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Nanotechnologies – Vocabulary

Platform for Ontology Engineering and Evolution for Nanotechnology

AUTOMATIC CONSTRUCTION OF NANOTECHNOLOGY ONTOLOGY STANDARDS

ICSU–CODATA WORKSHOP ON THE DESCRIPTION OF NANOMATERIALS, Ministère de l'Enseignement Supérieur et de la Recherché, Paris, France, 2012-02-23/24

Outline

- Introduction and motivation
- Development of example nano carbon nomenclature and integration of data in an ontology for nanomaterials
  - Nomenclature for NanoCarbon
  - Integration of physical/chemical properties and data in an OWL 2 ontology for NanoCarbon
  - Ontology evaluation and further development
- Ontology evolution process
  - Ontology learning
  - Ontology merging
  - Ontology updating
- Project structure
- Conclusions

Ontology Standards for Nanotechnology

- Ontologies are the central elements in any open e-infrastructure for information exchange across disciplines, organizational and geographical borders
- In the nanotechnology research field there is still no ontology standard in place, in spite of a strong need to coordinate and relate the diverse research conducted in this interdisciplinary field
- Ontologies are used to realise improved data integration and interoperability and can potentially bring big savings for both the industry and the public sectors
- Realising this potential requires efficient ontology construction, merging and evolution technologies

Ontology Standards for Nanotechnology, cont.

- The integration of people and applications into more efficient collaborative processes is central to the work on ontology engineering and evolution
- To make this happen, the applications and the information sources must all understand the annotations with respect to a common language, the ontology
- This ontology is an explicit and commonly accepted terminology standard that allows us to describe the content of data and services in a machine-processable and unambiguous way

Current stakeholders (new partners are welcome)

- Nanoscience, Nanomaterials and Nanotechnology
  - Norwegian Academy of Science and Letters, Standards Norway (ISO), Norwegian National Technical Committee (IEC), Norwegian technical universities, research institutes and industry. Cooperation (finance and technology) with Ministry of Trade and Industry and Ministry of Defense.
  - Broad outreach to international network in research, industry and finance.
- Computer Science and Information Technology
  - Oxford University, Manchester University, Karlsruhe Institute of Technology, Accenture (global)
- Computers and Law
  - Clifford Chance LLP, Norwegian Research Center for Computers and Law (NRCCL, University of Oslo), Simonsen Law, Arntzen de Besche

Project background

- Used the following documents
  - ISO/IEC 80004 Nanotechnology Vocabulary Series (specified in OWL2)
  - Nomenclature sp2 carbon nanoforms (I. Suarez-Martinez, N. Grobert, Chr. P. Ewels)
  - Informal standards, like the PAS, and scientific articles from the nanotechnology domain
- Ontology lifecycle model used
  - Both manual modeling tasks and automatic tool support
  - The ontology learning workbench (OWB) maps existing standards onto OWL2 (Ontology Web Language) structures and suggests new ontology structures from mining scientific domain documentation
  - Results from the OWB can be viewed, evaluated and modified with any ontology editor (e.g., Protégé)
  - Whereas the OWB speeds up the analysis of domain documents, the decisions on what to include in the final ontology still rests with the ontology modelers (nano domain experts)

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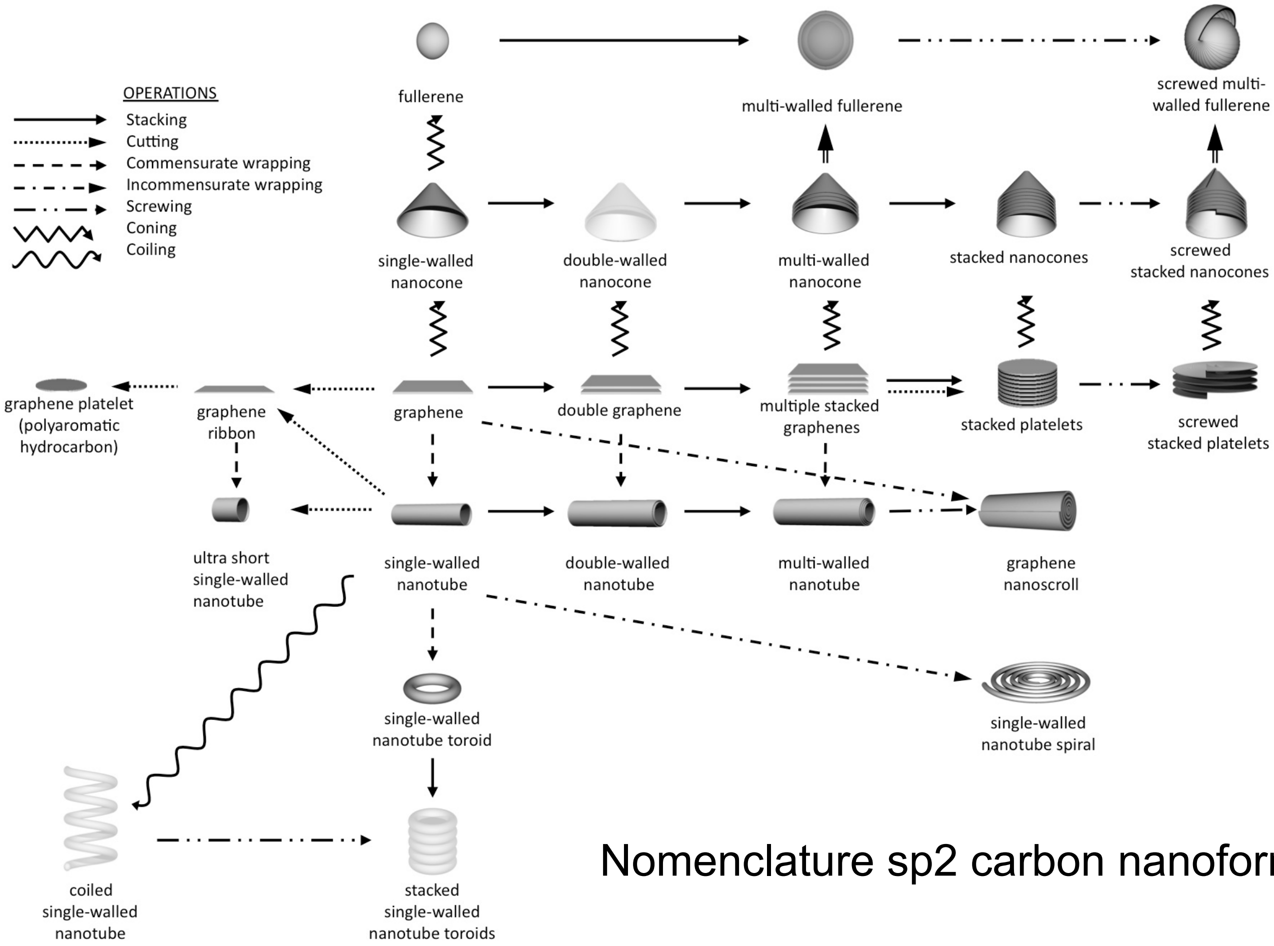
Difficulties with the use of ontologies

