R-NANO Research Unit of Advanced, Composite, Nano-Materials & Nanotechnology

Characterisation Ontology
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What is needed for Materials Characterisation Ontology

- persistent unique identifiers materials science resources;
- metadata standards for describing samples, processes, properties;
- common semantic models/ontologies to enable mapping between database schemas, information integration and semantic;
- laboratory information and provenance capture systems that capture the processes both in the laboratory as well as in the post-processing of the data.

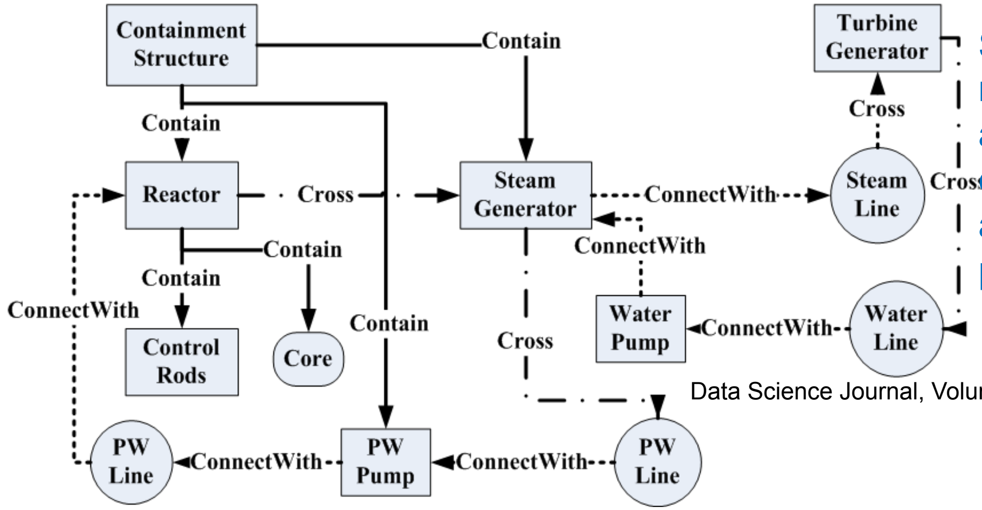
Materials Characterisation Ontology provides:

- rich machine-processable semantic descriptions;
- formal definitions of domains by defining classes, properties and relationships between them in Web Ontology Language (OWL);
- a basis to enable reasoning or deduction of new information. Ontologies enable semantic interoperability between resources, services, databases, and devices via inter-related knowledge structures.

Materials Characterisation Ontology will contribute to:

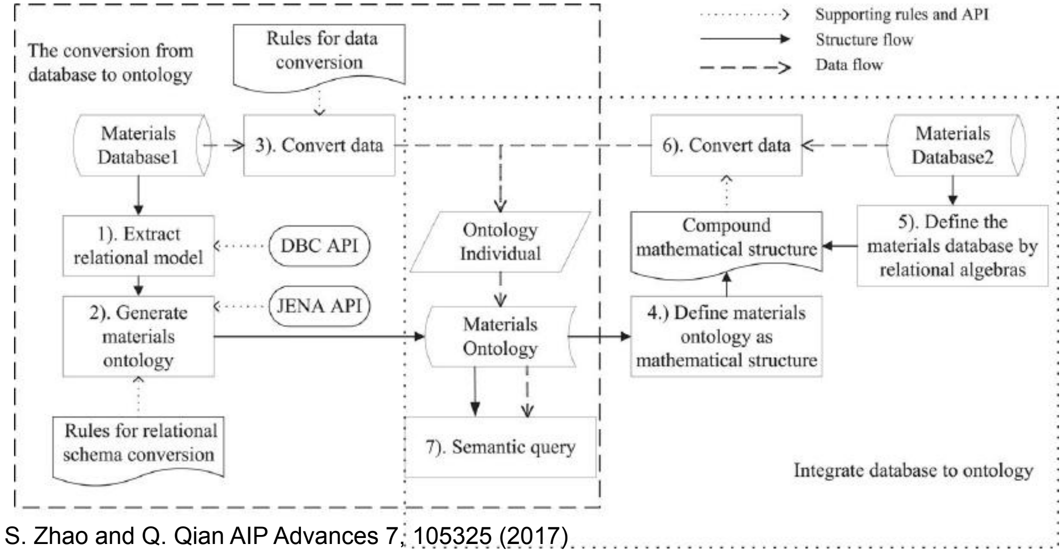
- Characterization digital data
- High throughput experiments
- High throughput characterization
- Cost reduction
- Reliable results
- Standard operation procedures (SOPs)
- Design of materials with improved characteristics
- Classification of techniques and acceleration of results
- Uniform query interface

