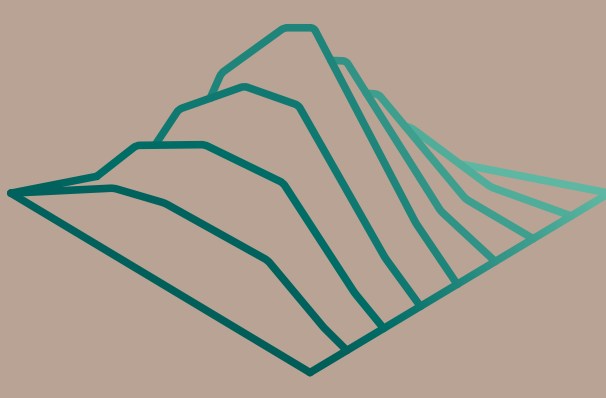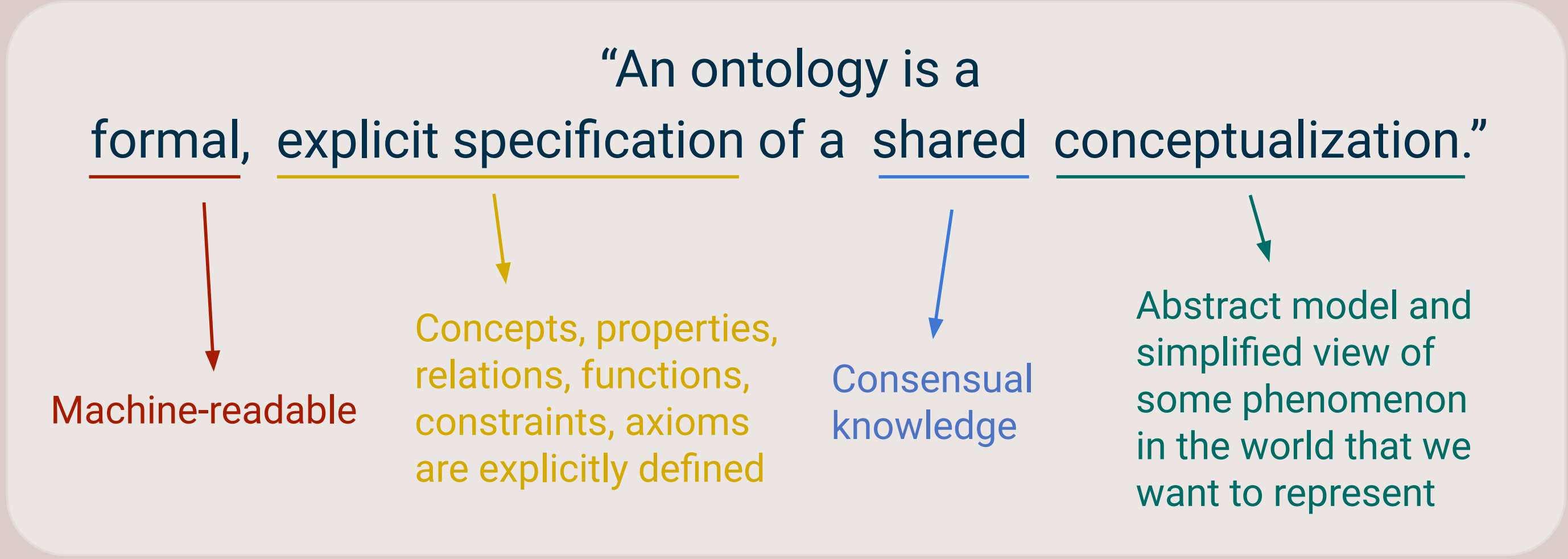# Ontologies
in Computational Materials Science

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NOMAD
NOVEL MATERIALS DISCOVERY

What is an ontology?

"An ontology is a formal, explicit specification of a shared conceptualization."

- **formal** → Machine-readable
- **explicit specification of a** → Concepts, properties, relations, functions, constraints, axioms are explicitly defined
- **shared** → Consensual knowledge
- **conceptualization** → Abstract model and simplified view of some phenomenon in the world that we want to represent

The NOMAD Meta Info

The NOMAD Meta Info is the meta data scheme for data in the NOMAD Archive – the largest database for normalized data in computational materials science.

