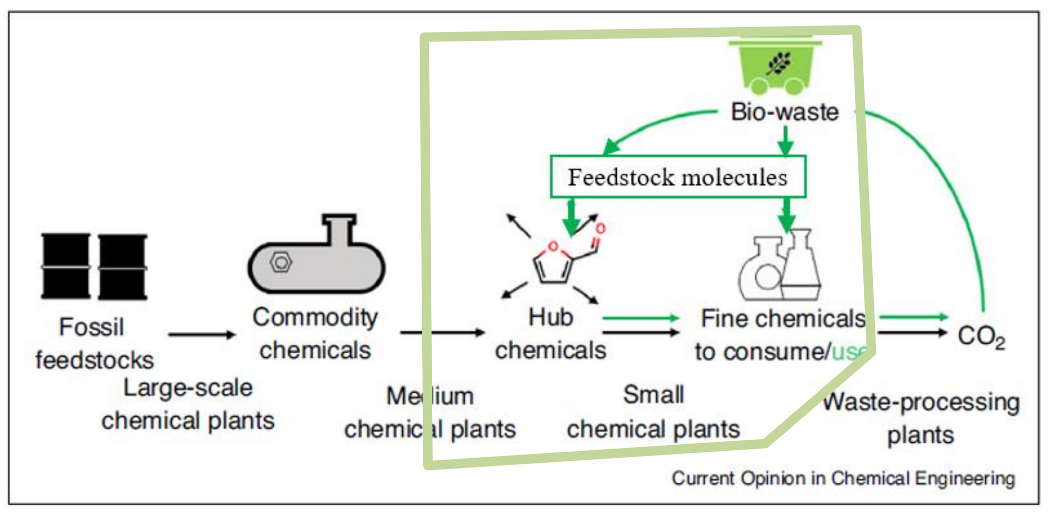
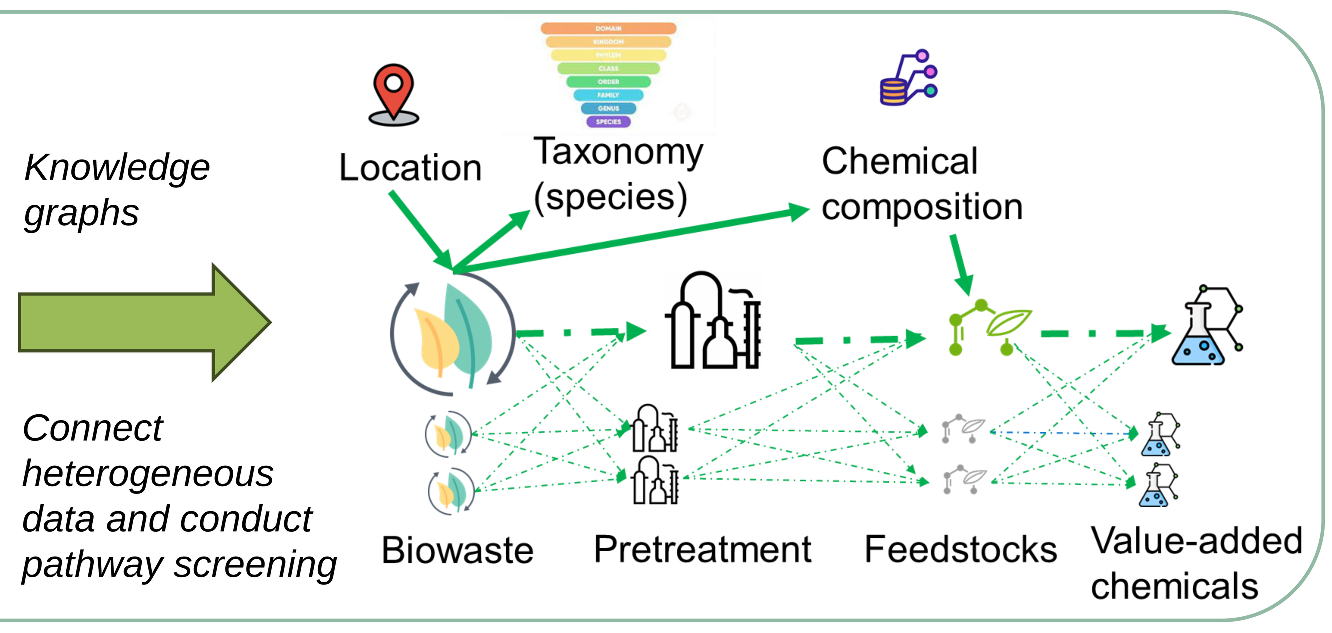
Knowledge graphs for the biowaste-to-chemicals domain

Adarsh Arun[1,2], Zhen Guo[2,3], Alexei Lapkin[1,2,3]

