iDMT
Innovation Centre in Digital Molecular Technologies

Access to data in a fully digital chemical lab

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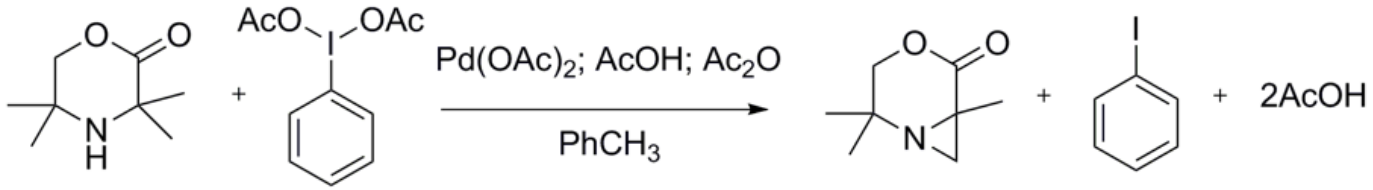
EUROPEAN UNION
European Regional Development Fund

UNIVERSITY OF CAMBRIDGE
AstraZeneca
SHIONOGI

What is Chemical Data

- Human readable vs machine readable chemical information




```
RInChI=0.03.1S/C10H11IO4/c1-8(12)
14-11(15-9(2)13)10-6-4-3-5-7-10/h3-7H,
1-2H3!C8H15NO2/c1-7(2)5-11-6(10)8(3,4)9-7/h9H,
5H2,1-4H3<>C2H4O2/c1-2(3)4/h1H3,(H,3,4)!C6H5I/
c7-6-4-2-1-3-5-6/h1-5H!C8H13NO2/c1-7
(2)5-11-6(10)8(3)4-9(7)8/h4-5H2,1-3H3<>2C2H4O2.
Pd/c2*1-2(3)4;/h2*1H3,(H,3,4);/q;;+2/p-2!C2H4O2/
c1-2(3)4/h1H3,(H,3,4)!C4H6O3/c1-3(5)7-4(2)
6/h1-2H3!C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3/d+
```

```
ProcAuxInfo=$$PAI0.01|1:2|1;1|2;1;
1|393|6E5|60:0.06;120:0.14;180:0.20;
240:0.32;300:0.40;360:0.52;420:0.70;
480:0.90;540:1.0;600:1.0|?;?;0.90|8.3E-7;
8.3E-7|0;0;0|4.2E-9:m:f;8.3E-6:m:f;
1.7E-6:m:f;1.5E-4:m:f|1E-5
```

Jacob et al. J Cheminform (2017) 9:23

- Reactants (nature and relevant properties)
- Products (nature and relevant properties)
- Reagents (solvent, catalyst, ligand, magic dust…)
- Reaction conditions (T, P, residence time, etc)
- Yield of main product as a function of time

