

OntoChem: Representing Chemical Mechanisms using OWL Ontologies

Problems with the Current Approach

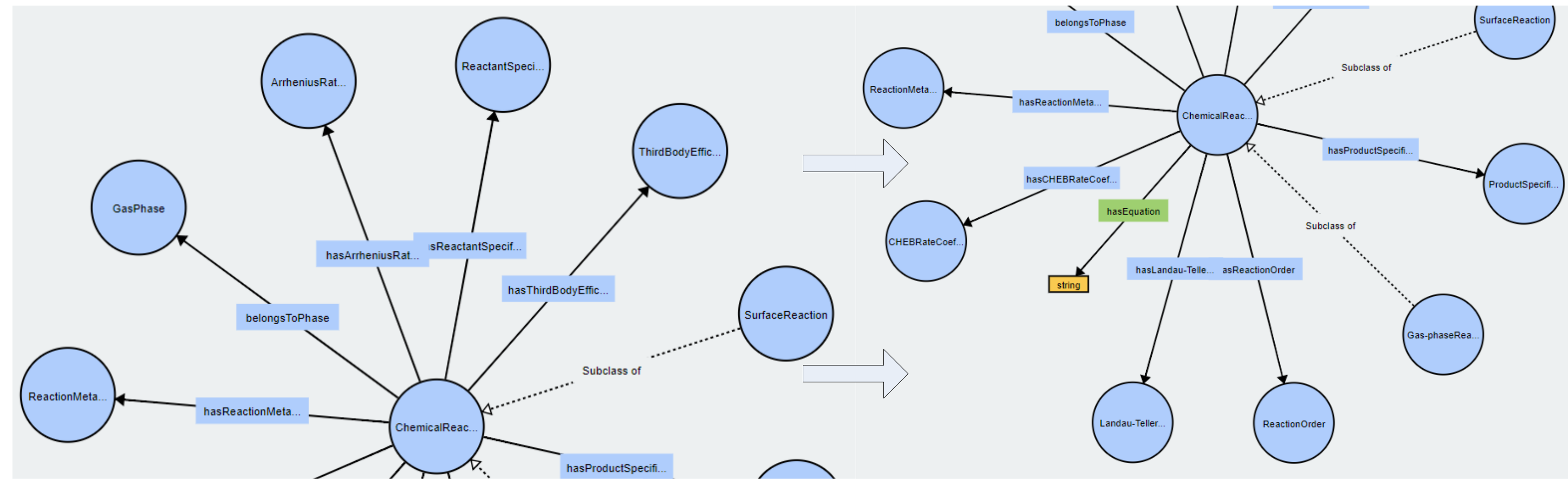
- Fragmentation/heterogeneity of data sources and tools
- Inconsistencies between data

Examples

• Inconsistencies in chemical models

- ❖ Discrepancies (up to 100 kJ/mol) in enthalpies of formation of same species in different models
- ❖ Many orders of magnitude discrepancy in the rates of the same chemical reactions in different models