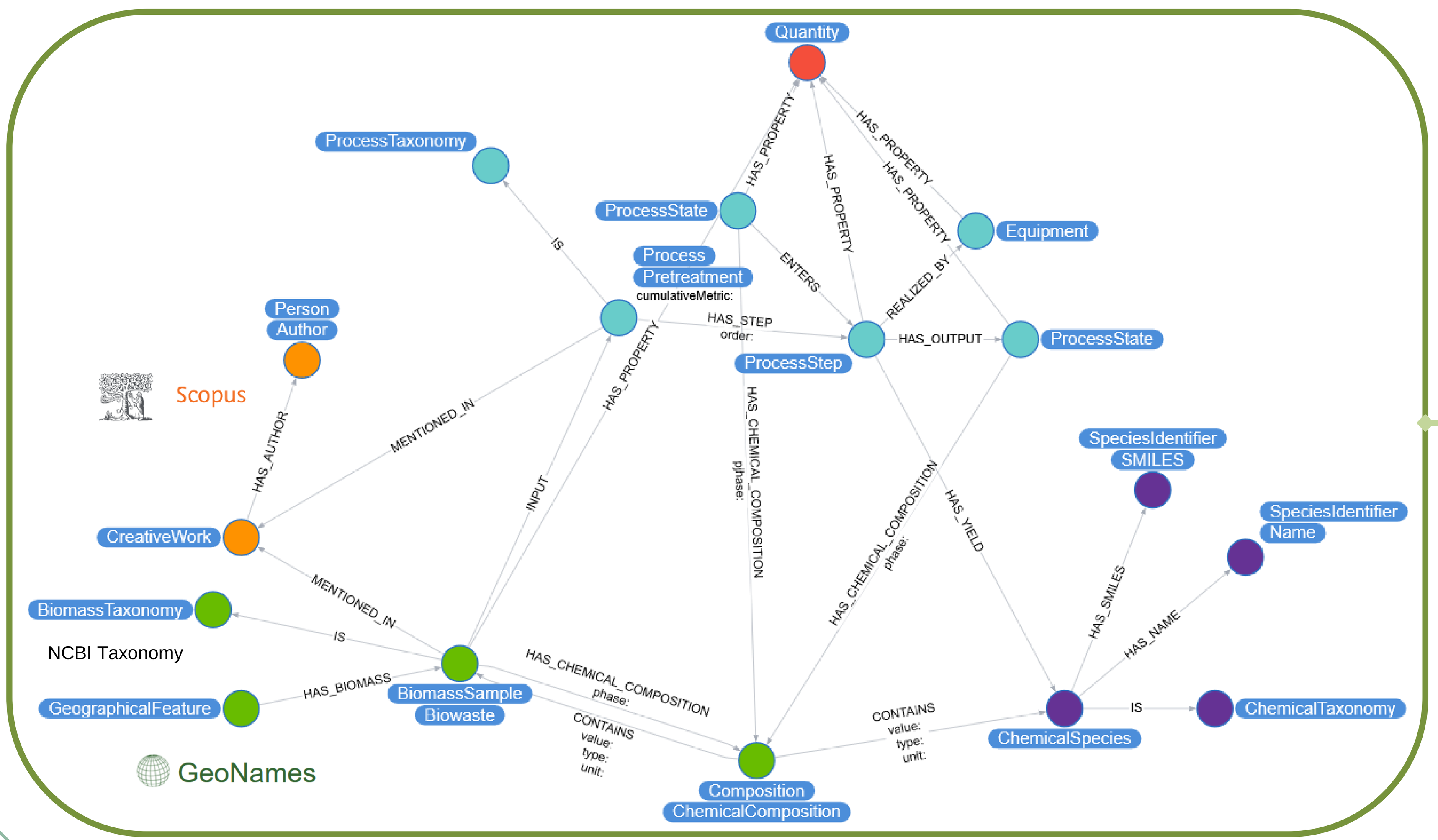
Introduction

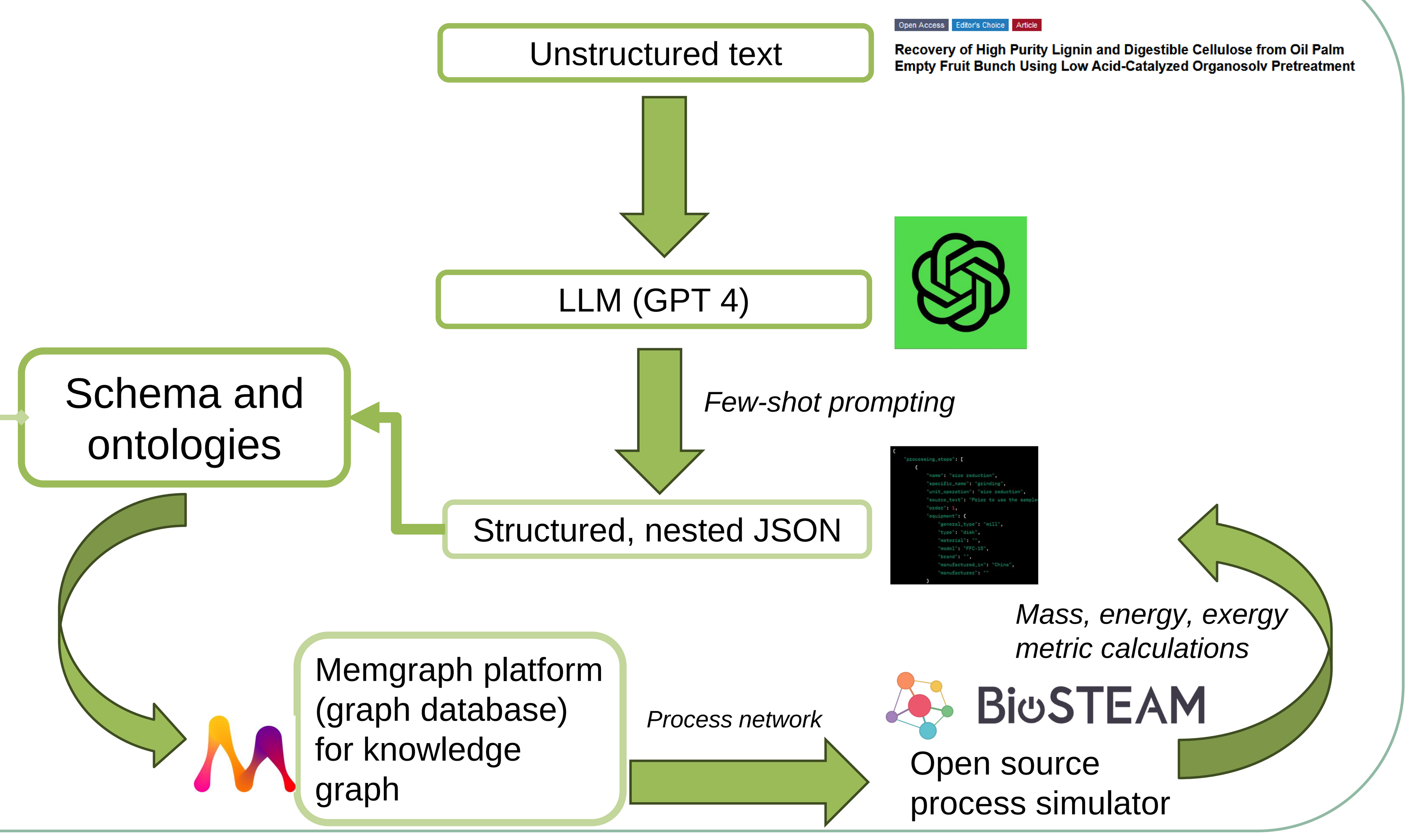
- Chemical value chain is still linear, heavily reliant on non-renewable fossil feedstocks
- Nearly 1.2 billion tons of biowaste are generated per year (majority are either landfilled or incinerated)
- What are the most sustainable pathways from biowaste to value-added chemicals and how can we find them?