Simplified examples



Simplified relationships among the components of a nuclear power plant

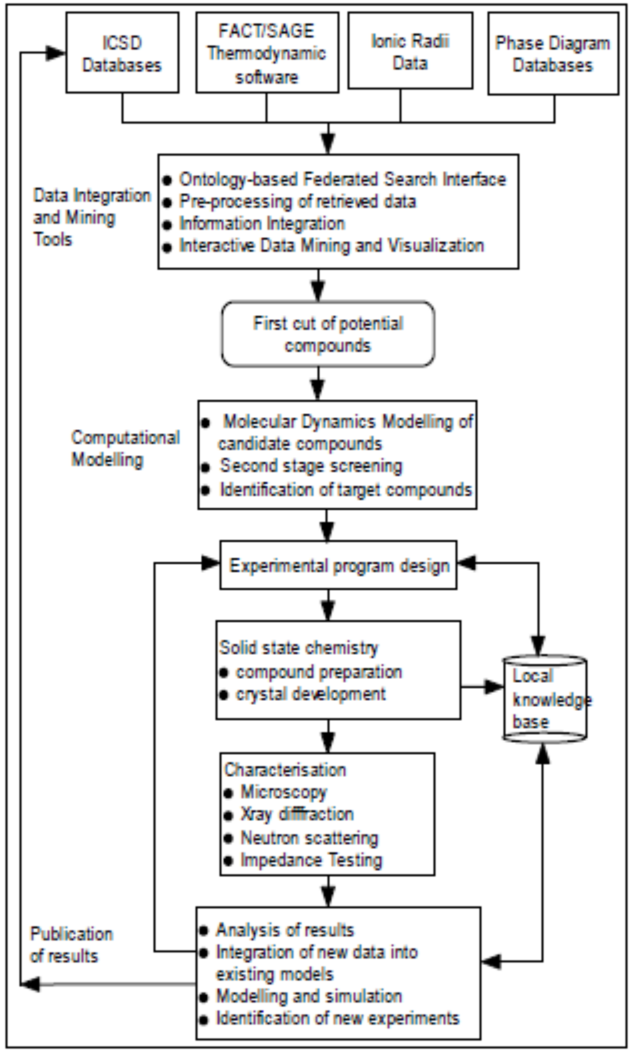
Data Science Journal, Volume 12, 13 January 2014



System architecture of the ontology based heterogeneous databases integration

S. Zhao and Q. Qian AIP Advances 7, 105325 (2017)

searching for novel oxygen ion conducting materials that can operate more efficiently at lower temperatures for longer durations



Cheung, Kwok, Drennan, John and Hunter, Jane (2008). Towards an Ontology for Data-driven Discovery of New Materials. In: Semantic Scientific Knowledge Integration AAAI/SSS Workshop, Stanford University, Palo Alto, CA, (9-14). 26-28 March, 2008.

