



The Center for Bright Beams Ontology Project

Kevin Nangoi
Paul Cueva
Alexander Bernstein
Will DeBenedetti

- An **ontology** is a **hierarchical machine-readable vocabulary** that formalizes the concepts in a particular discipline and *the relationships* between said concepts.
- Very roughly:
ontology = taxonomy + dictionary + relationships
- ‘Things + processes and how they are defined, organized, and relate to one another’

Why does CBB need an ontology?

- CBB is a large cross-disciplinary center that spans multiple institutions
- We need a central tool to permit cross-disciplinary collaborations that relate different concepts from different fields

The CBB ontology project seeks to foster team science between different institutions and disciplines

Target audience: First-year graduate students

**Answer:
All CBB grads and post-docs!**

Hosted by Cornell University

<https://webprotege.cbb.cornell.edu>

Best to illustrate with a few examples:

Examples: instrument, materials, process

What does an ontology look like?

Example: instrument, process, materials

Active Ontology x | Entities x | Individuals by class x | DL Query x

Annotation properties | Datatypes | Individuals

Classes | Object properties | Data properties

Class hierarchy: Scanning_Tunneling_Microscope

Annotations: Scanning_Tunneling_Microscope

Annotations +

definition [language: en]
A type of scanned probe microscope used for imaging the morphological and electronic structure of conductive surfaces. The microscope uses the tunneling current between the surface being imaged and a near-atomically-sharp metal probe to measure the distance between the tip and the surface. In the most common type of imaging, the tip is rastered across the surface while maintaining a constant tunneling current. The output image represents the position of the tip at every (x, y) location in the image. This form of imaging is typically referred to as constant height imaging; however, this is a simplification as the tip may assume different heights above, for example, different types of atoms.

dc:contributor [language: en]
Melissa A. Hines

'alternative term' [language: en]
STM

'useful_resource' [language: en]
Comprehensive introduction to scanning tunnelling microscopy that is suitable for first-year graduate students:
C. J. Chen, Introduction to Scanning Tunneling Microscopy (Oxford Univ. Press, New York, 2008).

'useful_resource' [language: en]
Modeling STM images to include tip effects:
<http://dx.doi.org/10.1103/RevModPhys.75.1287>

'useful_resource' [language: en]
Most common technique to model STM images
<http://dx.doi.org/10.1103/PhysRevB.31.805>

Description: Scanning_Tunneling_Microscope

Equivalent To +

SubClass Of +
● Scanned_Probe_Microscope

General class axioms +

SubClass Of (Anonymous Ancestor)

Instances +

Target for Key +

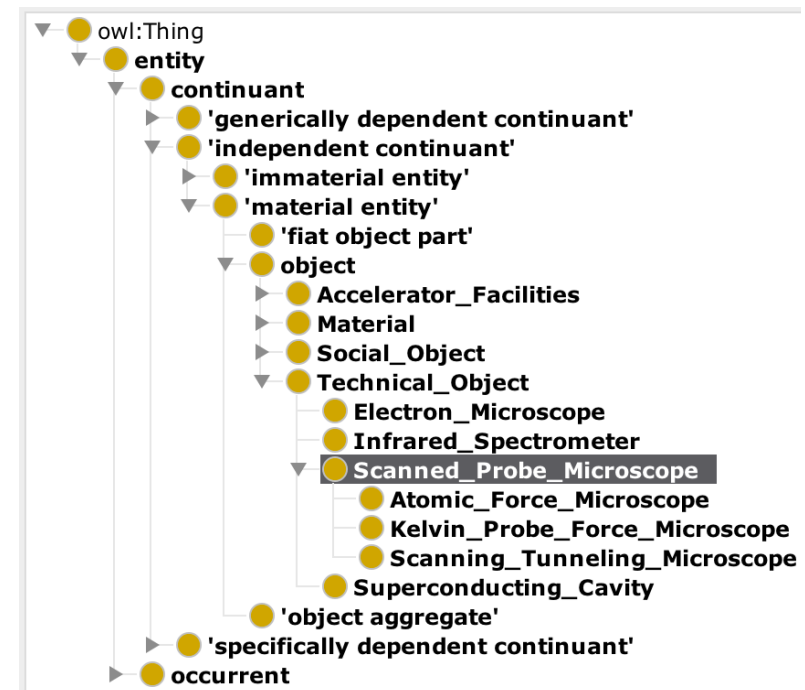
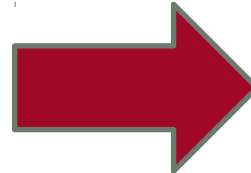
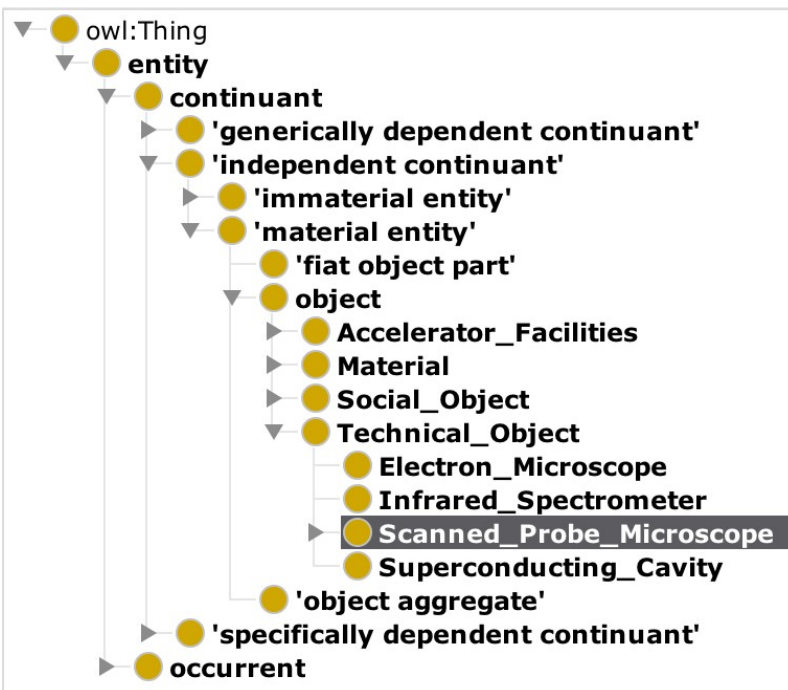
Things +
Processes