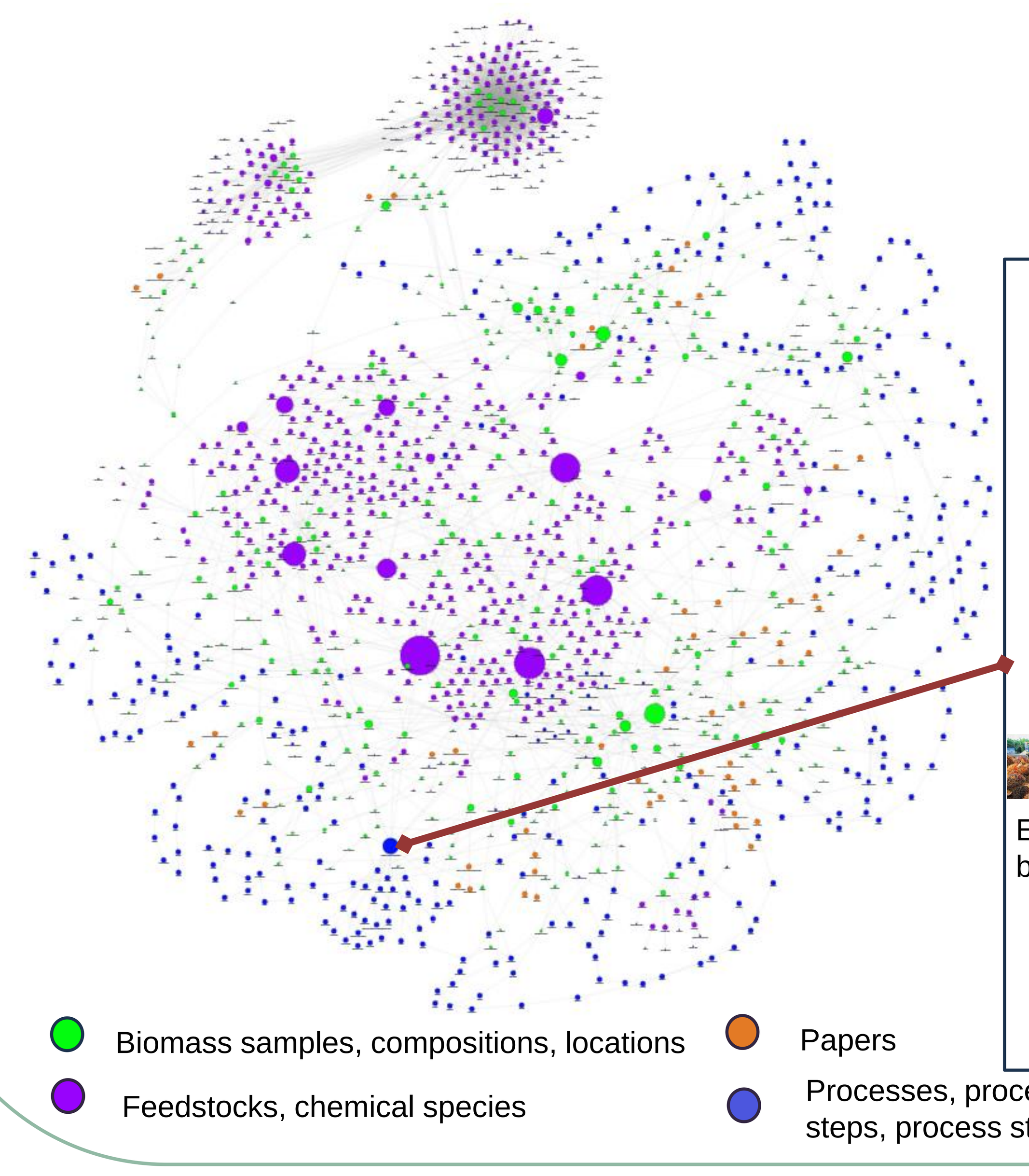
Methods

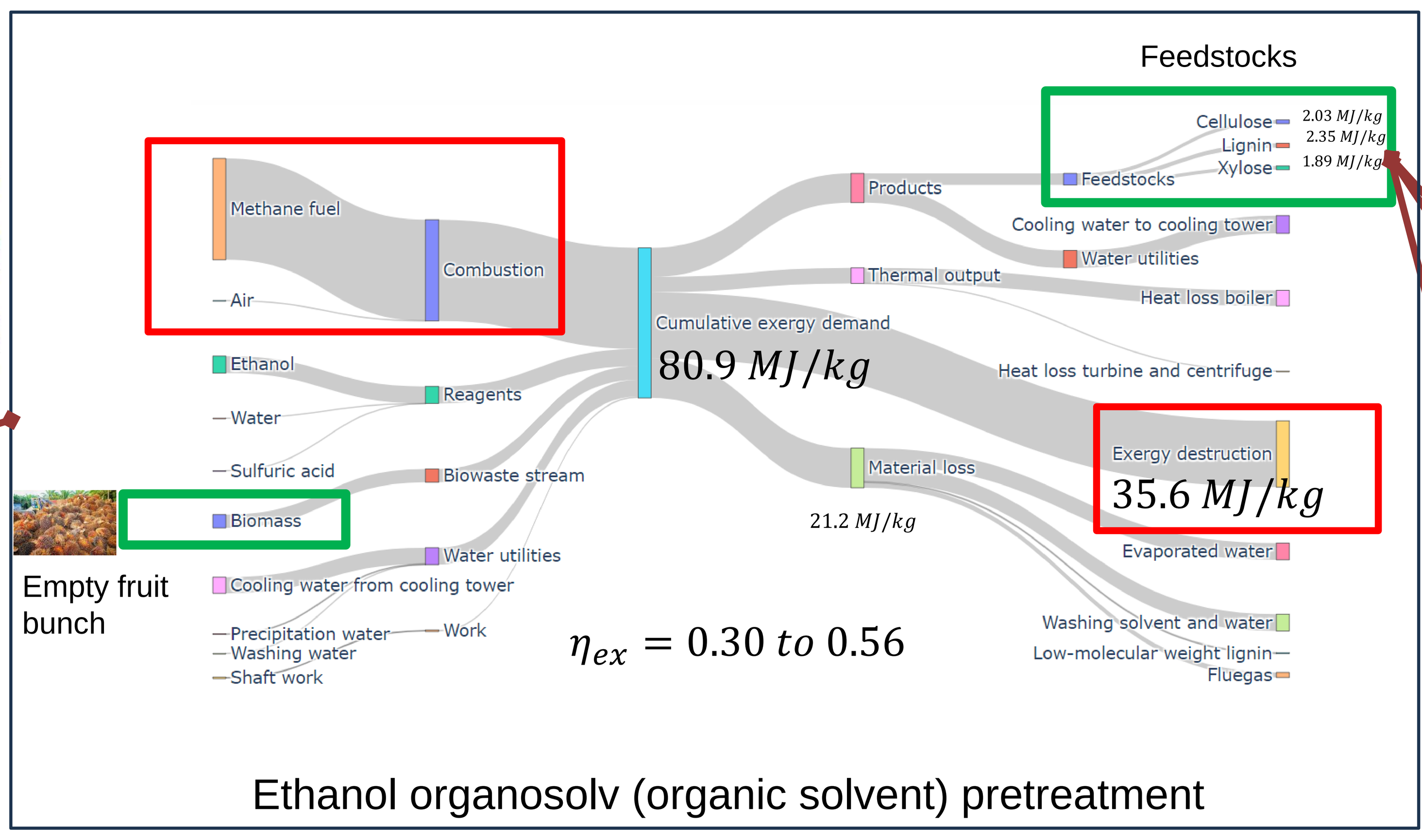




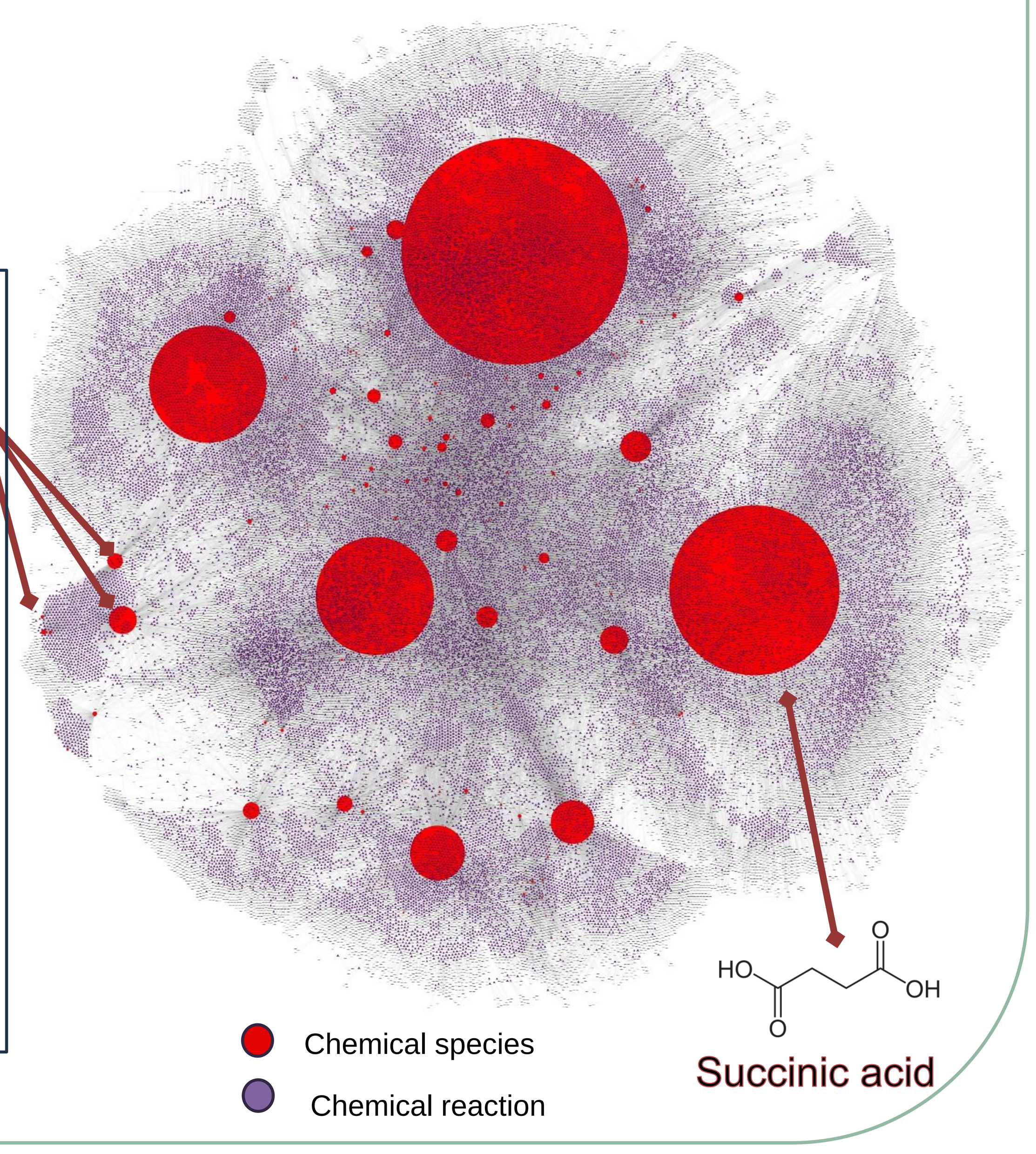
Results

- ~90 biomass samples (across 29 types) from oil palm residues to corn stover
- ~40 pretreatment processes (across 7 types) from organic solvent to ionic liquid
- ~ 120 feedstocks populated (from lignin to chitin)
- Facilitate pathway screening from biowaste to value-added chemicals like succinic acid, acetic acid, ethanol





Ethanol organosolv (organic solvent) pretreatment



Conclusions

- **Knowledge graphs** are crucial in representing and evaluating the space of possibilities or **pathways from biowaste to value-added chemicals** to establish a **circular chemical economy**
- **First of its kind knowledge graph** developed containing ~90 biomass samples, ~40 pretreatment process and ~120 feedstocks, allowing for pathway screening to **value-added chemicals** using **sustainability** metrics such as exergy

References

Arun A, Weber J, Guo Z, Lapkin A. Integration of biowaste into chemical reaction networks. ChemRxiv. Cambridge: Cambridge Open Engage; 2021; This content is a preprint and has not been peer-reviewed.