- Ontologies are being developed independently for different subdisciplines of nanotechnology
- New ontological elements (terminologies and definitions) continuously emerge from researchers and standardization groups
- Some old elements become irrelevant or find more popular corresponding synonyms
- The dynamic nature of this process requires continuous update of existing ontologies
- Collaboration between distinct subdisciplines requires safe techniques for merging of independently developed ontologies

Managing ontologies manually is not a simple task

Nomenclature for NanoCarbon

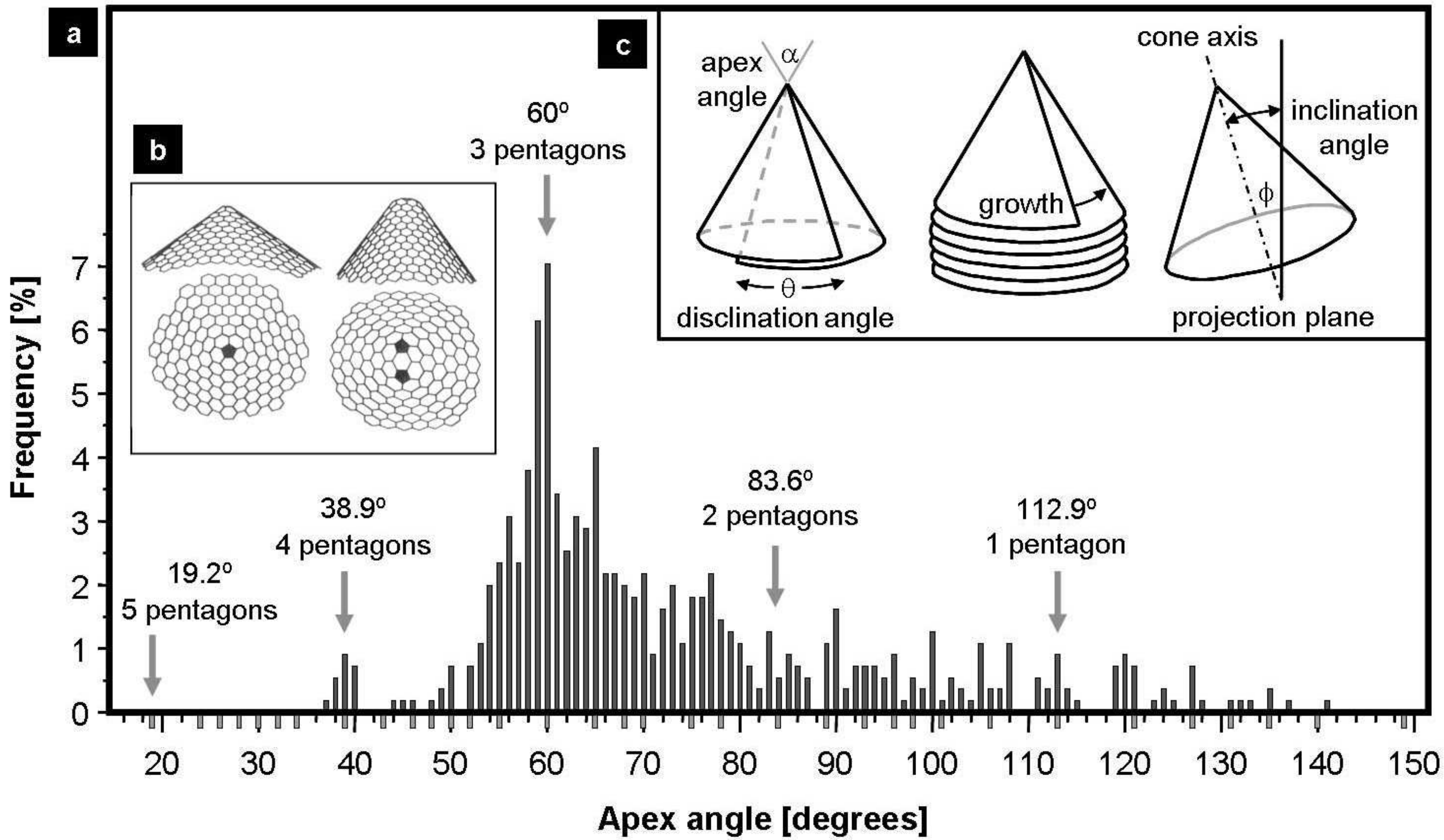


Nomenclature sp2 carbon nanoforms

Nomenclature for NanoCarbon, cont.

- The nomenclature is developed in accordance with the guidelines in; *Nomenclature for sp^2 carbon nanoforms*
- Exception: The term *helical nanocones* is used instead of *screwed stacked nanocones*, as we think the latter is incorrect; screwed cones cannot be exploded into single graphene cones – they concist of a single layer wrapped around itself. (See next picture)

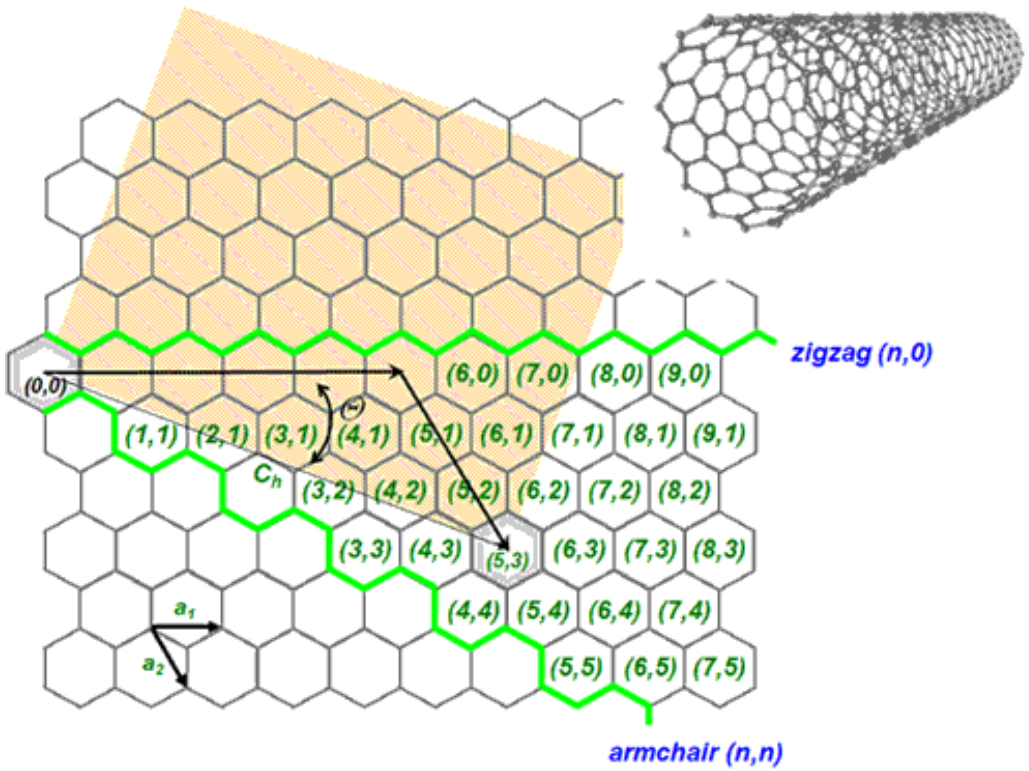
Nomenclature for NanoCarbon, cont.