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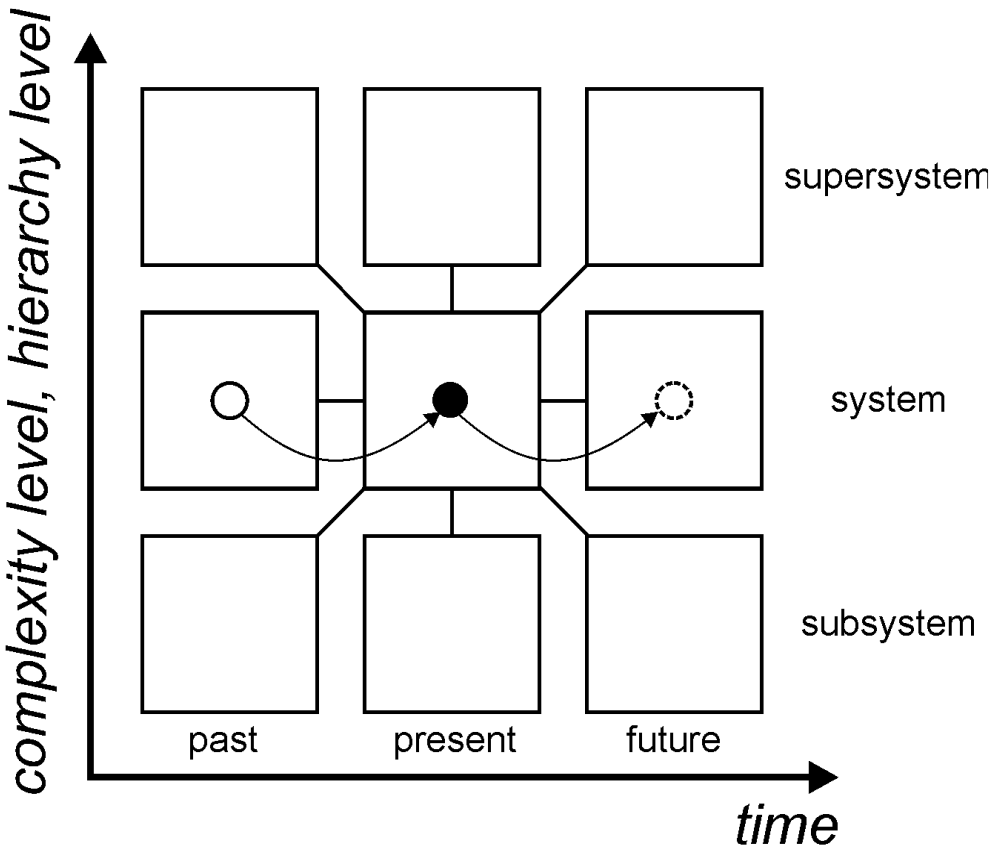
Chemical Reaction as a System



Description of interactions within complex hierarchical systems requires understanding of their intrinsic and emerging properties and their relation to scale and time.

The same description can be applied to a chemical reaction:

- Invariant properties of molecules
- Context-dependent properties of molecules
- Properties & phenomena dependent on time
- Properties & phenomena dependent on scale

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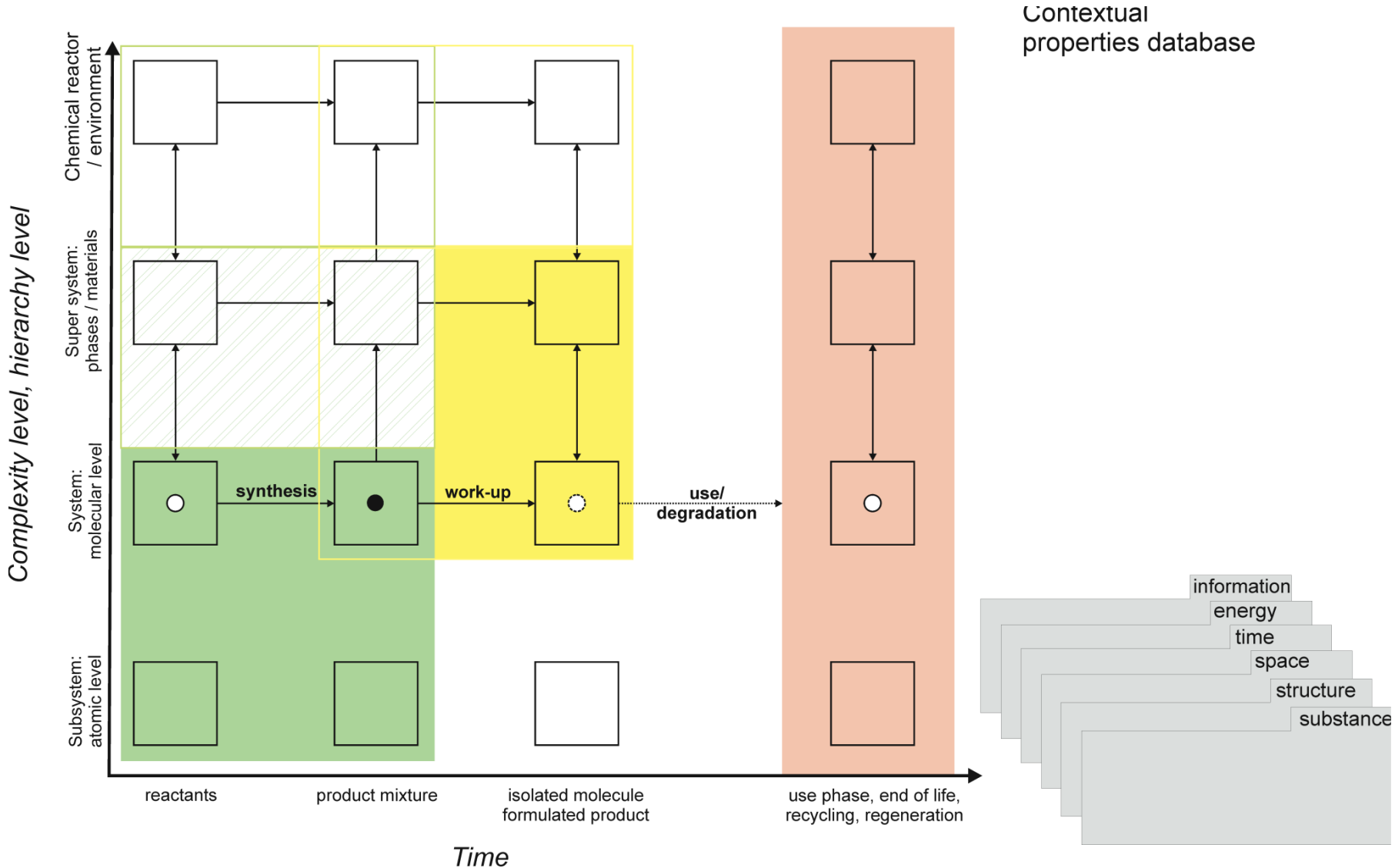
Chemical Reaction Context