There are currently four types of meta data that structure the data and assign relations between them:

Concrete values are the labels to the values (strings, scalars, vectors, …) parsed by parsers.
Sections represent different parts of a computer simulation.
Abstract types are mata data for meta data, they describe the type fo data that is labeled by a Concrete Value or a Section
Dimensions classify some meta data terms as integers that define the lengths of a dimension of a non-scalar Concrete Value

The NOMAD Meta Info contains 5 types of relations. 4 are shown as arrows. The 5th is the has reference which points from section to section.
→ Can be represented ontologically and linked to more semantic ontologies
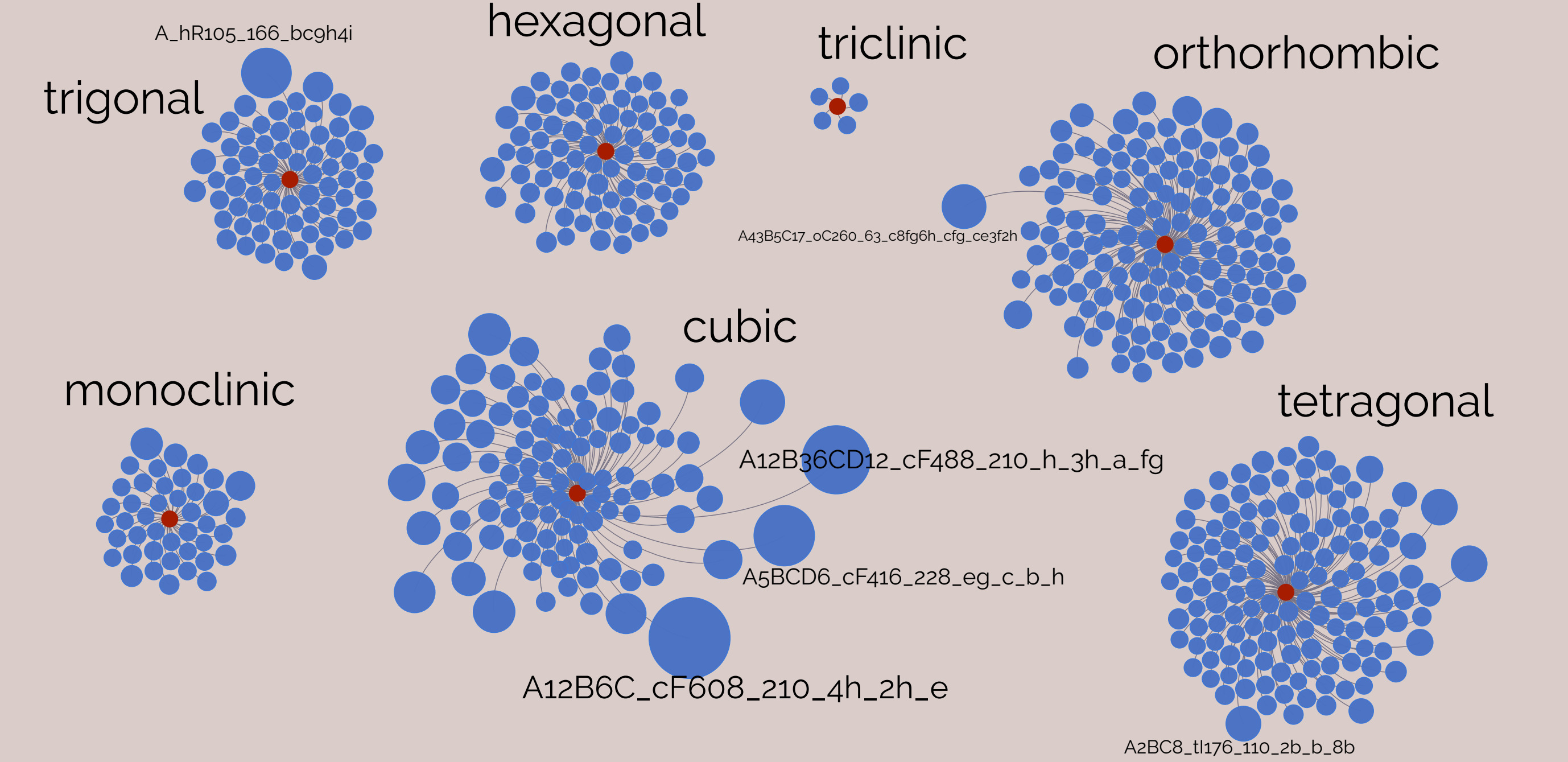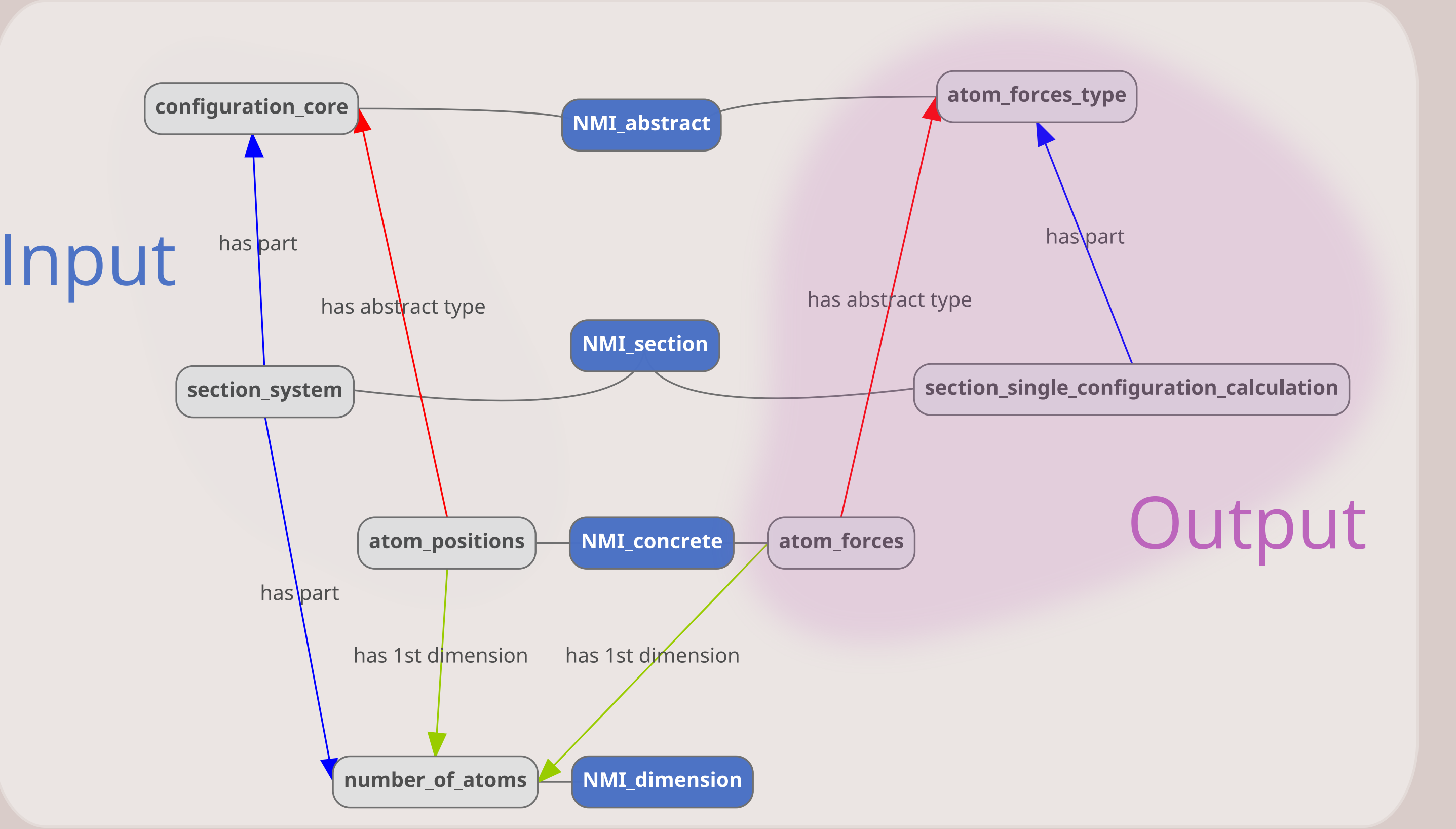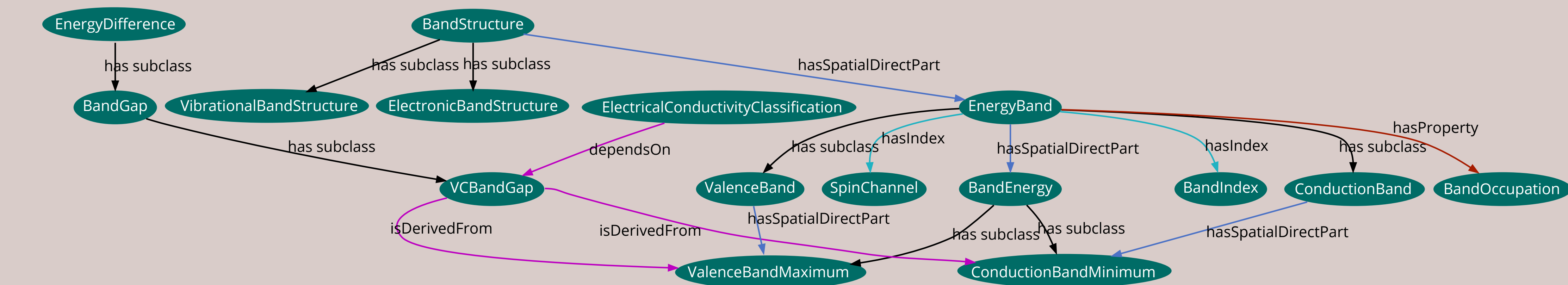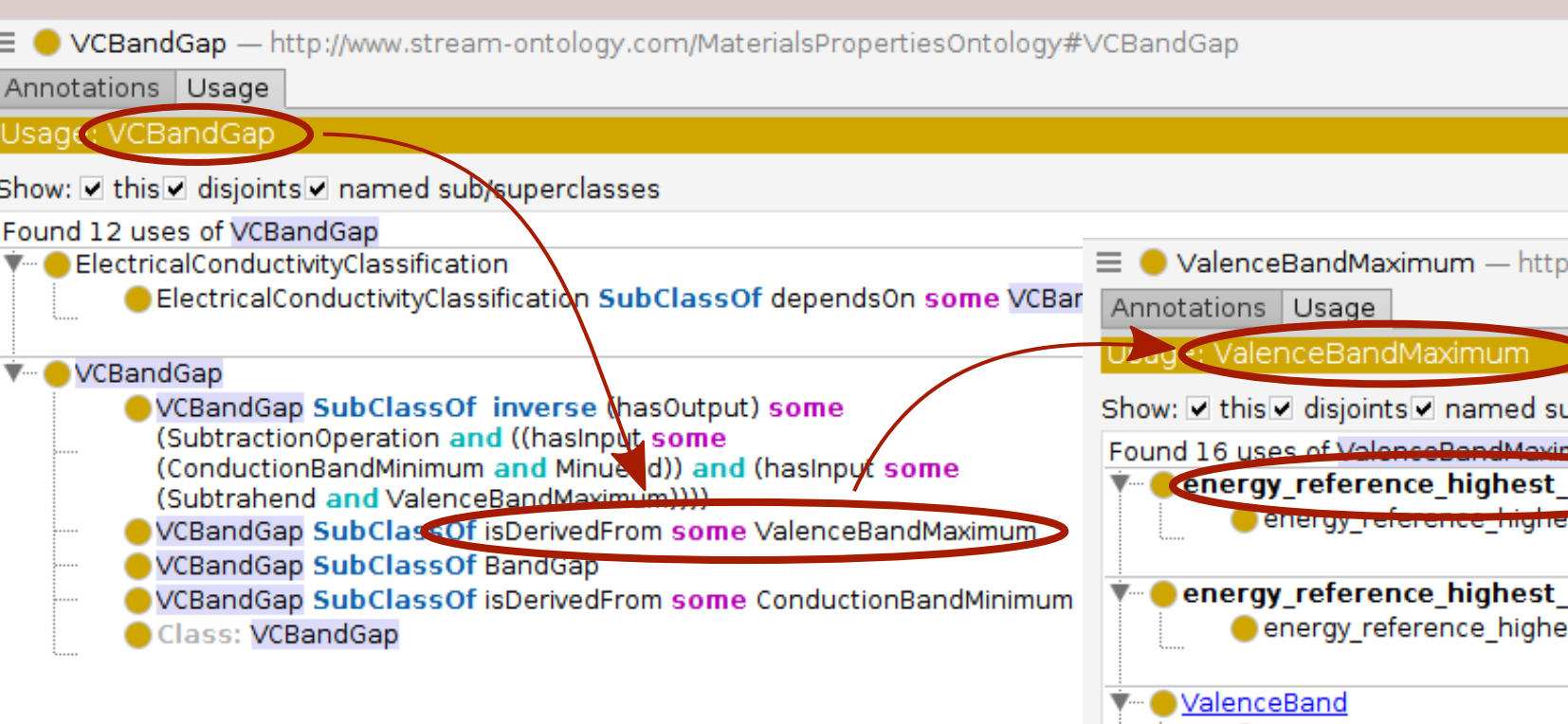