Single Walled Carbon Nano Tubes

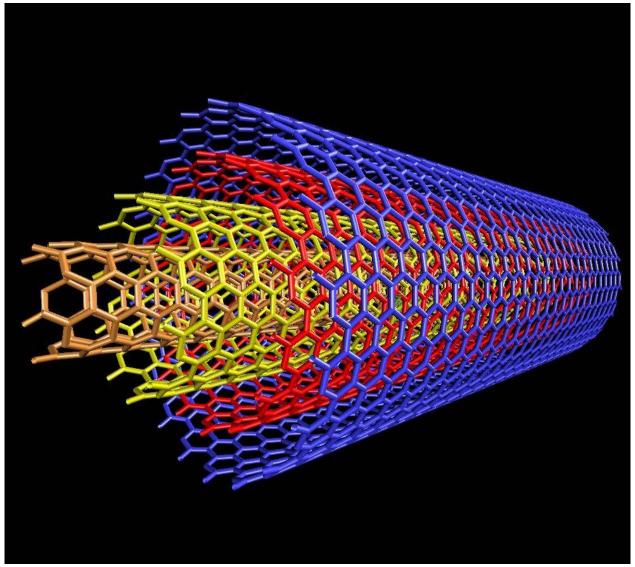
- SWNT[R13/L100/M6/N5] = Single Walled Carbon Nano Tube with Radius R = 13 nm, Length L = 100 nm and chiral vector (see next picture) (M,N) = (6,5)
- This specifies completely an open-ended tube without functionalized surface or defects. Suggestions to alternative syntax are welcome; e.g. SWNT_R{13}L{100}…etc

Chiral Vector



Multi-Walled Carbon Nanotubes

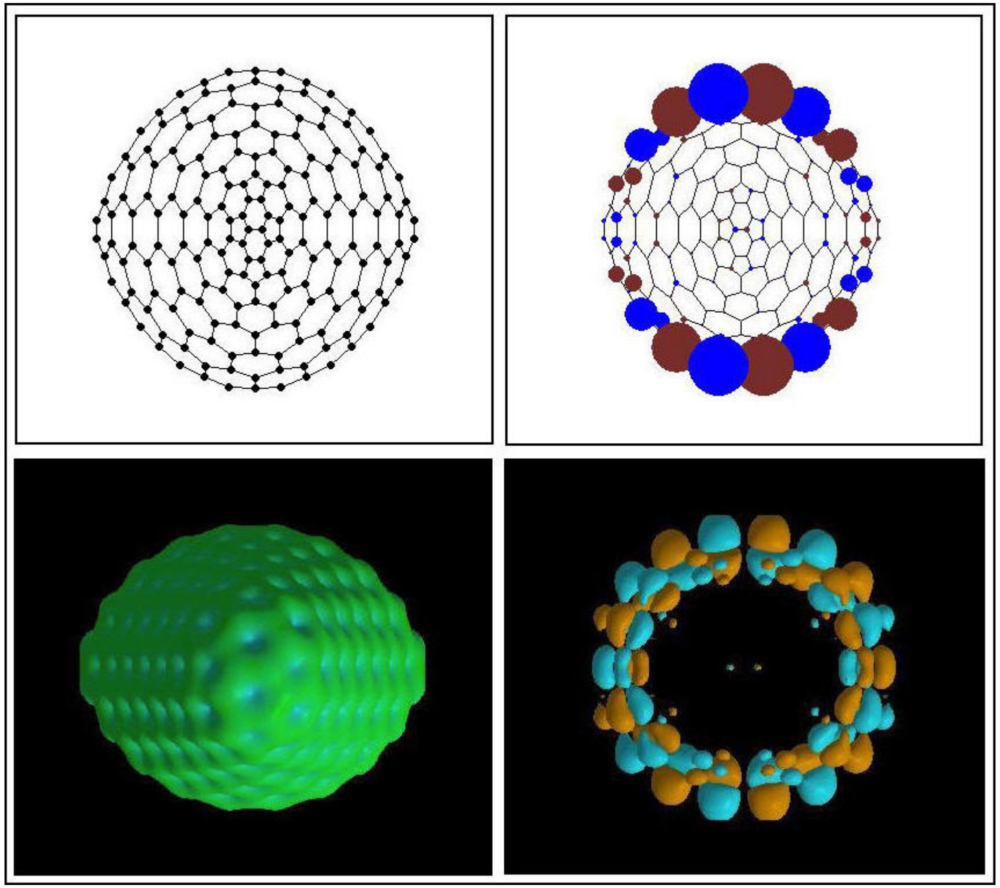
- MWCNT[R34/L460/M7/N1/W5] = Carbon Nano Tube with # Walls W = 5 where the outer wall has Radius R = 34 nm, Length L = 460 nm and chiral vector (M,N)=(7,1).



Graphene Cones

- Single Walled Carbon Nano Cones are called *Graphene Cones* in the ontology, as they can be transformed from graphene by removing 1 to 5 sectors of disclination angle 60° and rejoining the resulting dangling bonds.
- GC[D240/R250] = Graphene Cone transformed from circular graphene of Radius R=250 nm and total disclination angle D = 240° = 4 x 60°.

Integration of physical/chemical properties and data in an ontology for NanoCarbon