How they are defined

How they are related

Example: instrument, materials, properties, processes

Scanning Tunneling Microscope (STM)






Annotations in the ontology




Example: instrument, materials, properties

Annotations: Scanning_Tunneling_Microscope




Annotations +

definition [language: en]   




A type of scanned probe microscope used for imaging the morphological and electronic structure of conductive surfaces. The microscope uses the tunneling current between the surface being imaged and a near-atomically-sharp metal probe to measure the distance between the tip and the surface. In the most common type of imaging, the tip is rastered across the surface while maintaining a constant tunneling current. The output image represents the position of the tip at every (x, y) location in the image. This form of imaging is typically referred to as constant height imaging; however, this is a simplification as the tip may assume different heights above, for example, different types of atoms.

dc:contributor [language: en]   




Melissa A. Hines

'alternative term' [language: en]   




STM

'useful_resource' [language: en]   

Comprehensive introduction to scanning tunnelling microscopy that is suitable for first-year graduate students:
C. J. Chen, Introduction to Scanning Tunneling Microscopy (Oxford Univ. Press, New York, 2008).

'useful_resource' [language: en]   

Modeling STM images to include tip effects:
<http://dx.doi.org/10.1103/RevModPhys.75.1287>

'useful_resource' [language: en]   

Most common technique to model STM images
<http://dx.doi.org/10.1103/PhysRevB.31.805>

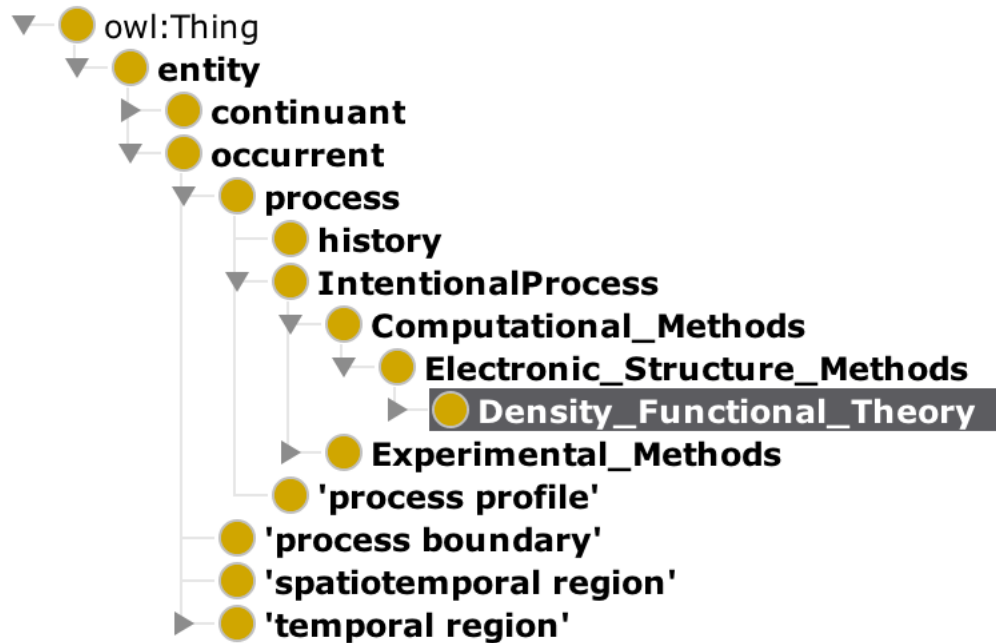
Description: Scanning_Tunneling_Microscope

Annotations include definitions, acronyms, and resources

Best way to share resources: include DOIs for useful papers!