Chemical Engineering & Processing. Process intensification, 50 (2011) 1027-1034

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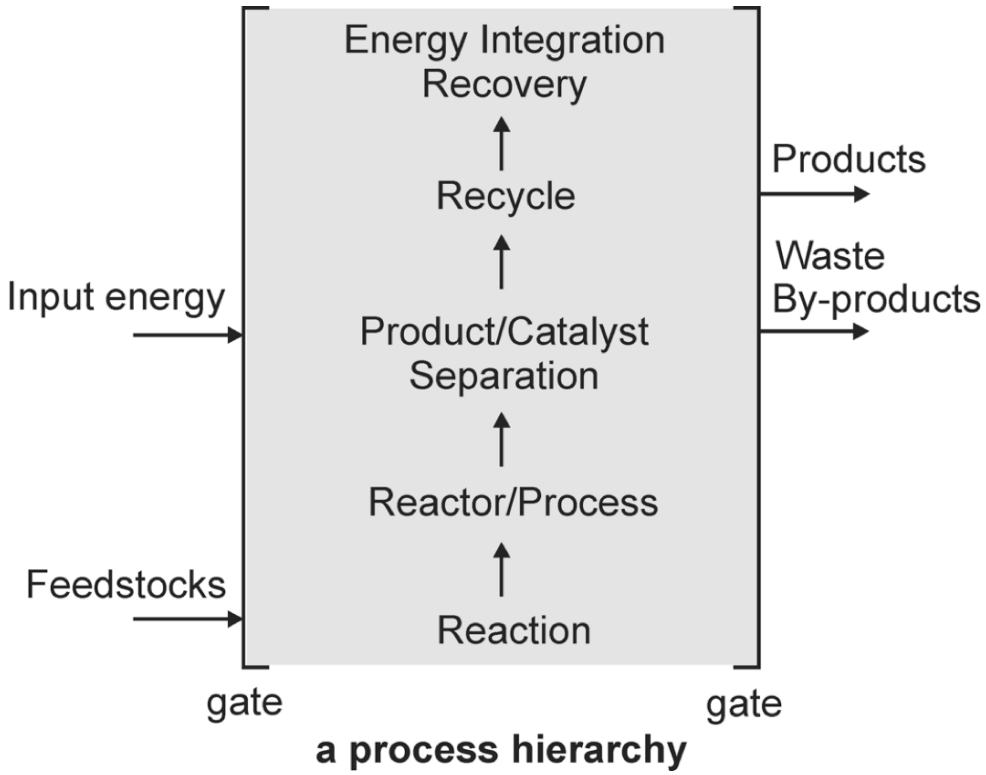
Process as a Hierarchical System



a process hierarchy

Data requirements for describing a process:

- All chemical species and their physico-chemical properties (under conditions in storage, feed, all process stages and final storage – multiple instances of specific 'context').
- All reactions (pathways [mechanisms], kinetics).
- Mass transfer (phases, rates of mass transfer in specific equipment).
- Heat transfer (phases, properties of fluids, rates of heat transfer in specific equipment).
- Impact of hydrodynamics on any properties.
- Neighbouring systems (for mass and energy integration).

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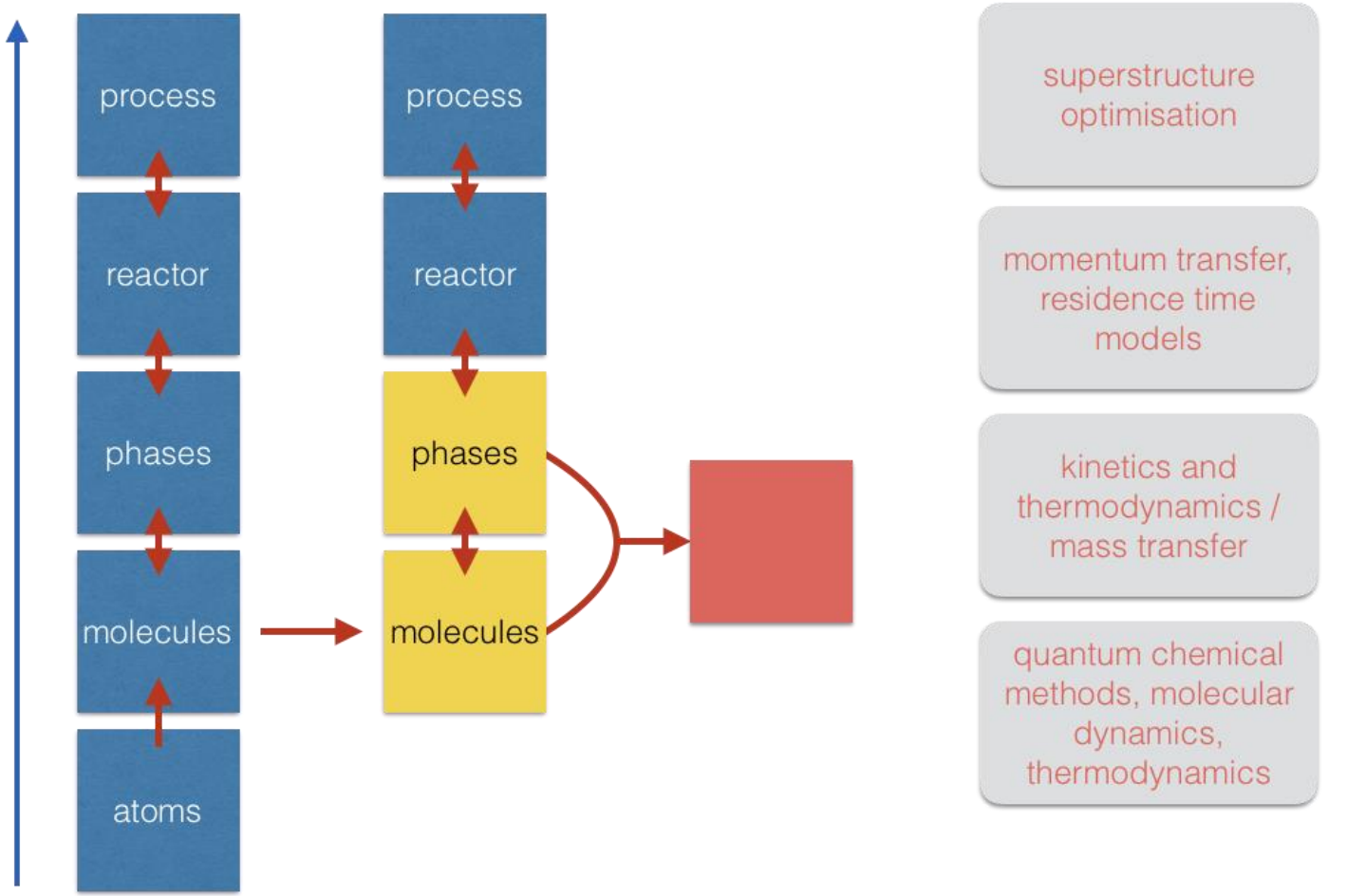
Process Context = Reaction + Equipment + Infrastructure