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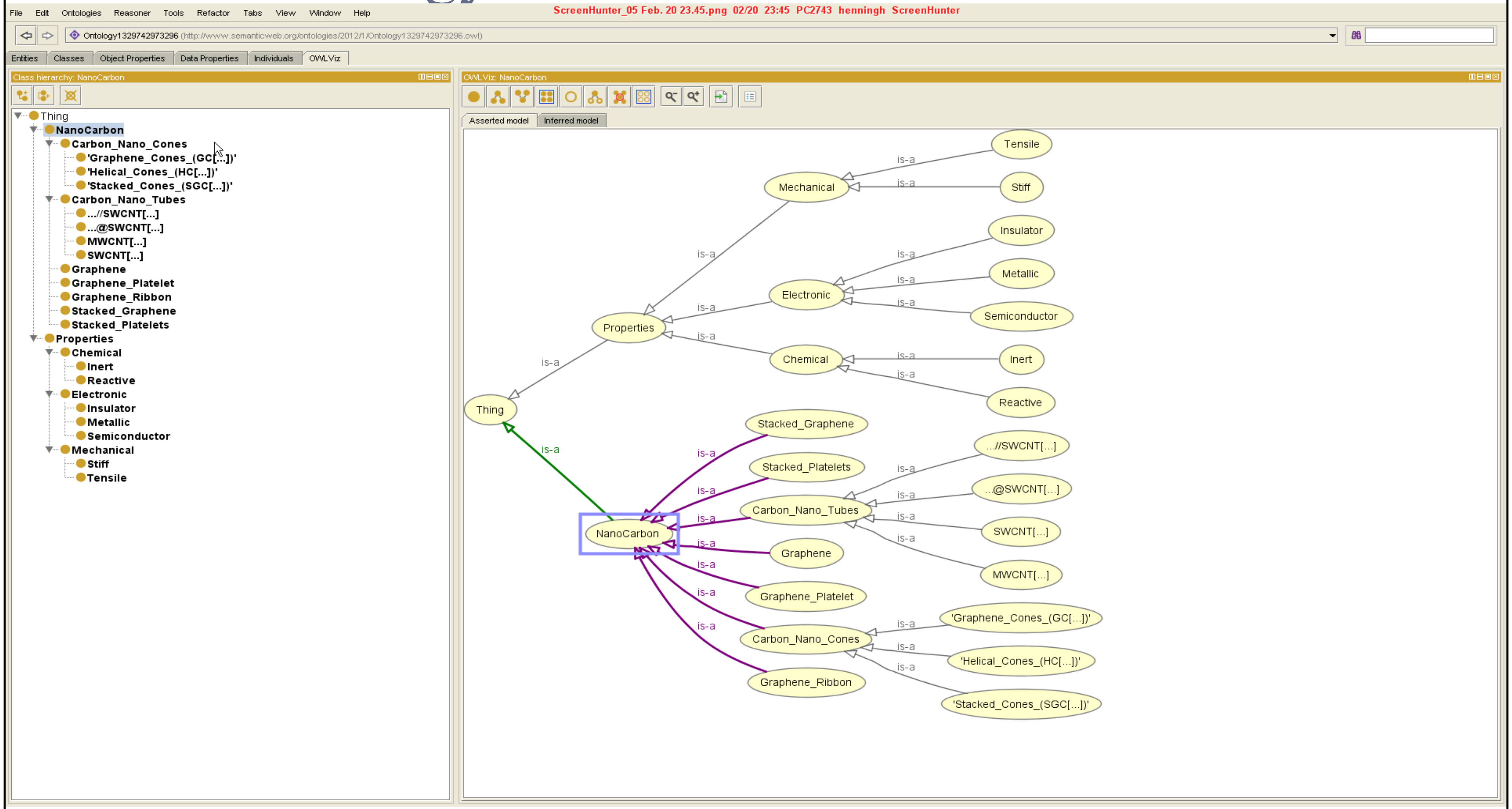
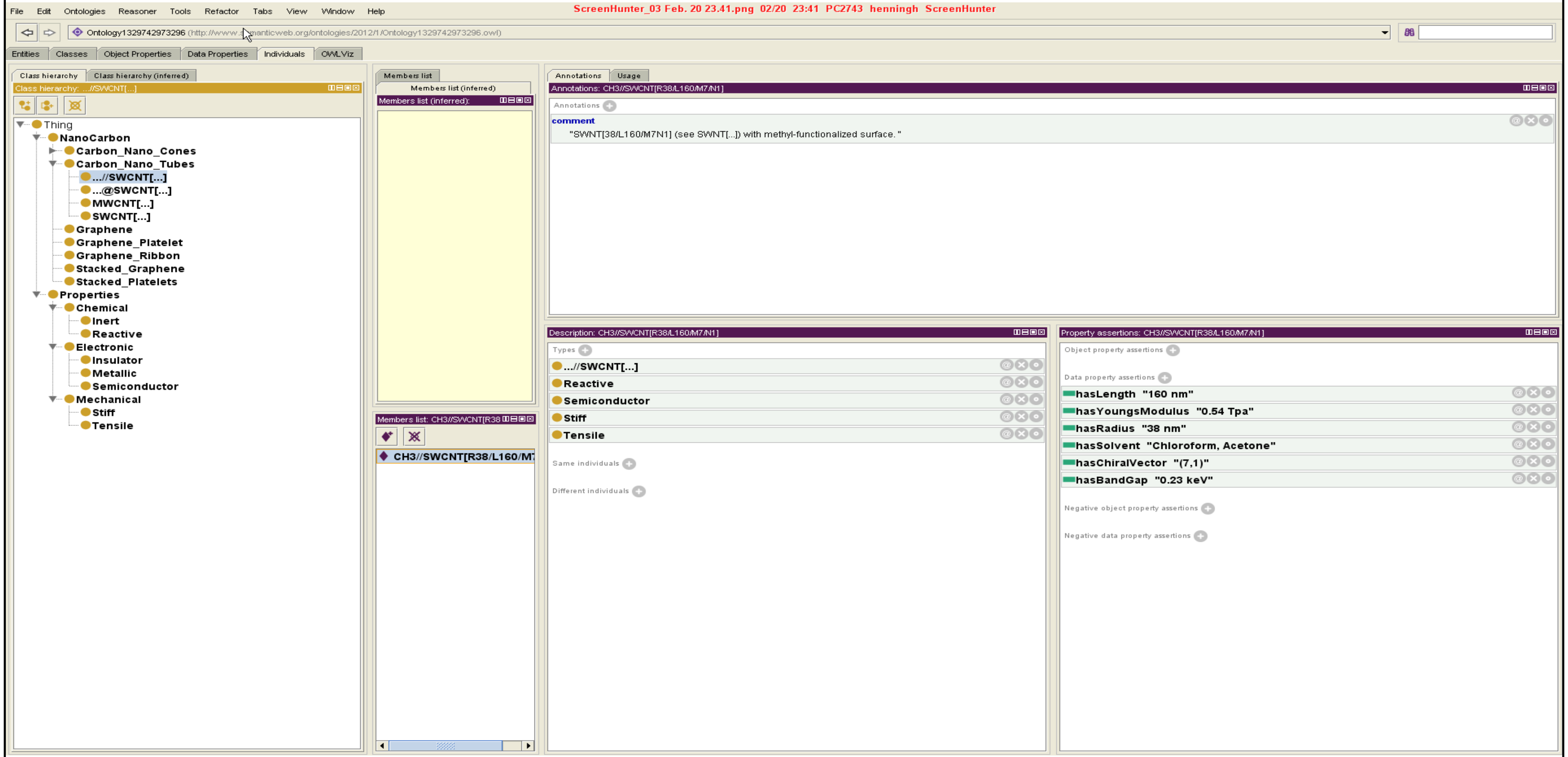
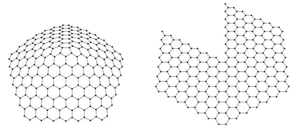
Model Ontology for Nano Carbon