Guo, Z., Yan, N., & Lapkin, A. (2019). Towards circular economy: integration of bio-waste into chemical supply chain. *Current Opinion in Chemical Engineering*, *26*, 148–156. https://doi.org/10.1016/j.coche.2019.09.010/

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CDI Chemical Data Intelligence

Building Sustainability into Business Models: Clean Tech Adoption Incentives and Internal Carbon Pricing for Multi-Unit Firms

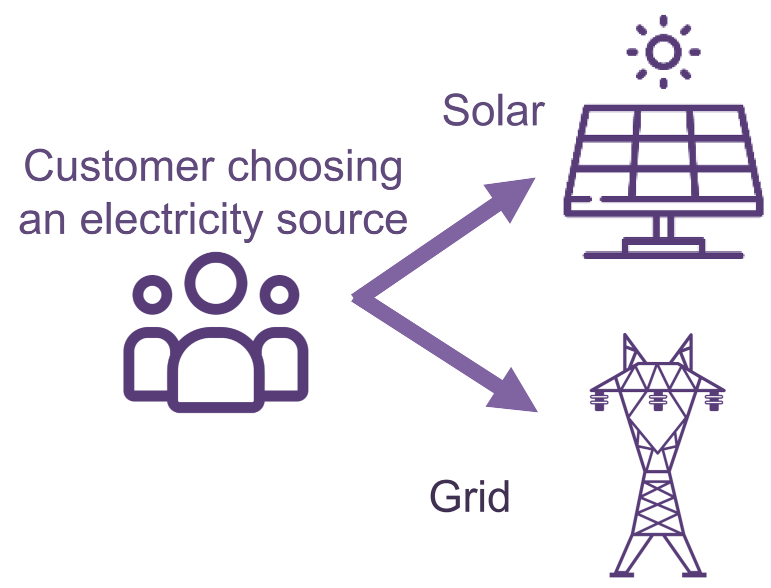
[J. Lemuel Martin[1], K. R. Preethi[2], S. Viswanathan[2], Yan Wang[1]]

Introduction

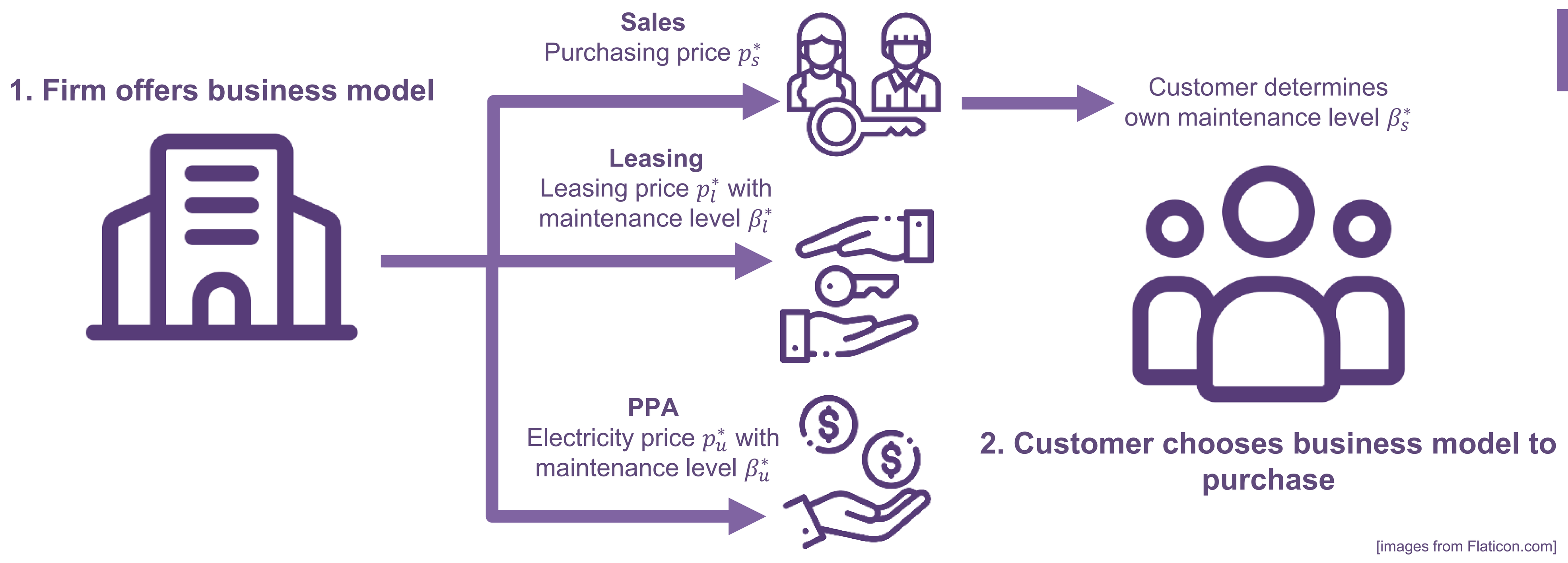
A game theoretic approach to business model design illustrates strategic interactions with the goal of aligning player incentives, from firms to customers. Using price as a key lever, we investigate the impact of integrating sustainability with game theoretic business models, namely: (1) alternative business models to incentivize clean technology adoption, and (2) internal carbon pricing structures for multi-unit firms.