Another example

Example: instrument, process materials,



Annotations: Density_Functional_Theory



Annotations 

definition [language: en]



An electronic structure method that has been popular in solid-state physics since the 1970s. However, DFT was not considered accurate enough for calculations in quantum chemistry until the 1990s, when the approximations used in the theory were greatly refined to better model the exchange and correlation interactions. Computational costs are relatively low when compared to traditional methods, such as exchange-only Hartree–Fock theory and its descendants that include electron correlation.

Despite recent improvements, there are still difficulties in using density functional theory to properly describe intermolecular interactions (of critical importance to understanding chemical reactions), especially van der Waals forces (dispersion); charge transfer excitations; transition states, global potential energy surfaces, dopant interactions and some other strongly correlated systems; and in calculations of the band gap and ferromagnetism in semiconductors.

'definition source' [language: en]



https://en.wikipedia.org/wiki/Density_functional_theory

'useful_resource'

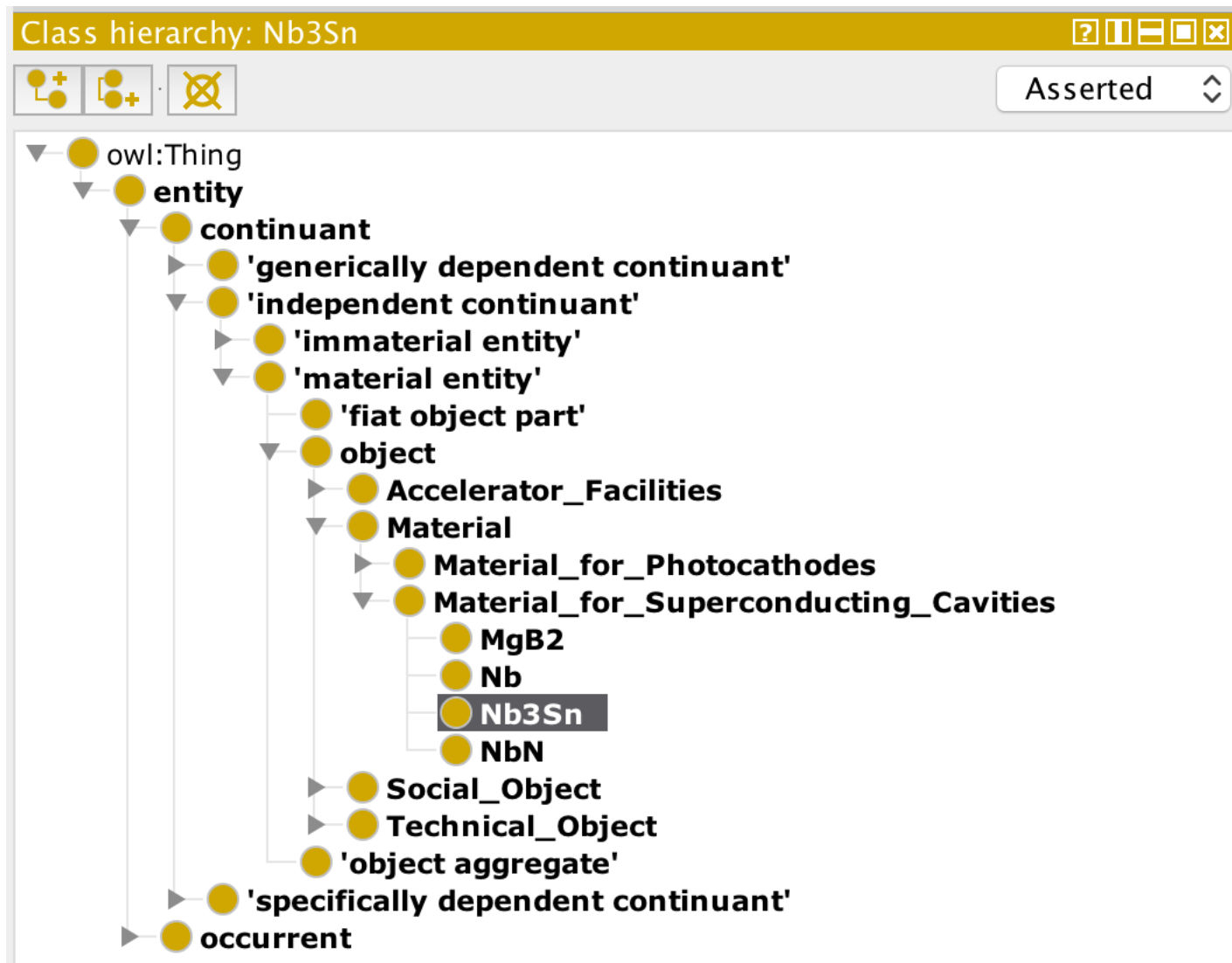


Conceptual review of density functional methods.