Materials Characterisation Ontology Building

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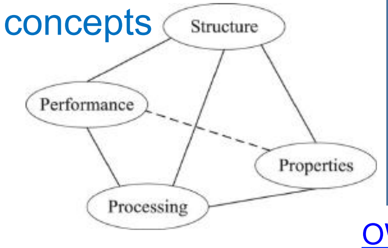
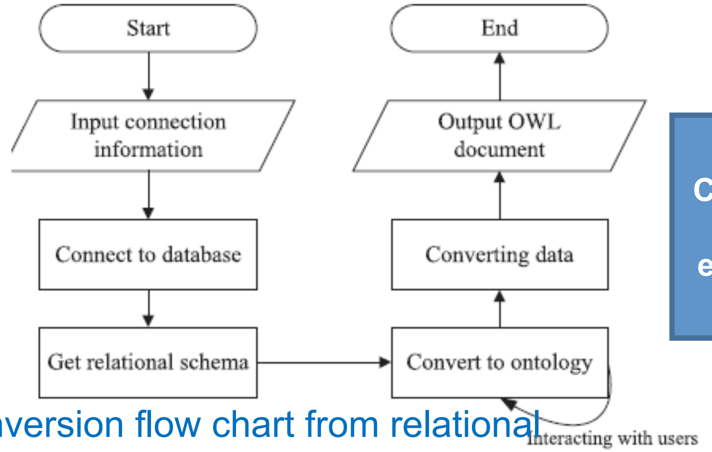
Materials science tetrahedron for root concepts



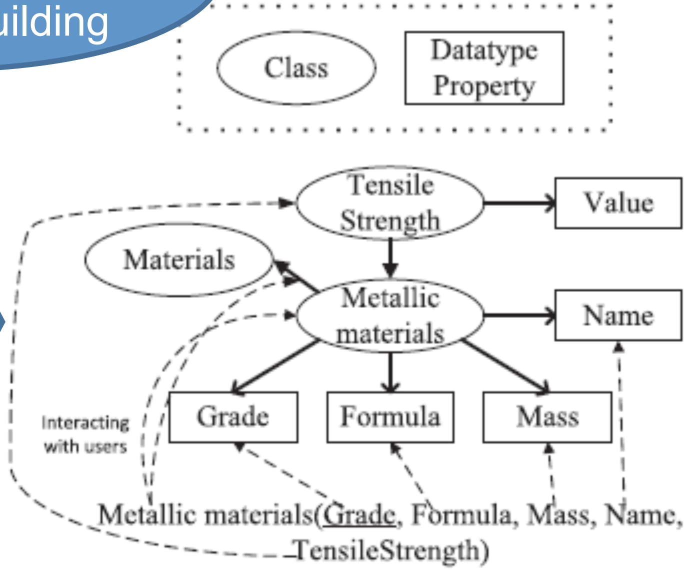
owl:Class
material, structure, properties, processing and performance