DESIGNING INCENTIVES FOR CLEAN TECH ADOPTION (Application: Rooftop Solar Systems)

1 RESEARCH QUESTION: What alternative business models can solar power firms utilize to increase solar power adoption, and when would one model be preferred over the other?



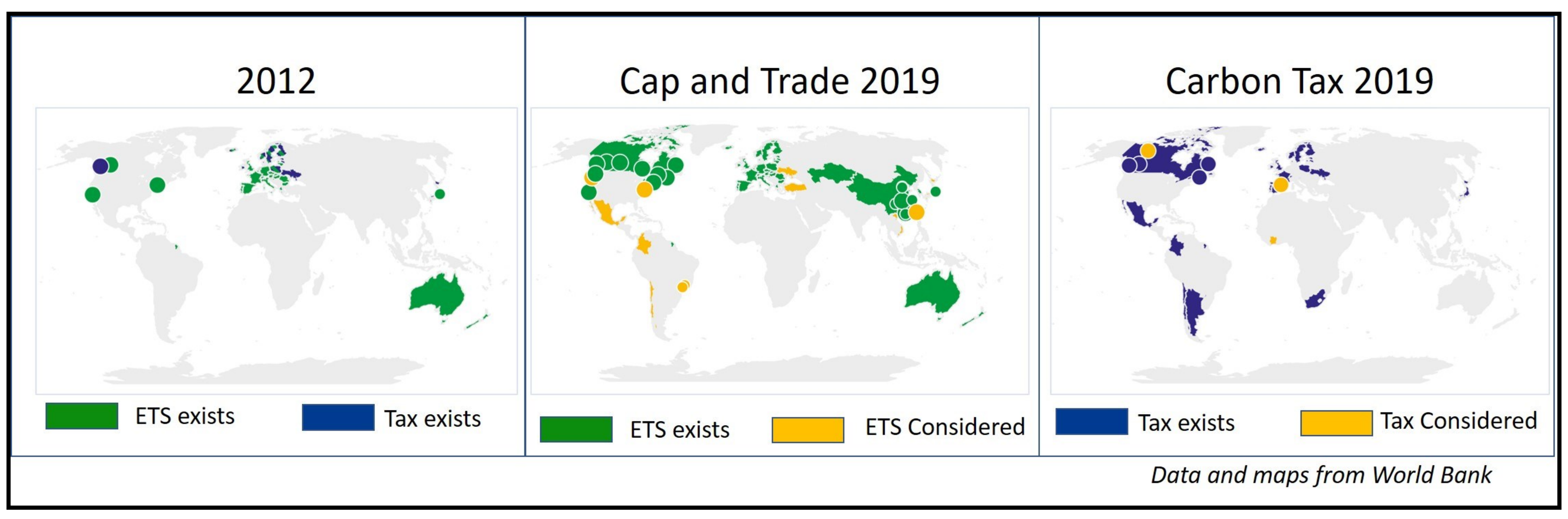
2 METHODOLOGY: We develop a game theoretic analysis of alternative business models for solar panel adoption. The model could be customized in other clean tech contexts where products are offered as a service.



3 FINDINGS AND FUTURE APPLICATIONS:

- Under a single representative (homogenous) customer(s), leasing and PPA yield the same benefits for both firm and customer.
- Under customers heterogeneous in demand and/or solar generation, both leasing and PPA are required and in fact hybrid pricing models are required as well.
- We develop algorithms to determine the optimal pricing for each model, which can leverage data-driven approaches to generate further market insights.

INTERNAL CARBON PRICING IN MULTI-UNIT FIRMS



1 RESEARCH QUESTION: How should the internal carbon tax rate be set in a multi-business unit company such that (1) low carbon technology investments are encouraged, and (2) future regulation is accounted for without crippling present business?

2 METHODOLOGY: We develop a game theoretic model involving the central decision maker who sets the internal carbon tax rate based on a carbon reduction (SBTi) target, and several business units who possibly face stiff competition from other companies who do not have any carbon tax.

$$Firm\ Profits = \sum SBU\ profits + \sum Carbon\ tax\ from\ SBU$$

$$\Pi = \sum \underbrace{(a-bq)q}_{\text{Revenue}} - \underbrace{cq}_{\text{Production Cost}} - \underbrace{f(v)}_{\text{Abatement cost}} - \underbrace{Eq(1-v)\tau}_{\text{Tax paid to the firm by the SBU}} + \sum \underbrace{Eq(1-v)\tau}_{\text{Tax collected by the firm}}$$

3 FINDINGS AND FUTURE APPLICATIONS:

- Uniform internal carbon tax rates achieve best firm profit but can cripple emission intensive and/or competition challenged business units (EICCUs).
- Non-uniform tax rates with lower taxes for EICCUs can reduce short term firm profits but avoids crippling EICCUs and prepares all units for future regulations.
- A customized model can be built for Singapore. If contextual data is available, the model can be applied to generate insights and inform policy.

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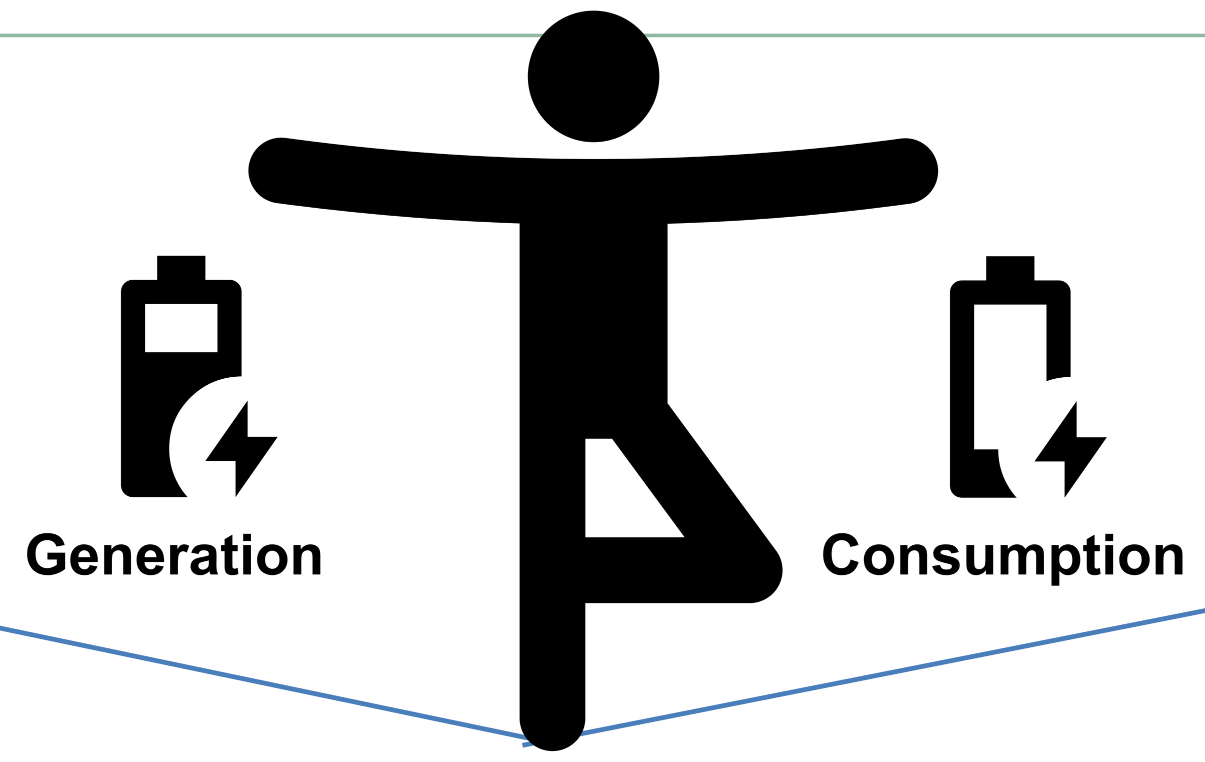
IRP4 Phase 1 – A retrospective

