

Demonstrator 19: Materials Databases Integration using the Materials Design Ontology

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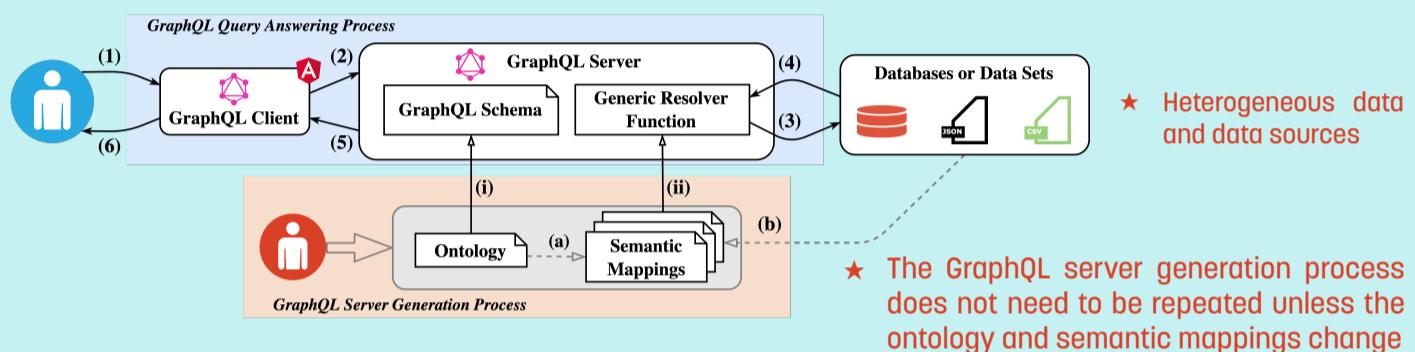
Introduction

In the materials design domain, much of the data from materials calculations is stored in different heterogeneous databases with different data and access models. Therefore, integrating data from different sources is challenging. As ontology-based access and integration alleviates such issues, we developed the Materials Design Ontology (MDO) for increasing interoperability among computational materials databases. Then we introduced a generic framework (OBG-gen) for using GraphQL in which a global domain ontology informs the generation of a GraphQL server that answers requests by querying heterogeneous data sources. By using MDO in this framework, we can generate a GraphQL server for data integration among heterogeneous computational materials databases. Additionally, we introduced a method (ToPMine-FTCA) for ontology extension and applied it in the materials science domain.

Approaches

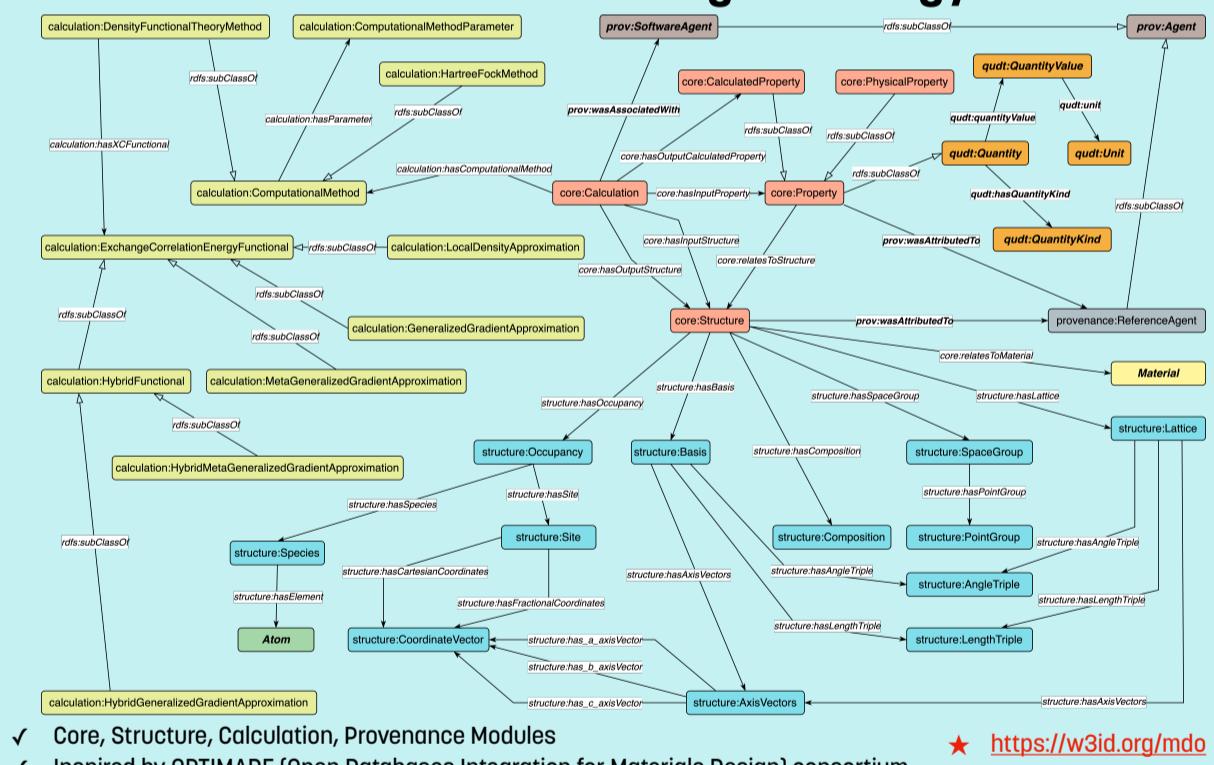
- ✓ A GraphQL-based framework for data access and data integration
- ✓ Ontology-based GraphQL server generation (OBG-gen)
 - ✓ Ontology-based GraphQL schema generation
 - ✓ A generic resolver function
- ✓ Materials Design Ontology (MDO)
- ✓ An approach for ontology extension (ToPMine-FTCA)