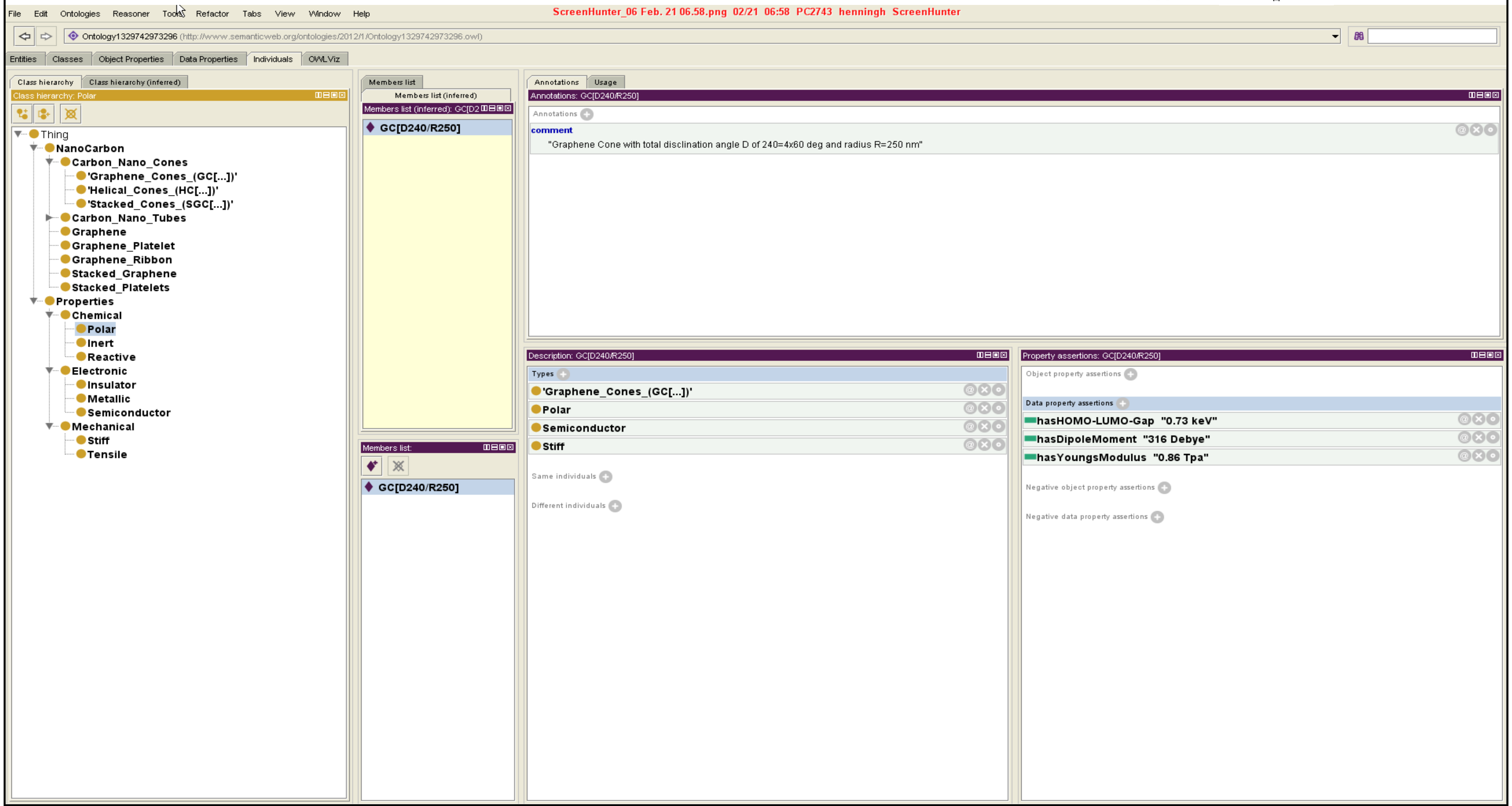


Representation of Nano Carbon entities. Below: SWNCT with methyl-functionalized surface



Graphene Cone





Heterogeneities in ontologies for nanotechnology

- Heterogeneity can be:
  - assembly of higher order structures not having same size with disparate geometric arrangements,
  - that represents dissimilar level of perfection.
  - both static and dynamic.
- Transferability to other systems / challenges:
  - Hierarchical structure is probably possible, but the shape of this is likely to be material dependent.
  - Should also be compatible with other relevant nomenclature
    - Eg. crystallographic in the case of crystals can be formed
    - Chemical (eg, self-organizing forms)
    - Biological (eg, PDB database, gene sequences, etc.) when such building blocks included in nanostructures.

Heterogeneities in ontologies for nanotechnology

- Heterogeneities and structural defects can hardly be addressed through the ontology alone.
- Complete specification in these cases can however be achieved by a link under Datatype Properties in the OWL2 interface to a molecular file, e.g. in Protein Data Bank (PDB) format.
- The molecular file defines the complex completely, and can be displayed graphically. If possible, a standard naming convention is still desirable for these cases.

Ontology evaluation and further development (input from ICSU CODATA workshop attendes)

- Is the nomenclature convenient? Complete specification through nomenclature alone seems infeasible due to e.g. the pletora of topological variations at the open ends of tubes and cones.

- Building model ontologies is a good method to test nomenclatures. For example, integration of numerical data requires a more specific nomenclature than qualitative properties.

- Further development requires expert input on dependencies of physical/chemical properties on structural details.

Project: Ontology Engineering and Evolution for Nanotechnology

- A **collaborative environment** to support the use and development of nanotechnology ontologies
  - **To learn** new ontological elements
    - highlighting **emerging terms** among researcher and standardization groups
    - identifying **relations** between them
  - **To combine** ontologies
    - helping to **merge existing ontologies** from different subdisciplines of nanotechnology
    - locating **overlapping** and **conflicting** regions
  - **To update** ontologies
    - finding ontology elements that become **out-of-date** or are **irrelevant** for researchers and standardization groups
    - identifying elements that should be **renamed**
    - identifying new elements that should be **included**

Ontology Learning

- Goal: (semi-)automatically identify and extract relevant concepts and relations from a given corpus to form an ontology
- Documents are parsed; indexed and subject to statistical analyses for concept extraction;
- This produces statistical reports including
  - suggestion scores (how often has a candidate term been suggested), and
  - the suggested neighborhood in an existing ontology

Ontology Merging

- Some ontologies are developed in totally different scientific and industrial contexts
- However, the inter-disciplinary nature of the field requires collaboration between academics and industrial partners
- Safe merging of ontologies is important and tools are needed to
  - detect possible inconsistencies
  - assist in the repair of these inconsistencies

Merging of Ontologies

Ontology Merging
- Merging ISO/IEC 80004 Vocabulary Series ontologies with other ontologies for nanotechnology