[Keck-Voon Ling,[1,2] Sanjib Panda,[1,3] Hoay Beng Gooi,[1,2] P.N. Suganthan,[1,2] Weng Khuen Ho,[1,3] Rusli,[1,2] King Jet Tseng,[1,4] Eddy Foo Yi Shyh,[1,2] Gehan Amaratunga,[1,5] Jan Maciejowski[1,5], *et al*]

Introduction

IRP4 Phase 1, also called **Integrated Chemical and Electrical Systems Operation (ICESO)**, investigated how the CO_2 emissions from electricity supplied to chemical plants can be minimised in Jurong Island. The research was carried out over 5 years, ending in October 2018. The project significantly advanced how electrical power systems for an industrial park can be controlled in near real-time to enhance efficiency and reduce CO_2 emissions while retaining the security of supply. The work was foundational for the **J-Park Simulator**, which later became **the World Avatar**.

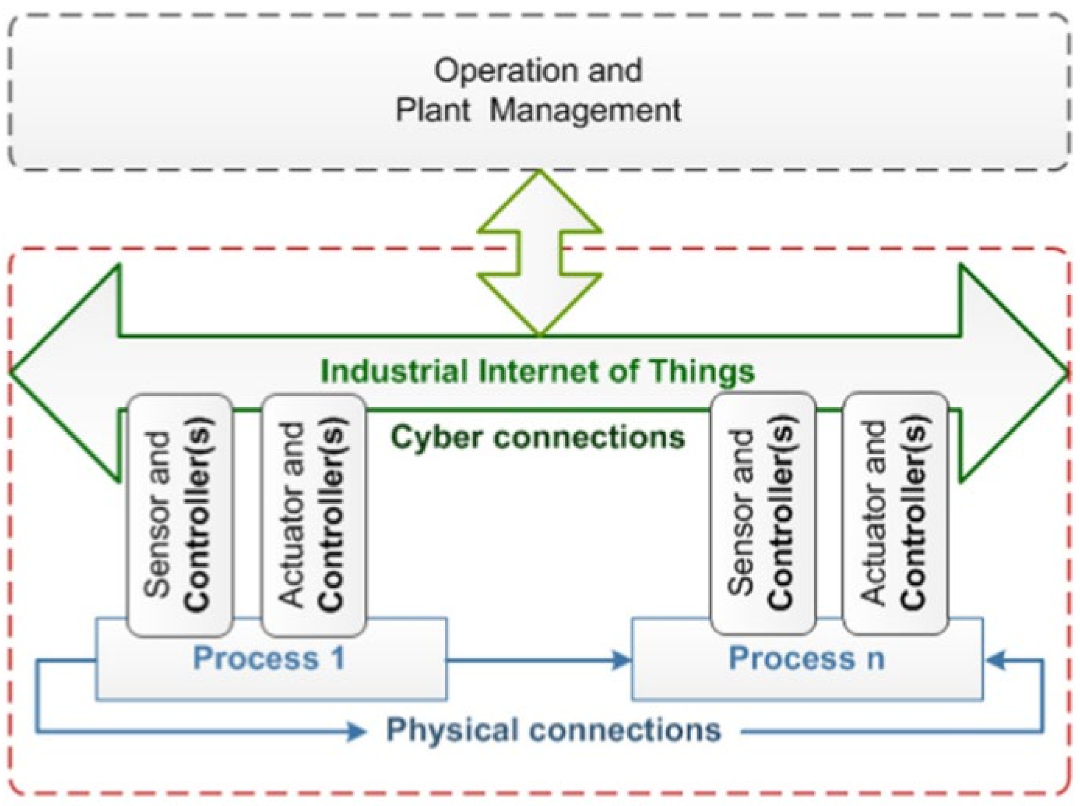
With electricity generation, the standard practice is to generate **large reserves** in case of an unexpected surge in demand or other disruption to the power distribution system. However, it is more efficient to have **smaller reserves** if everything works as expected. So, we walk a tightrope, balancing **generation** with **consumption** and **reserves** with **risk.**



ICESO focused on the Jurong Island electrical sub-network to optimise the coordination of energy **generation** and **consumption** within the electrical and chemical systems. It sought to discover how **tighter integration** of the electrical supply network and chemical plant load can **reduce the carbon footprint** of the chemical industry.

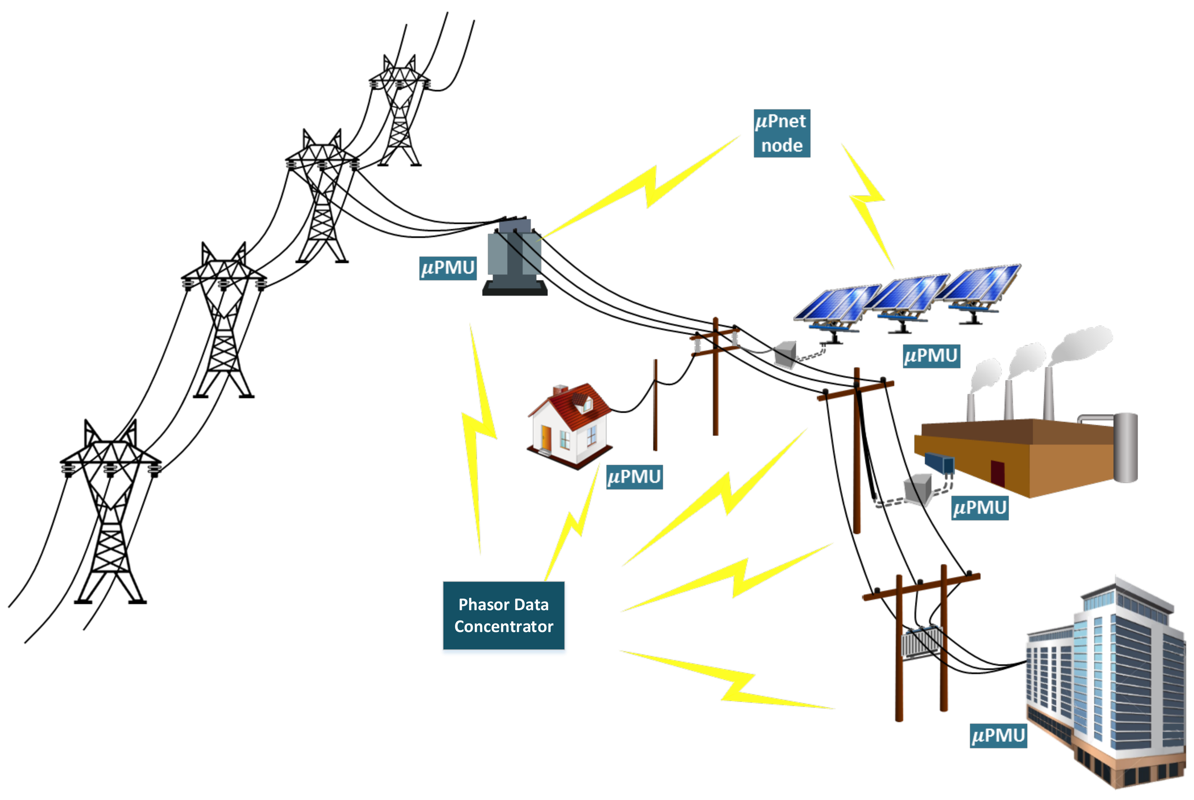
IRP 4.1: Fast algorithms to solve model predictive control problems [(a)]