The Crystal Structure Ontology

Semantically represent crystal structures and their symmetries
Extract for crystal symmetry at class level
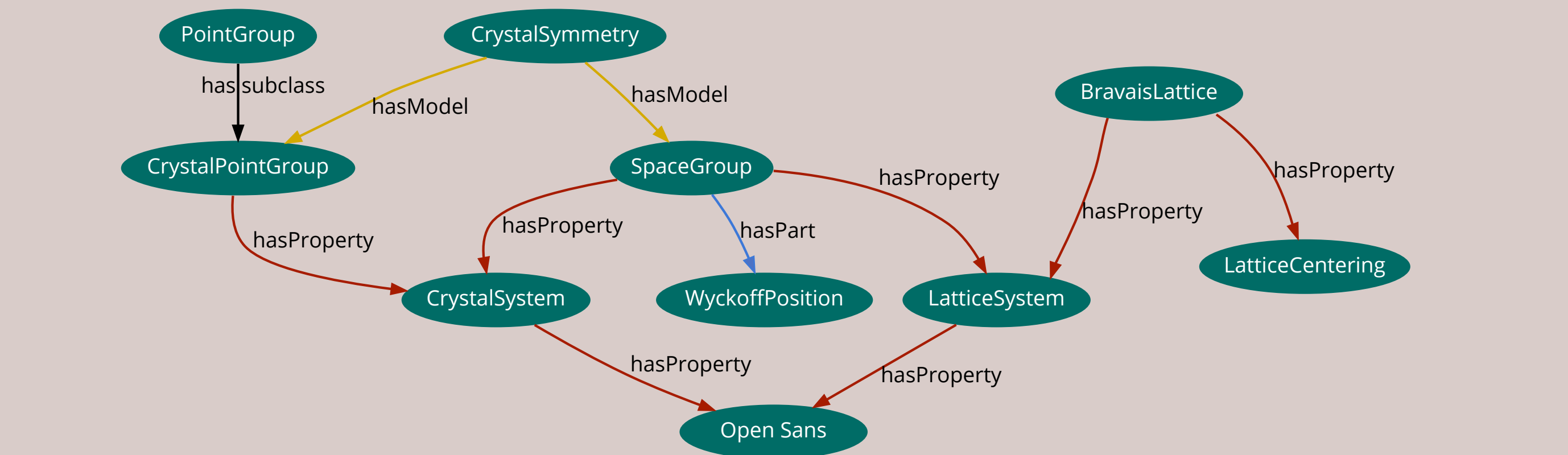
Ontology can be instantiated with AFLOW Library of Crystallographic Prototypes
Querying this knowledge graph allows visualization as network:
Prototypes (blue) size-scaled by number of atoms clustered in crystal systems (red)

## The Materials Properties Ontology

Application: Search for a better solcar cell material

1st step:
Use ontology editor/viewer to find relevant terms
(here: Protégé)

2nd step:
Choose a dataset from NOMAD
(here: *Hybrid organic inorganic Perovskites*)
DOI: 10.17172/NOMAD/2017.03.15-1