OWL Web Ontology Language Reference

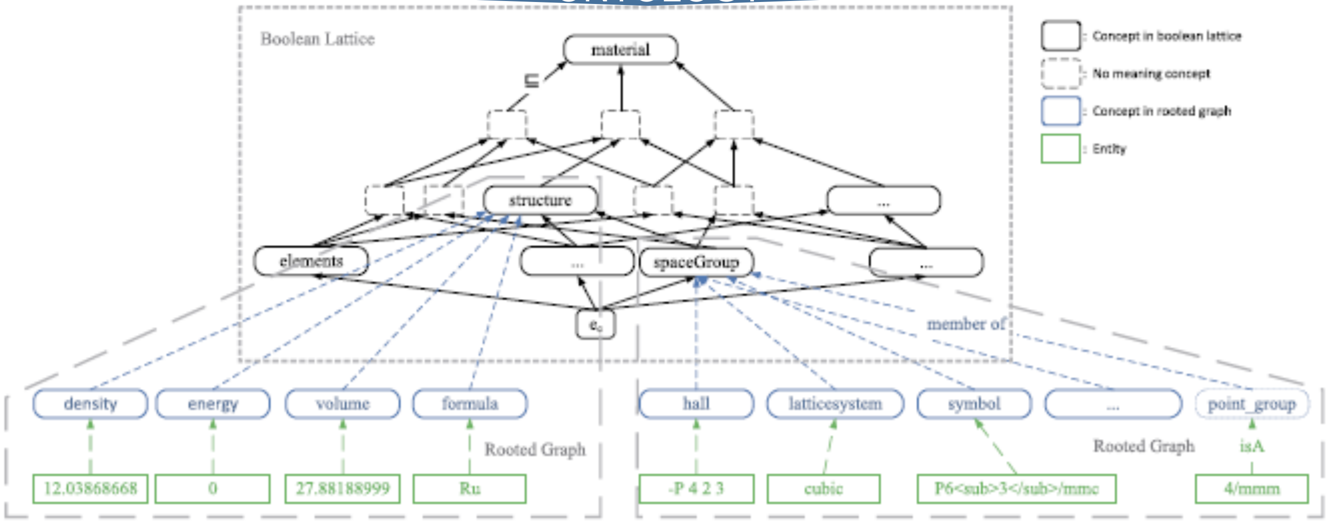


Conversion flow chart from relational database to OWL based ontology

Conversion example



INTEGRATE DATABASES TO ONTOLOGY



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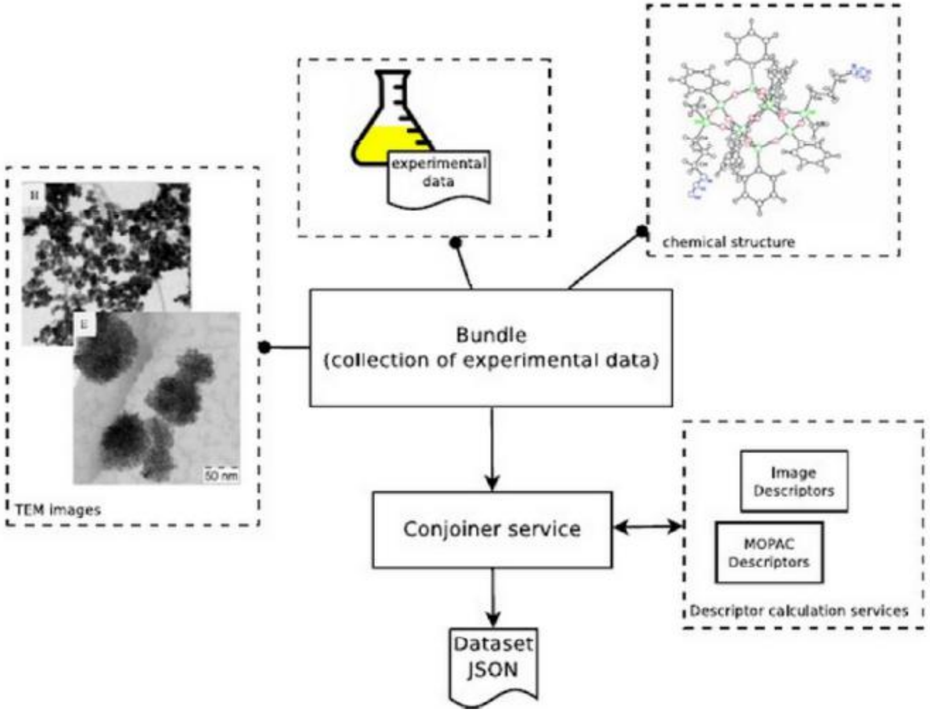
The example of Jacpot-enanomapper



Schematic representation of Jaqpot Quattro's Conjoiner service. Heterogeneous data is processed and standardised for the algorithm services.

NTUA's implementation of ontology in combination to an application tool (https://enanomapper.net/) which can:

- **Predict adverse effects of engineering nanomaterials (ENM)**
- **Focus on risk management and safety assessment of ENM**
- **Promote even more the applications of ENM**
- **Cover the broad range of applications in multiple fields**
- **Aid in the establishment of in silico approaches thus being cost and time effective**
- **Be open source**
- **Enhance the collaboration of modeling and research groups**
- **Harmonize the databases, ontology and modeling infrastructures**
- **Reduce the animal testing**
- **Aid in the design of new safer products of reduced risk**

Chomenidis C, Drakakis G, Tsiliki G, Anagnostopoulou E, Valsamis A, Doganis P, Sopasakis P, Sarimveis H, J Chem Inf Model. 2017 Sep 25;57(9):2161-2172