Indexing
- Split documents into text units
- Store each unit in a search index

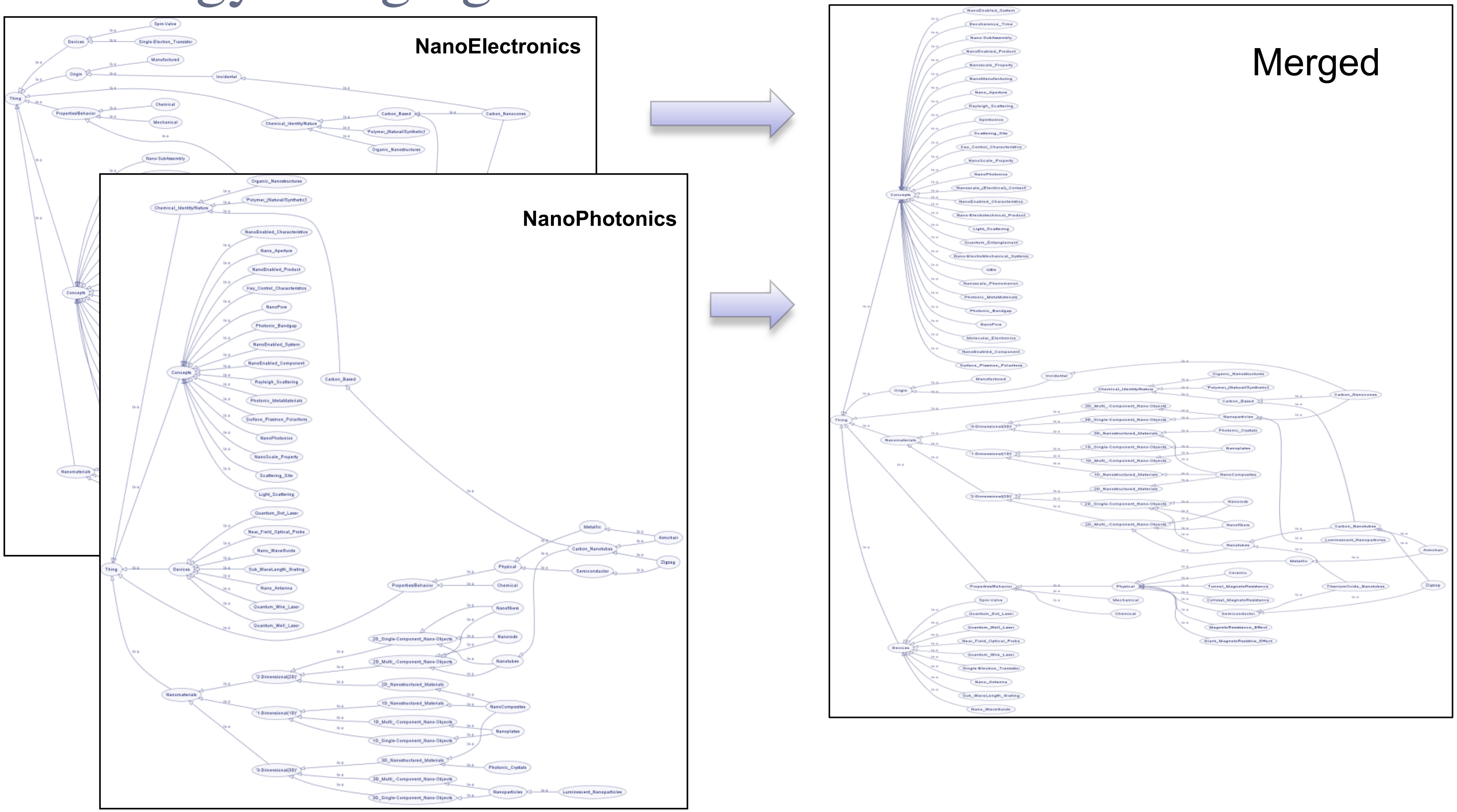
Information Retrieval
- Retrieve and concatenate textual paragraphs that are related to concepts in the basis ontology
- Stores the result set size for each concept

Keyword extraction
- Extracting phrases and terms that are prominent in the concatenated texts

Evaluation of results
- Export of results to an excel spread sheet for human inspection

