MAMBO: the Materials And Molecules Basic Ontology

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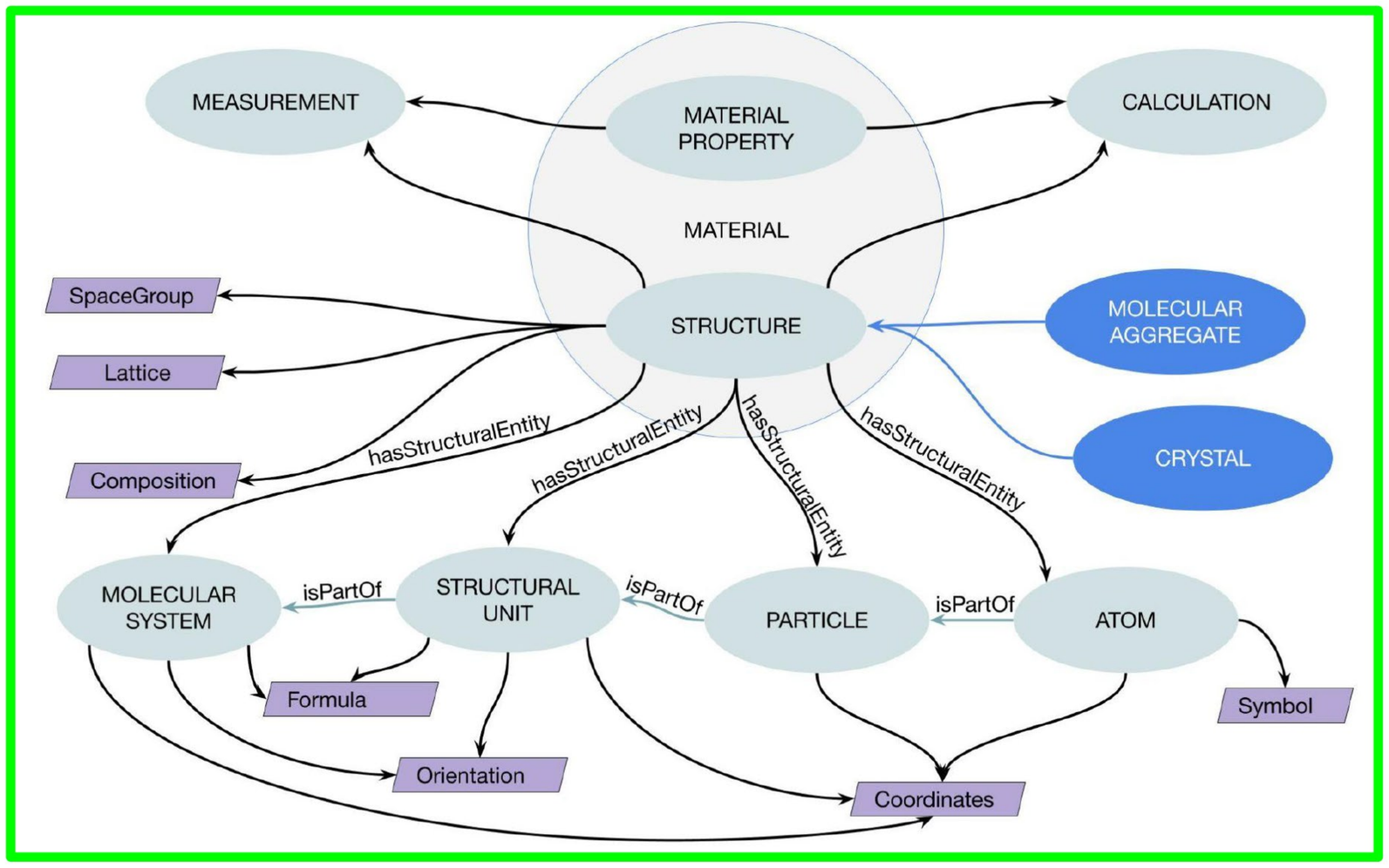
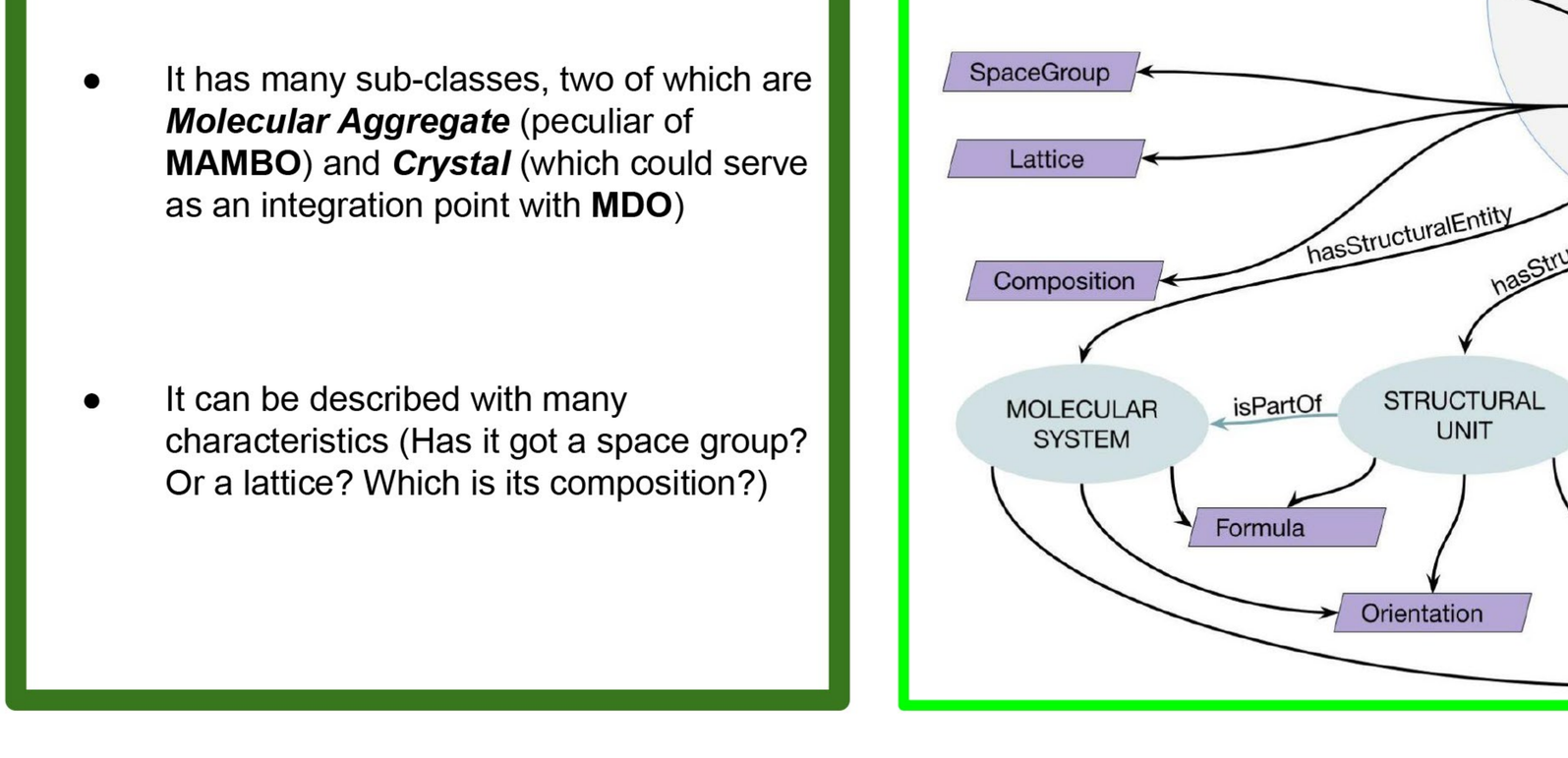
MAMBO is an ontology for molecular materials and their applications in real-life scenarios
MAMBO has been developed focusing on novel materials with functional properties, with particular attention to the nanoscale

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 collects the parameters of their respective methods
- A similar relationship will be developed with the ***Structure*** class