GraphQL-based Data Integration and OBG-gen

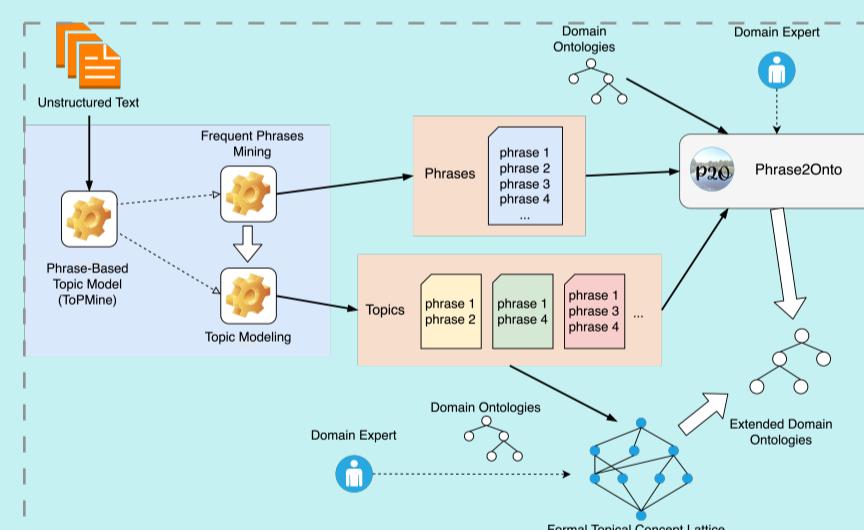


- ✓ Given an ontology and semantic mappings, after steps (i) and (ii), a GraphQL server is ready to setup
- ✓ Documented domain-interested queries (1) are translated to GraphQL queries validated against the schema (2)
- ✓ The generic resolver function accesses the data sources (3) and combines, structures the data (4)
- ✓ Finally, the result is returned to the user (5, 6)

MDO (Materials Design Ontology)



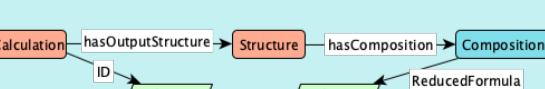
ToPMine-FTCA



- ✓ Phrase-based topic model, formal topical concept analysis, domain expert validation
- ✓ Applied for extending NanoParticle Ontology, eNanoMapper ontology and MDO
- ✓ Phrase2Onto user interface supporting domain expert validation

GraphQL Query Example

- ✓ Setup a GraphQL server based on MDO by using OBG-gen
- ✓ List Calculations (integrated and semantic query)
 - Get all the calculations where reduced chemical formula contains the Titanium (Ti) element
 - Contain several query fields



Client-Side and Server-Side

The screenshot shows the Client-Side and Server-Side interface:

Client-Side: An Angular-based Web application with a search bar ('elements CONTAINS "Ti"') and a 'Query' button. Below it is a table of IRI links:

IRI	Action
http://example.com/calculation/10676	Download
http://example.com/calculation/8390	Download
http://example.com/calculation/31023	Download
http://example.com/calculation/19423	Download
http://example.com/calculation/27974	Download

Server-Side: The corresponding GraphQL query code:

```
query calculation_query{  
  CalculationList(  
    filter:  
      { hasOutputStructure:  
        { hasComposition:  
          { ReducedFormula: { _like: "%Ti%" } } } }  
  )  
  {  
    ID  
    hasOutputStructure{  
      hasComposition{  
        ReducedFormula  
      }  
    }  
  }  
}  
Items per page: 5 1 - 5 of 55 < < > >>
```

Notes:

- ✓ Angular-based Web application
- ✓ User-specified query entity and filter expressions
- ✓ Avoid writing filter expressions in the GraphQL syntax
- ✓ Download result as json files

Ongoing and Future Work

- ✓ Ontology alignment in the materials science domain
- ✓ Natural Language-based queries