superstructure optimisation

momentum transfer, residence time models

kinetics and thermodynamics / mass transfer

quantum chemical methods, molecular dynamics, thermodynamics

Reactants ***Products*** ***Use phase*** → *End of Life*

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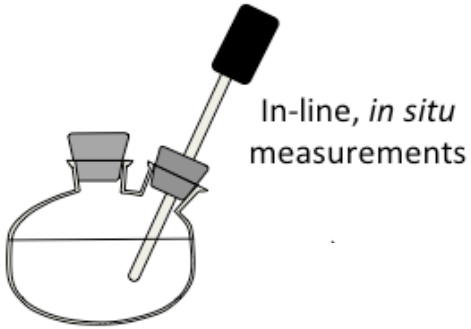
How to Manage Data in a Fully Digital Lab

Experiment Coding
Translation of DoE into automated experiment formulation
Equipment ontology



Automated experimental system

Data Ontology
Classification of experimental observations

Chemical Data:
Reaxys
ELNs
QC results
Reaction mechanisms
Thermodynamic properties
Molecular descriptors
Environmental impact factors
Toxicity data
….

Chemical Ontology
Relationships between data elements

Chemical Knowledge:
Kinetic model hypothesis
Formulation properties hypothesis
Bio-activity model
Reactivity pattern hypothesis
….

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What Should iDMT Build?

Innovation Centre in Digital Molecular Technologies (iDMT) is a project co-funded by the European Regional Development Fund (ERDF), AstraZeneca, Shionogi and the University of Cambridge.

iDMT is an open innovation platform for collaborative R&D projects in the areas of:

- Artificial Intelligence in Molecular Technologies
- Robotic Equipment for Chemical Synthesis
- Algorithms and Tools for Digital Process Development

- High-throughput experiments will generate data (reaction outcomes)
- Formulation robot will generate data (formulation properties)
- Flow synthesis robots will generate data (optimal reaction conditions)
- QC methods and MD methods will generate data
- ML / AI algorithms will use the data
- What is the architecture for storing and maintaining the data?