Extending ontology
- Incorporating the accepted suggestions into the ontology

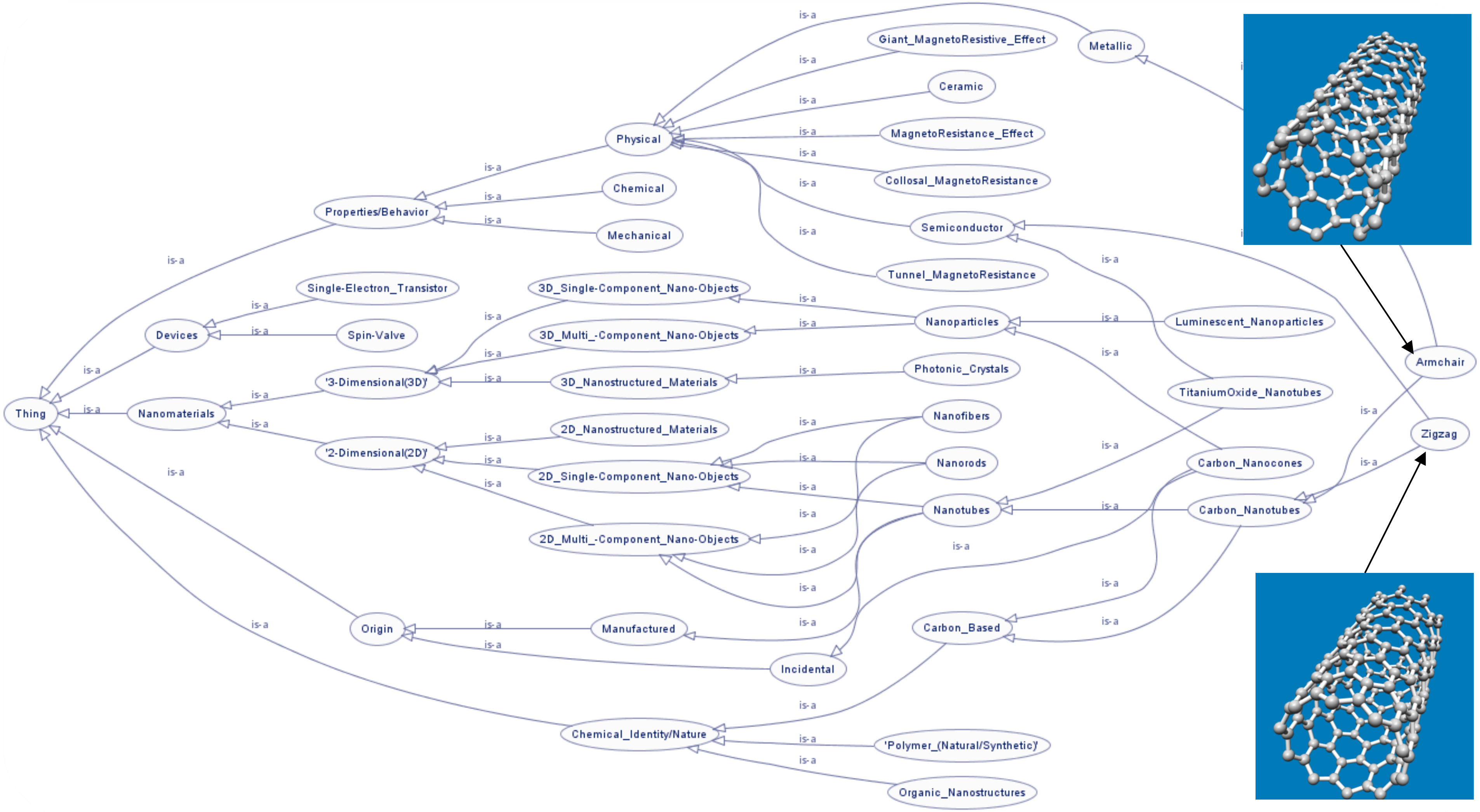
Ontology Merging



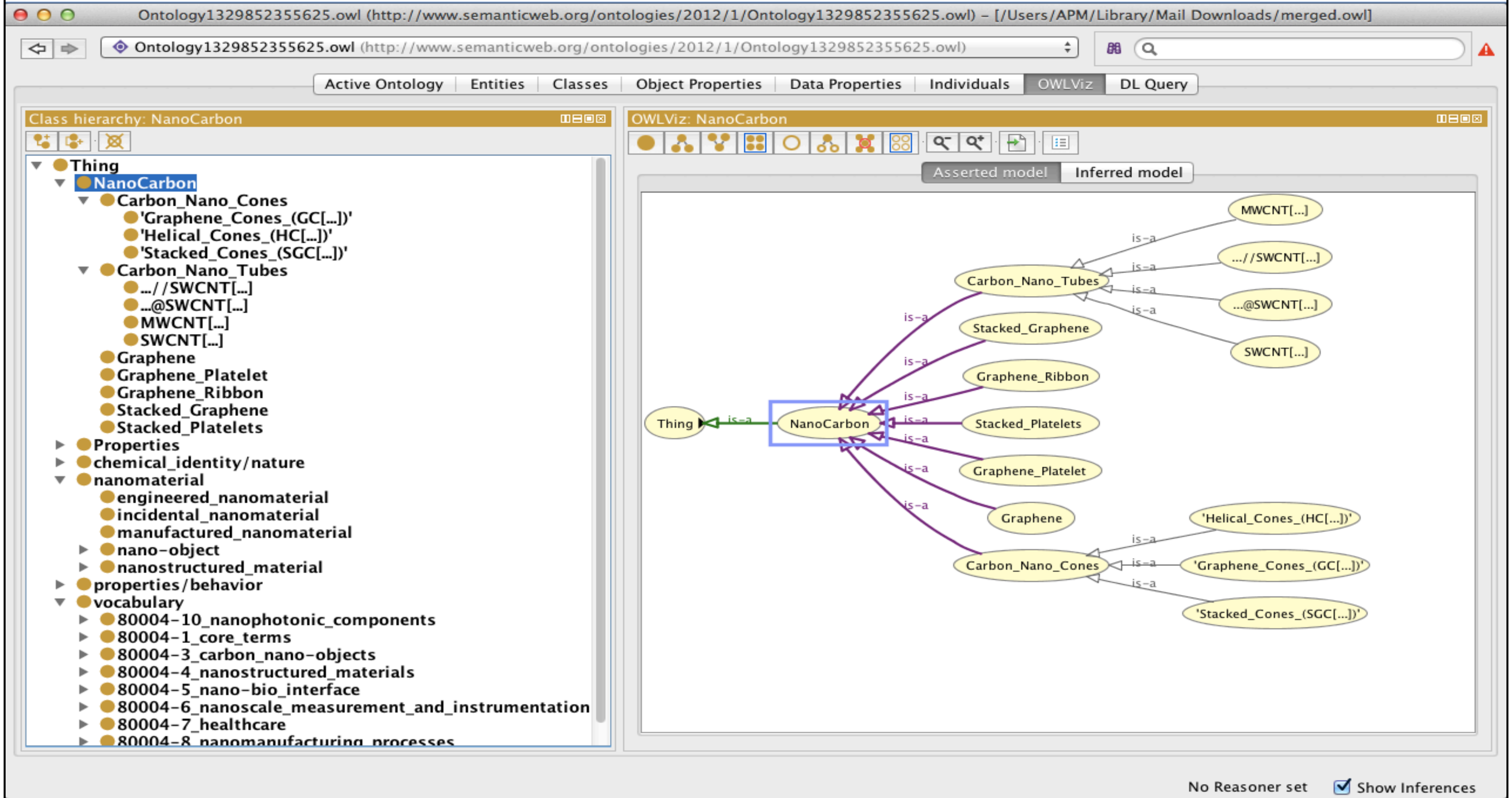
Ontology Updating

- Ontologies evolve naturally
- Most industries experience that ontologies are very dynamic and grow over time
- Manual update is complex; costly and time consuming
- Document analysis tools can suggest the removal; renaming; or inclusion of new terms in an ontology

Extending the ontology (1)



Extending the ontology (2)



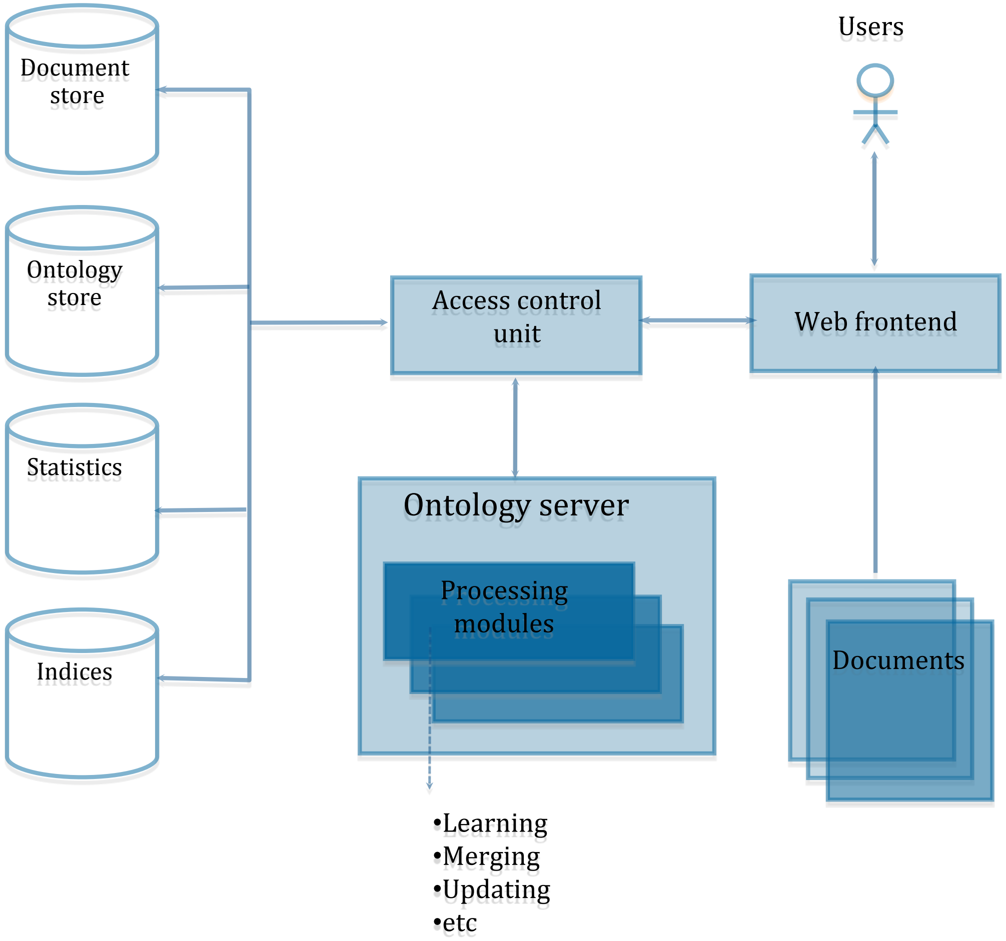
Integrating these techniques

- Learning, merging and updating ontologies are relevant for all cases of nanotechnology
- Industrial collaborators need a unified tool-supported platform integrating all of these aspects of ontology design
- Research collaborators can contribute with cutting-edge techniques and benefit from tests in real-case scenarios
- An iterative development process that gradually integrates the techniques can mitigate risks and offer real benefits to all concerned