Ontological Modelling of Chemical Reactions



The Power of an Ontology

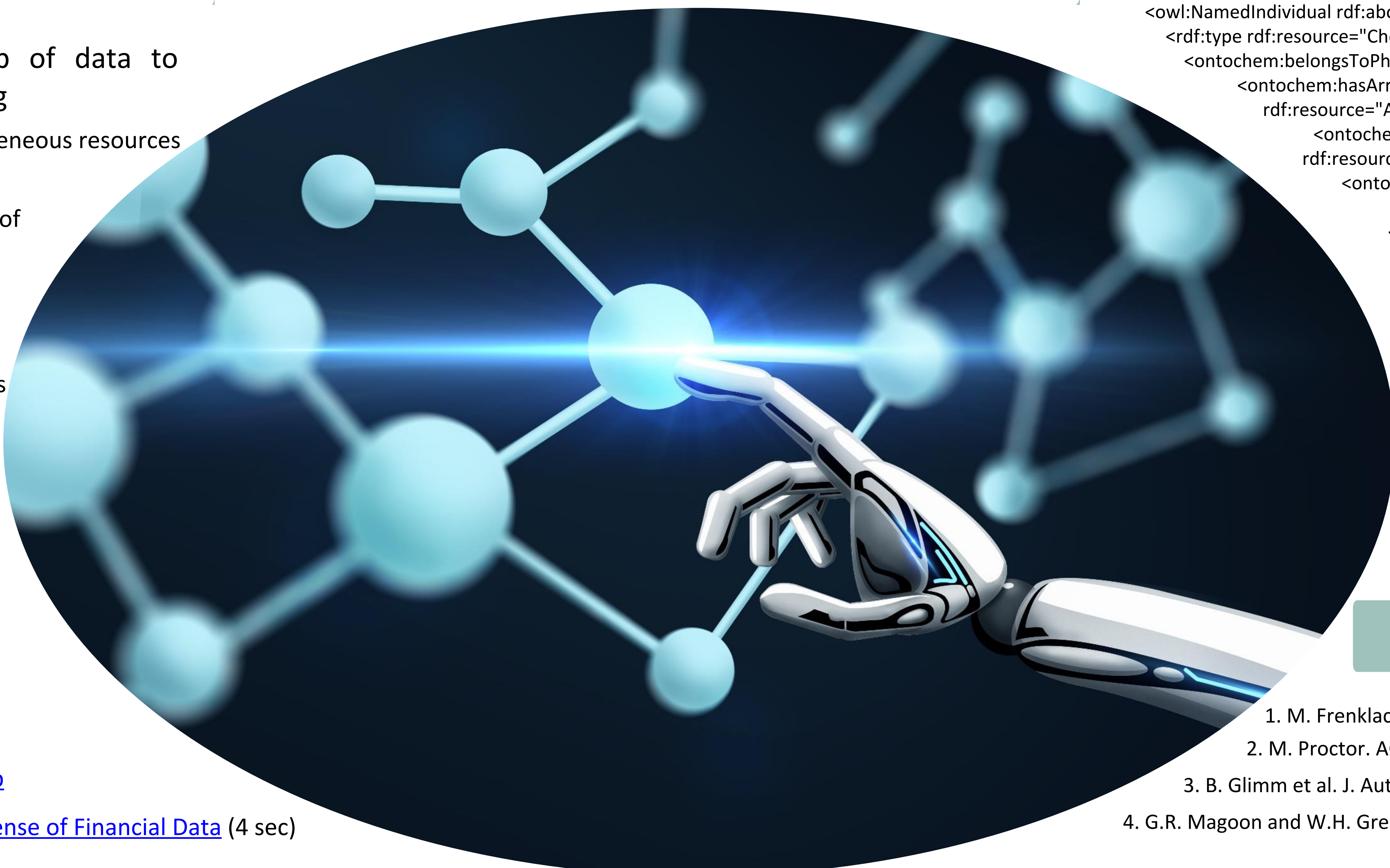
Machines do the work

- An ontology sits on top of data to ensure a common meaning
 - ❖ Integrate and query heterogeneous resources within and across a domain
 - ❖ Natural language processing of unstructured literature
- Simplifies software engineering
 - ❖ Easy development of services
 - ❖ Reuse of existing resources
 - ❖ Advanced query
 - ❖ Automation of tasks
- Extensible
 - ❖ Re-use and extend existing ontologies
 - ❖ Standardisation via W3C

Examples

- ❖ How [Google powers the Web](#)
- ❖ FIBO: [A New Way to Make Sense of Financial Data](#) (4 sec)

Molecule Formulae Meet Artificial Intelligence



OWL Representation of Reactions

```
<owl:NamedIndividual rdf:about="ChemicalReaction_25796139006455_1">
  <rdf:type rdf:resource="ChemicalReaction"/>
  <ontochem:belongsToPhase rdf:resource="Phase_25796138875779"/>
  <ontochem:hasArrheniusRateCoefficient
    rdf:resource="ArrheniusRateCoefficient_25796139015942"/>
  <ontochem:hasProductSpecification
    rdf:resource="ProductSpecification_25796139137857"/>
  <ontochem:hasEquation rdf:datatype="xsd:string">
    O2 + H [=] O + OH</ontochem:hasEquation>
  <ontochem:isReversible rdf:datatype="
    xsd:string">yes</ontochem:isReversible>
</owl:NamedIndividual>
```

