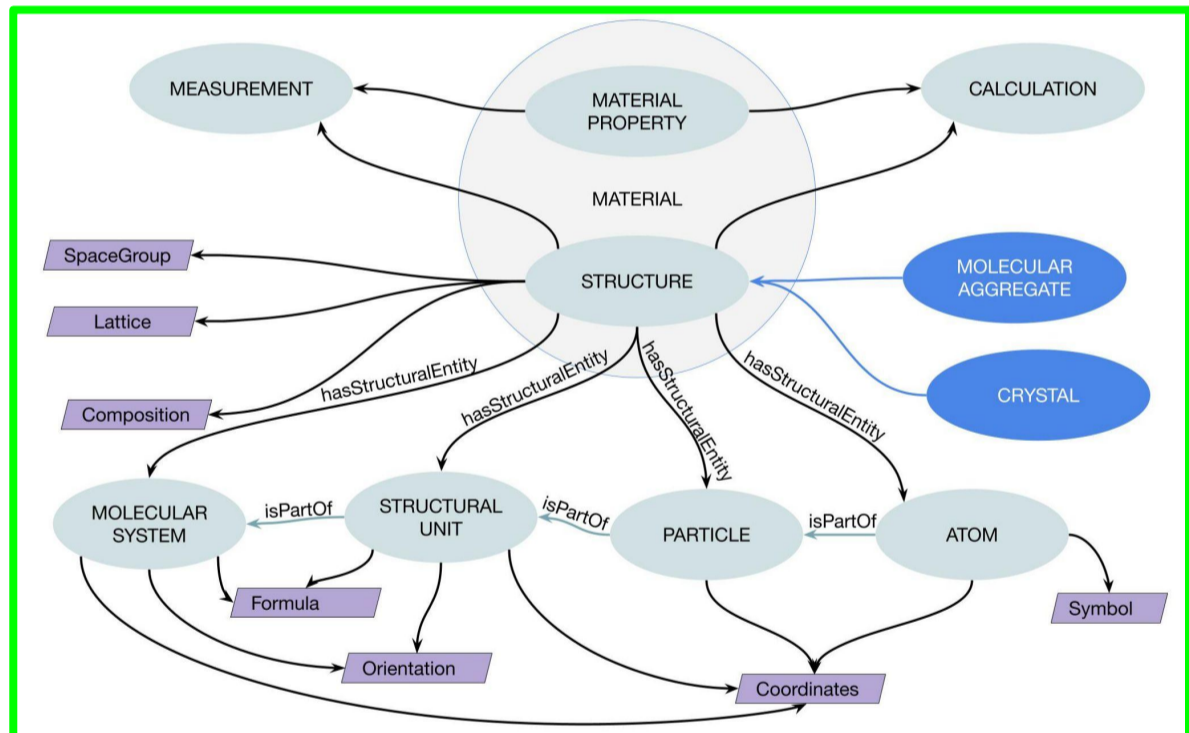
MAMBO is an ontology for molecular materials and their applications in real-life scenarios

MAMBO has been developed focusing on novel materials with functional properties, with particular attention to the nanoscale

It's still a work-in-progress, but it's expected to enable the systematic integration of computational and experimental data in specific domains, with a strong emphasis on the applications of data-driven frameworks for the design of novel materials with tailored characteristics

The two figures below represent two of **MAMBO's** main hierarchies and their relation with the core of the ontology: the one dealing with the structural characteristics of a **Material (Structure)** and the twin hierarchies representing computational and experimental workflows (**Calculation** and **Measurement**, respectively)

- A **Structure** is composed by one or more structural entities
- It has many sub-classes, two of which are **Molecular Aggregate** (peculiar of **MAMBO**) and **Crystal** (which could serve as an integration point with **MDO**)
- It can be described with many characteristics (Has it got a space group? Or a lattice? Which is its composition?)



- A **Property** is summarised as its value and its name
- A **Property** can be determined with a **Measurement** or a **Calculation**.
- Both have a corresponding **Method** class, which collects the different, related methods and techniques.
- Both collect the parameters of their respective methods
- A similar relationship will be developed with the **Structure** class