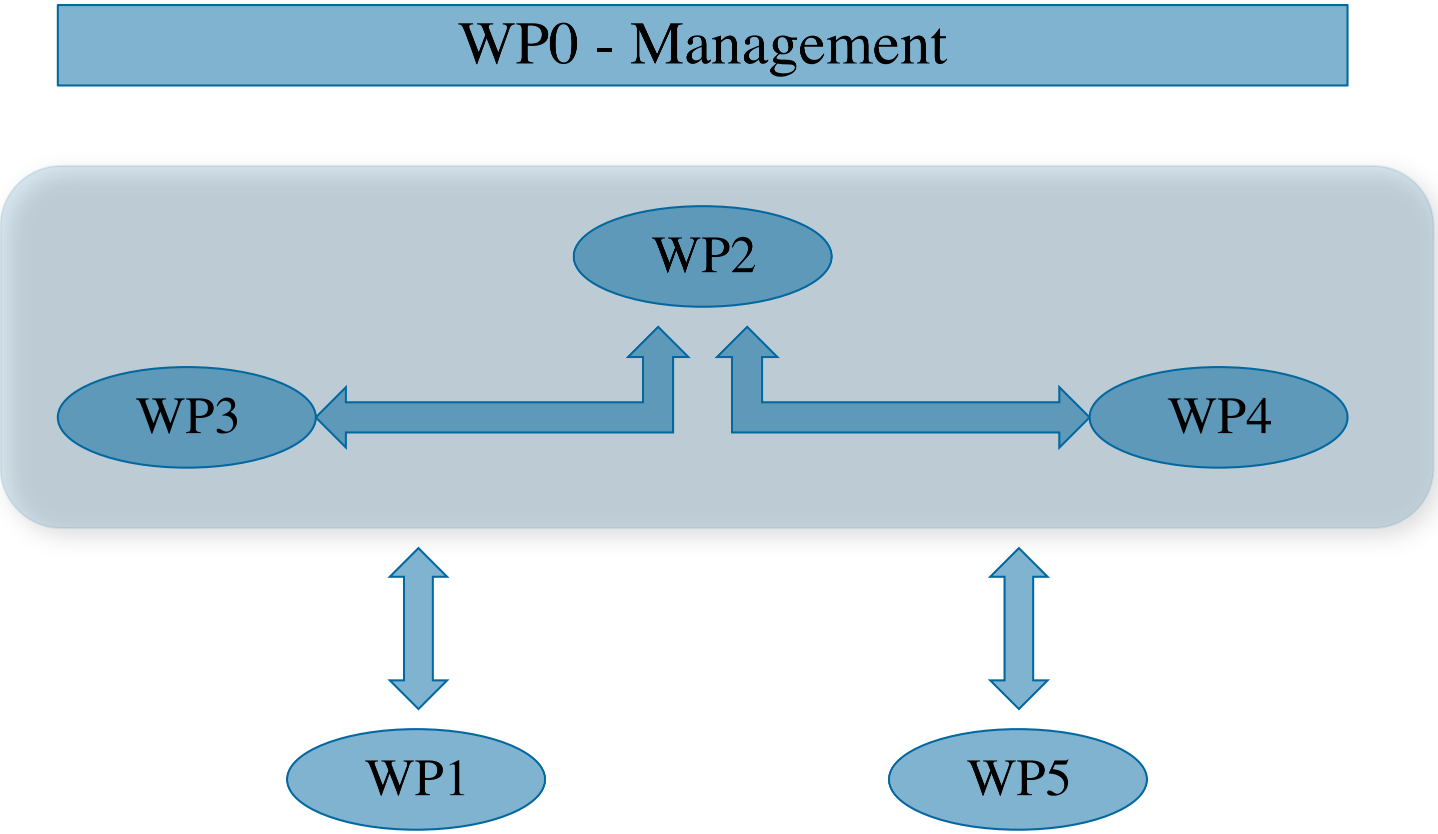
Project: Ontology Engineering and Evolution for Nanotechnology

- Goal:
  - To provide a collaborative environment for the development and use of ontologies and the integration of advanced techniques for ontology design
  - To demonstrate ontology learning in the nanotechnology domain
- Approach:
  - Development of a core basis and subsequent incorporation or more sophisticated components
  - Use of existing ontologies in nanotechnology as a case study to support the development
- Ontology basis:
  - ISO/IEC TS 80004 Nanotechnology Vocabulary Series
  - IUPAC nomenclatures (InChI)
  - Crystallographic/chemical/biological nomenclatures
  - Gene Ontology (GO) and other ontologies, e.g. NPO
- Document corpus:
  - Documents on nanotechnology in relevant fields
  - Working documents from ISO/TC 229, IEC/TC 113, CEN/TC 352, OECD WPMN

Platform architecture



Project structure



Project structure

- WP0 – Project management
  - NQCG
- WP1 – Ontology Evolution Platform
  - NQCG
- WP2 – Integrated Ontology Evolution Framework
  - Oxford/Manchester: Prof. Ian Horrocks and Prof. Uli Sattler
- WP3 – Ontology Learning and Extraction
  - KIT: Prof. Rudi Studer
- WP4 – Collaborative Ontology Engineering
  - Oxford/Manchester: Prof. Ian Horrocks and Prof. Uli Sattler
- WP5 – Ontology Engineering for the Nanotechnology Domain
  - NQCG: Dr. Henning Heiberg-Andersen

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Project structure

- WP1 – Ontology Evolution Platform
  - Specification, design and implementation of the platform
- WP2 – Integrated Ontology Evolution Framework
  - Representation language and structures
- WP3 – Ontology Learning and Extraction
  - Data acquisition, linguistic processing, ontology learning, trend-detection
- WP4 – Collaborative Ontology Engineering
  - Composition and decomposition framework for collaborative engineering
- WP5 – Ontology Engineering for the Nanotechnology Domain
  - Use case study and evaluation aspects

Integrated Ontology Evolution Framework

- Integrated ontology representation language
  - extension of OWL 2 to handle information about
    - provenance
    - trust of ontology components (e.g., axioms and modules)
    - composition of an ontology
  - so as to allow
    - representation of uncertainties
    - a more powerful OWL 2 import and export mechanism

Ontology Learning and Extraction

- Tools and techniques for detection of occurrences of ontology components (classes, individual, etc) in natural language text
  - Data acquisition: document crawlers and data infrastructure for textual knowledge
  - Linguistic processing
  - Ontology learning and mapping
  - Ontology-based trend detection
    - identify trends and emerging topics in newly published documents

Collaborative Ontology Engineering

- Development of methods that allow independent manipulation of parts of ontologies with subsequent re-integration into the overall ontology
- Ontology decomposition, version control and reconciliation
  - analysis of the logical modular structure of the ontologies
  - support for version management
  - support for conflict resolution

Conclusions

- Ontology learning should be used as an effective tool in
  - Development of standard nanotechnology terminologies and nomenclature systems
  - Maintenance of standard nanotechnology terminologies and nomenclature systems
  - Harmonization of different standard nanotechnology terminologies and nomenclature

- Collaborative ontology engineering platform can effectively assist ICSU
  - Construct and maintain nomenclature systems for nanoscience and nanotechnology
  - Collaborative environment to support the use and development of nano ontologies
  - Internet platform for collaboration and cooperation in nano research and development

- A broad representation of experts should take part in this work
  - ICSU, CODATA and Scientific Unions like IUPAC
  - Materials Research Societies
  - ISO/TC 229 and IEC/TC 113
  - OECD Working Party on Manufactured Nanomaterials and WPN
  - IP5 Foundation Projects (EPO, JPO, KIPO, SIPO, USPTO)
  - World Intellectual Property Organization (WIPO)
  - National academies of science and national standards development organizations
  - Organizations involved in developing classifications for nanotechnology
  - Leading scientific journals and publishers in relevant domains