3rd step:
Filter for materials with band gap > 1.0 eV *
→ reduces number of materials in dataset by factor 10
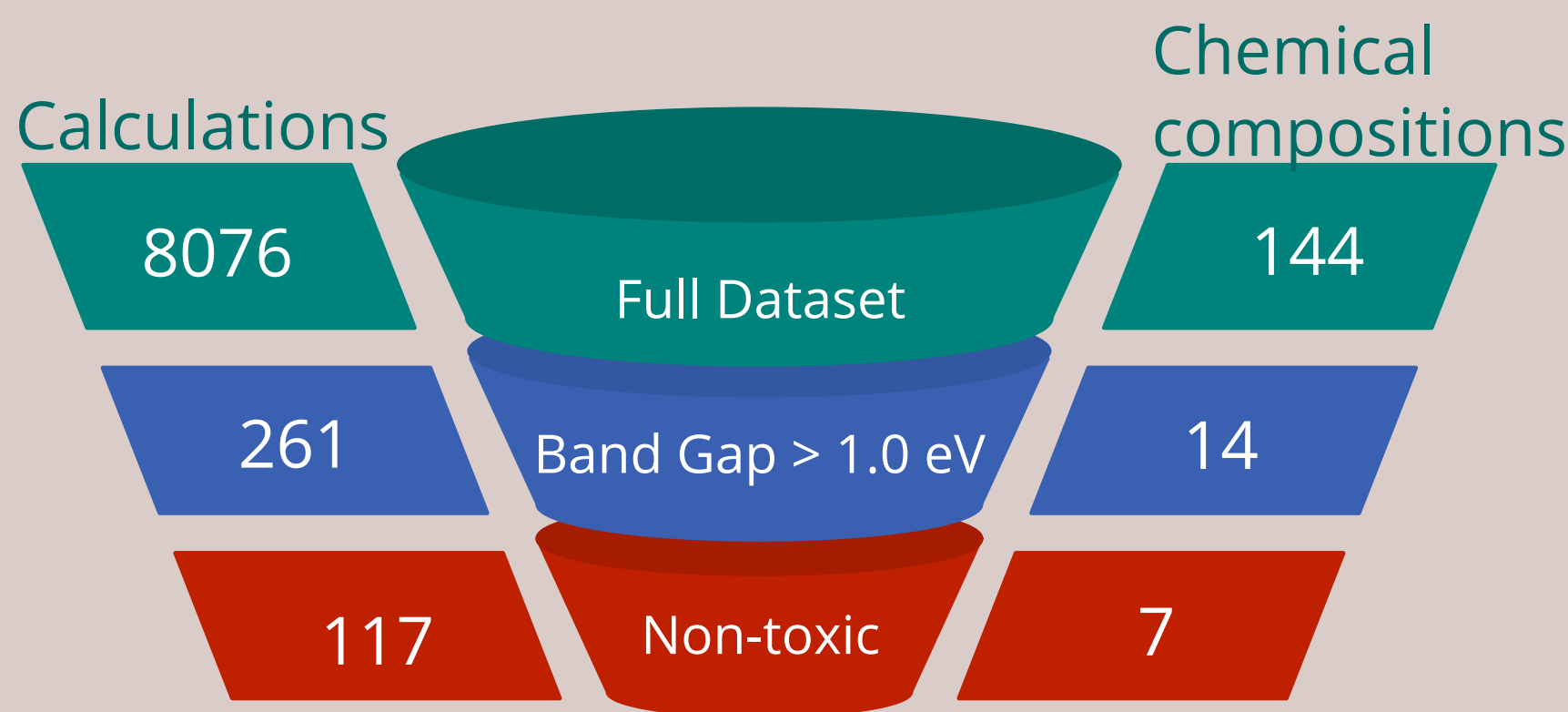
4th step:
Filter out all materials containing elements that cause some intoxicating effect according to Wikidata

* According to the Shockley Queisser criterion for maximum efficiency of solar cell, the optimal band gap is ~ 1.3 eV .

Calculations	Full Dataset	Chemical compositions
8076		144
261	Band Gap > 1.0 eV	14
117	Non-toxic	7