Achieved:
- Automated power distribution system management and control
- Quadratic programming solver based on alternating direction method of multipliers



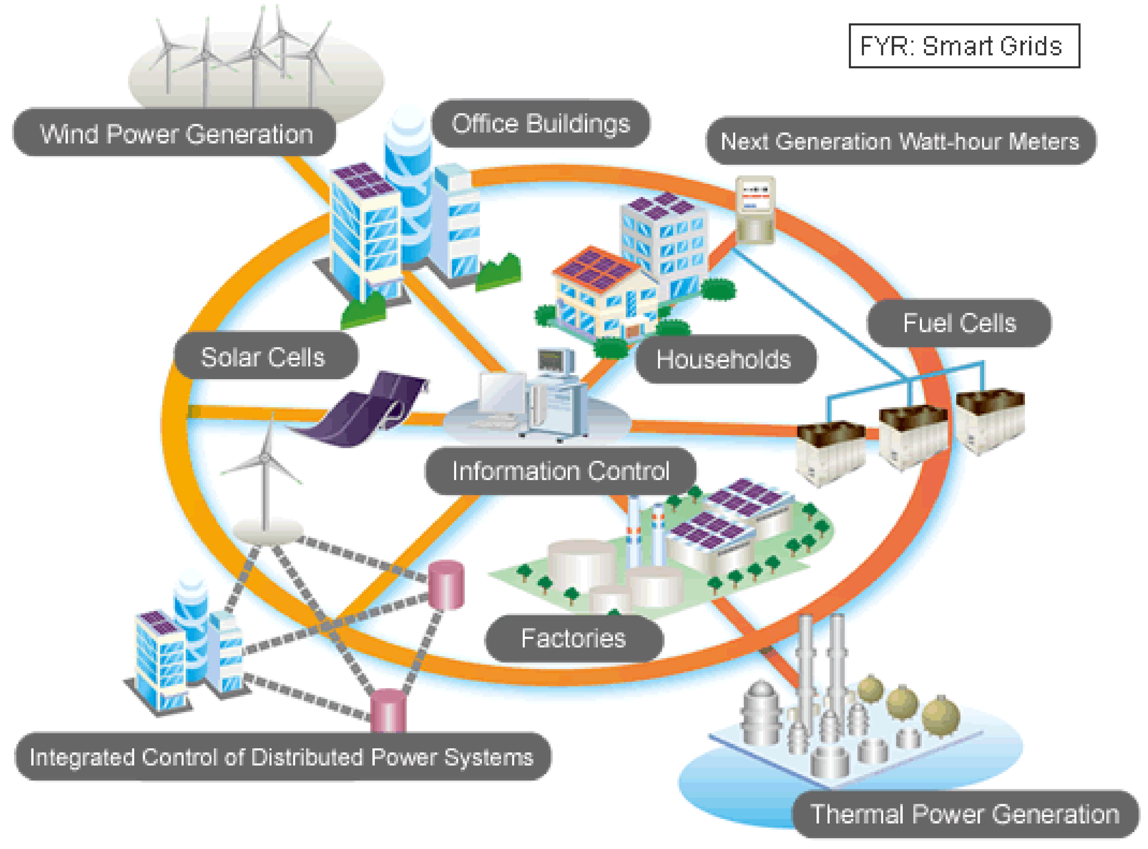
IRP 4.2: Extend model predictive control to non-linear and hybrid models [(b)]

Achieved:
- Model predictive control for energy efficiency in industrial parks
- Use of μPMU in smart grids for data gathering
- Robust state estimation for power systems



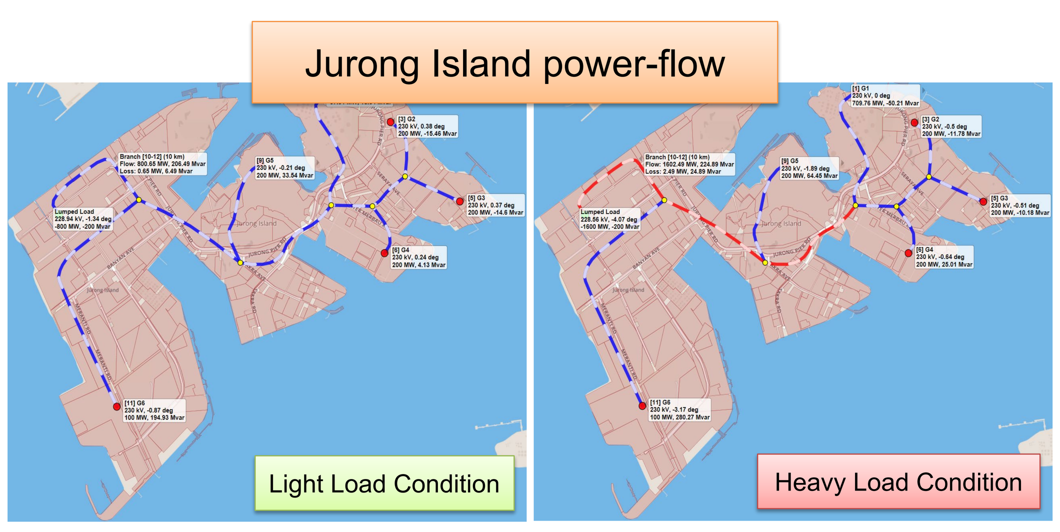
IRP 4.3: Model and control power generation networks with chemical process loads [(c)]

Achieved:
- Simulation with OPAL-RT (hardware-in-the-loop)
- Optimal scheduling of combined cycle gas turbines
- Power demand and electricity price forecasting
- CO_2 emission incorporated optimal power flow



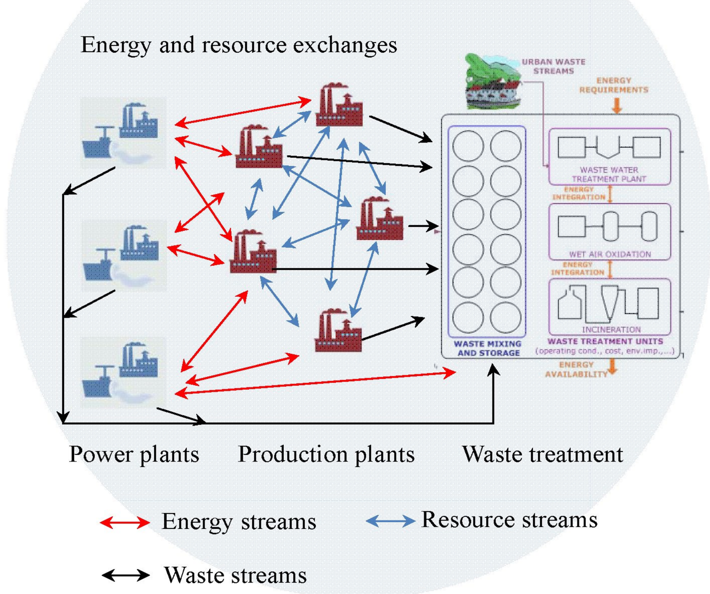
IRP 4.4: Model chemical process load and local electrical network akin to Jurong Island [(d)]