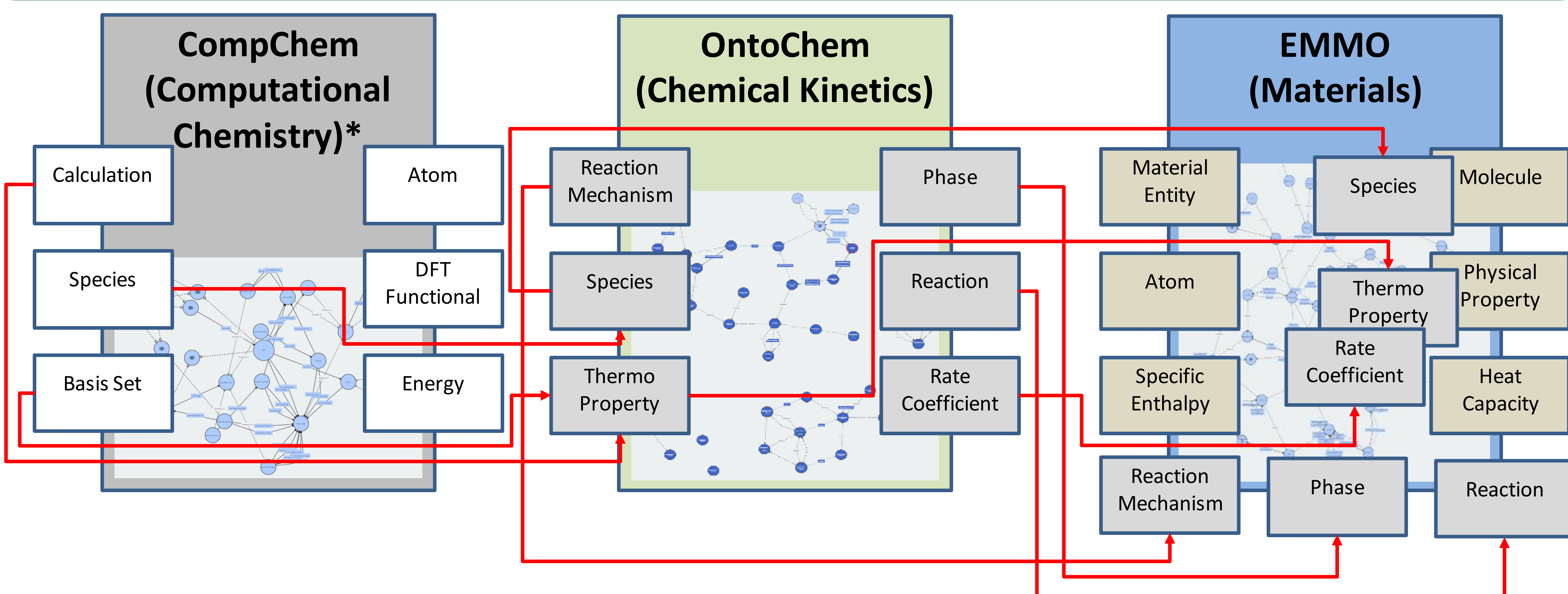
Acknowledgements

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References

1. M. Frenklach. Proc. Combust. Inst. 31 (2007), 125–40.
2. M. Proctor. AGTIVE'11, Springer-Verlag (2012), pp. 2–2.
3. B. Glimm et al. J. Automat. Reason. 53 (3) (2014), pp. 245–269.
4. G.R. Magoon and W.H. Green. Comput. Chem. Eng. 52 (2013), 35–45.

OntoChem with CompChem and EMMO



* This is a slightly modified version of the Gainsville Core Ontology.