<http://dx.doi.org/10.1021/cr990029p>

A typical example

Example: instrument, process materials



A typical example

The screenshot shows the Protege ontology editor interface. The browser address bar displays the URL: `bfo (http://purl.obolibrary.org/obo/bfo/2.0/bfo.owl)`. The active ontology is identified as `Nb3Sn` with the URL `http://purl.obolibrary.org/obo/bfo.owl#Nb3Sn`.

The left pane shows the **Class hierarchy: Nb3Sn** tree. The root is `owl:Thing`, which branches into `entity`. Under `entity`, there are several subclasses: `continuant`, `'generically dependent continuant'`, `'independent continuant'`, `'immaterial entity'`, `'material entity'`, `'fiat object part'`, `object`, and `'specifically dependent continuant'`. The `object` class further branches into `Accelerator_Facilities`, `Material`, `Social_Object`, and `Technical_Object`. The `Material` class branches into `Material_for_Photocathodes` and `Material_for_Superconducting_Cavities`. The `Material_for_Superconducting_Cavities` class branches into `HgB2`, `Nb`, `Nb3Sn` (highlighted), and `NbN`. The `Material_for_Photocathodes` class branches into `'object aggregate'` and `occurrent`.

The right pane shows the **Annotations: Nb3Sn** section, which is currently empty. Below it, the **Description: Nb3Sn** section shows the following relationships:

- Equivalent To: +
- SubClass Of: +
 - `Material_for_Superconducting_Cavities`
- General class axioms: +
- SubClass Of (Anonymous Ancestor):
- Instances: +
- Target for Key: +
- Disjoint With: +

At the bottom right, there is a status bar that reads: "No Reasoner set. Select a reasoner from the Reasoner menu" and a checked checkbox for "Show Inferences".

This is where you come in!

Annotations: Nb3Sn 🔍 📄 🗑️

Annotations +

Grad students and post-docs need to populate the ontology

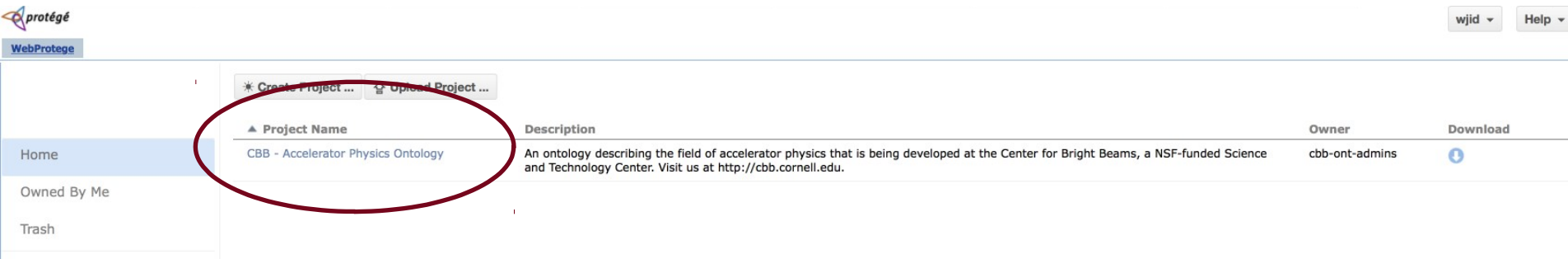
Some details to start

1. First create an ontology username and password here:


<https://webprotege.cbb.cornell.edu>

2. Email ontology admins for editing rights

cbb-ontology-admin-1@list.cornell.edu



The screenshot shows the WebProtege interface with a table of ontology projects. The 'Project Name' column is circled in red, highlighting the entry 'CBB - Accelerator Physics Ontology'. The table has columns for Project Name, Description, Owner, and Download.

| Project Name | Description | Owner | Download |
|------------------------------------|---|----------------|---|
| CBB - Accelerator Physics Ontology | An ontology describing the field of accelerator physics that is being developed at the Center for Bright Beams, a NSF-funded Science and Technology Center. Visit us at http://cbb.cornell.edu . | cbb-ont-admins |  |

All grads + post-docs complete 10 entries per year

Start by logging in and looking at ontology

Where to begin?



First create an ontology username and password here:

<https://webprotege.cbb.cornell.edu>

Questions about the ontology project? Ask an admin!

cbb-ontology-admin-1@list.cornell.edu