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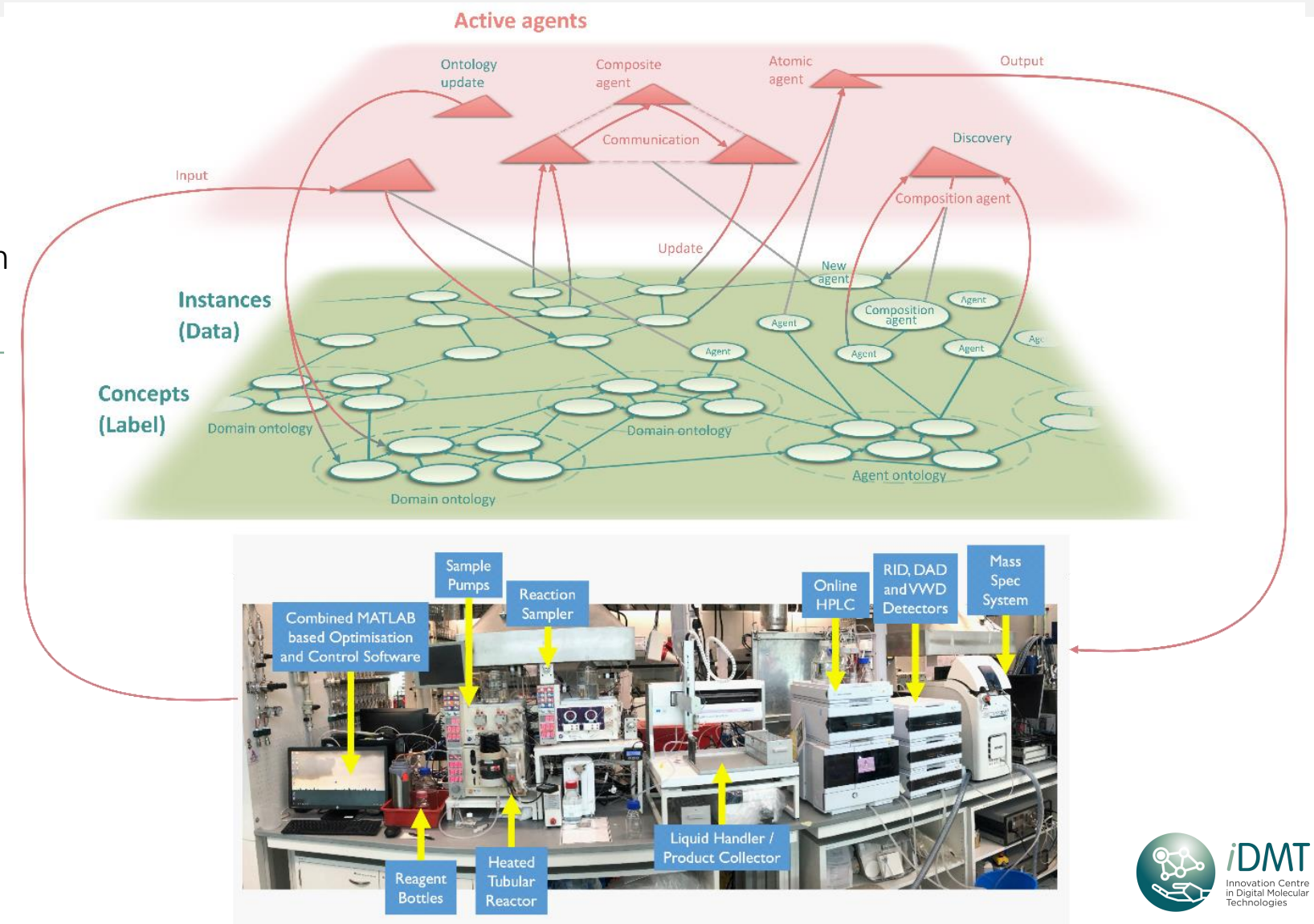
COMO/CARES/PIPS Knowledge Graph Technology

Who has the knowledge to develop such architecture

Partnership:

- Prof. Markus Kraft / COMO Group
- PIPS Data2Knowledge Project



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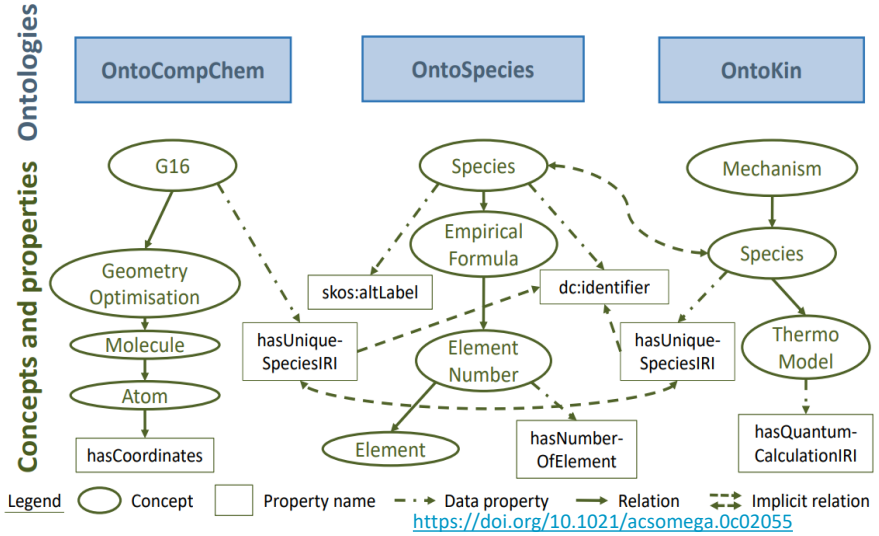
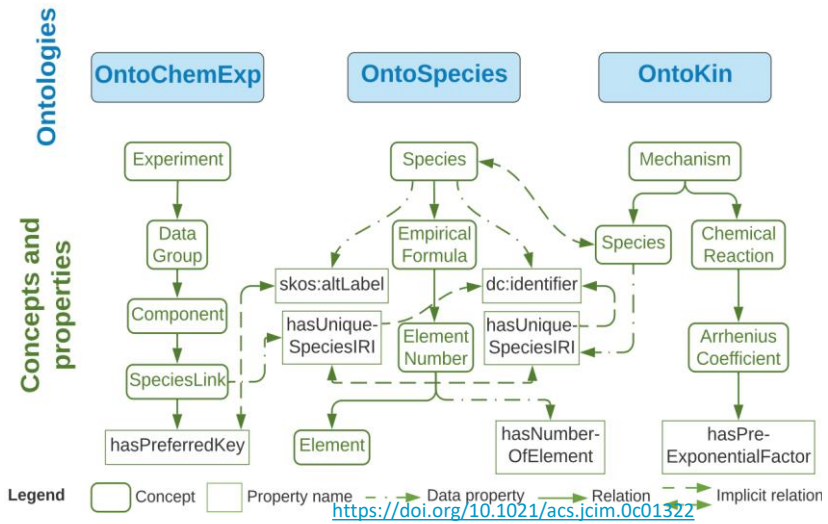
COMO/CARES Knowledge Graph Technology

- OntoSpecies – chemical species identification https://doi.org/10.1016/j.compchemeng.2020.106813
- OntoKin – chemical kinetic mechanisms https://doi.org/10.1021/acs.jcim.9b00960
- OntoCompChem – quantum chemistry calculation results https://doi.org/10.1021/acs.jcim.9b00227
- OntoChemExp – chemistry experiment data https://doi.org/10.1021/acs.jcim.0c01322

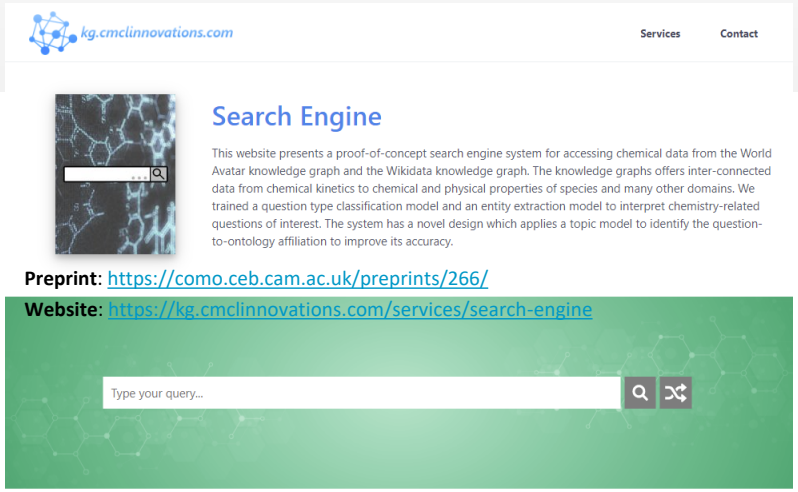
- All above ontologies are linked via OntoSpecies for unique chemical species identification



https://doi.org/10.1021/acsomega.0c02055



https://doi.org/10.1021/acs.jcim.0c01322



Preprint: https://como.ceb.cam.ac.uk/preprints/266/

Website: https://kg.cmclinnovations.com/services/search-engine

Example Questions

- General Computational Quantum Chemistry
- Kinetics & Thermodynamic
- Reactions & Mechanisms
- Molecule Classes
- Conditional Queries
- Queries by SMILES
- Molecule Properties

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