Achieved:
- Modelled NTU microgrids on OPAL-RT Hypersim
- Biodiesel plant operation study
- Near-real-time analysis and representation of power-flow



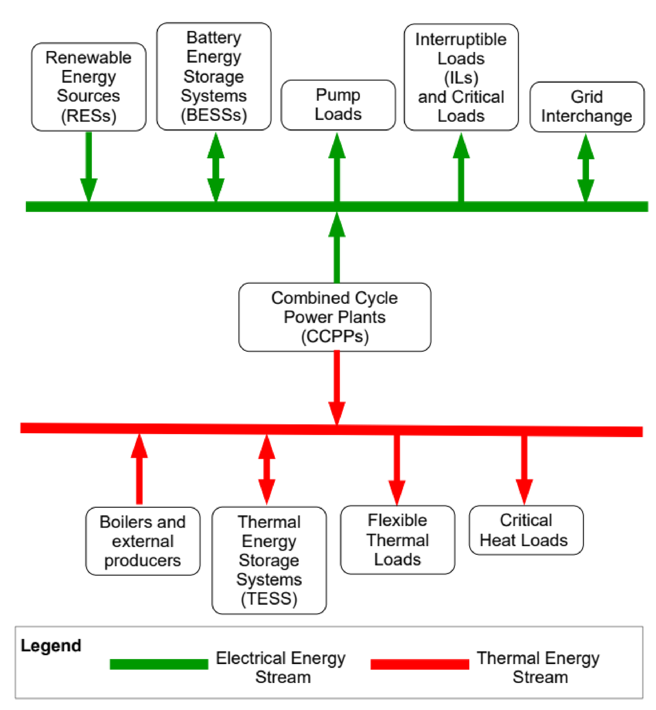
IRP 4.5: Model building, integration, and maintenance [(e)]

Achieved:
- Implementation of power system models in OPAL-RT environment
- Interface between J-park Simulator, OPAL-RT, and PowerWorld



IRP 4.6: Demonstration of proposed algorithms on pilot scale [(f)]

Achieved:
- Combined most effective methodologies within the J-Park simulator to assess performance within a chemical plant processing environment
- Tested power grid control and data analytics aspects



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[a] https://doi.org/10.1016/j.isatra.2015.08.008
[b] https://doi.org/10.1109/APPEEC.2015.7381051
[c] https://doi.org/10.22260/ISARC2014/0006
[d] http://dx.doi.org/10.13140/RG.2.2.18676.86400
[e] https://doi.org/10.23919/ECC.2018.8550187
[f] https://doi.org/10.32657%2F10220%2F49894

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Knowledge Engineering of Crystalline Materials

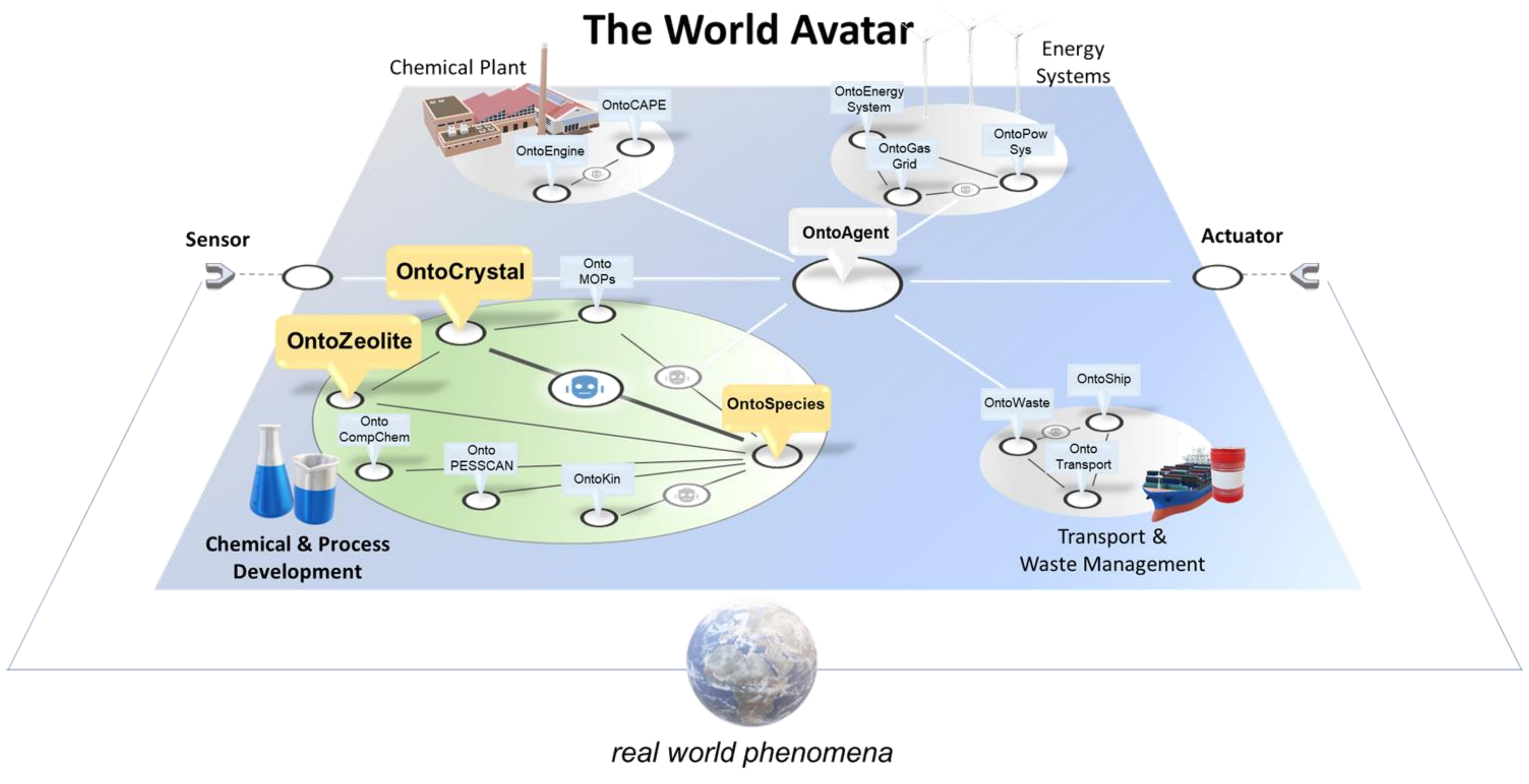
Pavlo Rutkevych,[1] Aleksandar Kondinski, [1] Srishti Ganguly,[1] Feroz Farazi,[2] Markus Kraft[1,2,3,4,5]

The World Avatar (TWA)

The World Avatar is a digital twin of the world. It uses semantic web technology to build dynamic knowledge graphs for various applications. The materials part of TWA currently includes ontologies for Chemical Species, Chemical Reactions, Metal Organic Polyhedra (MOPs), and Digital Laboratory.

The presented ontology for crystals (OntoCrystal) links together and expands this set of ontologies. The data is accessed through a SPARQL query or a specially designed agent with a user interface.

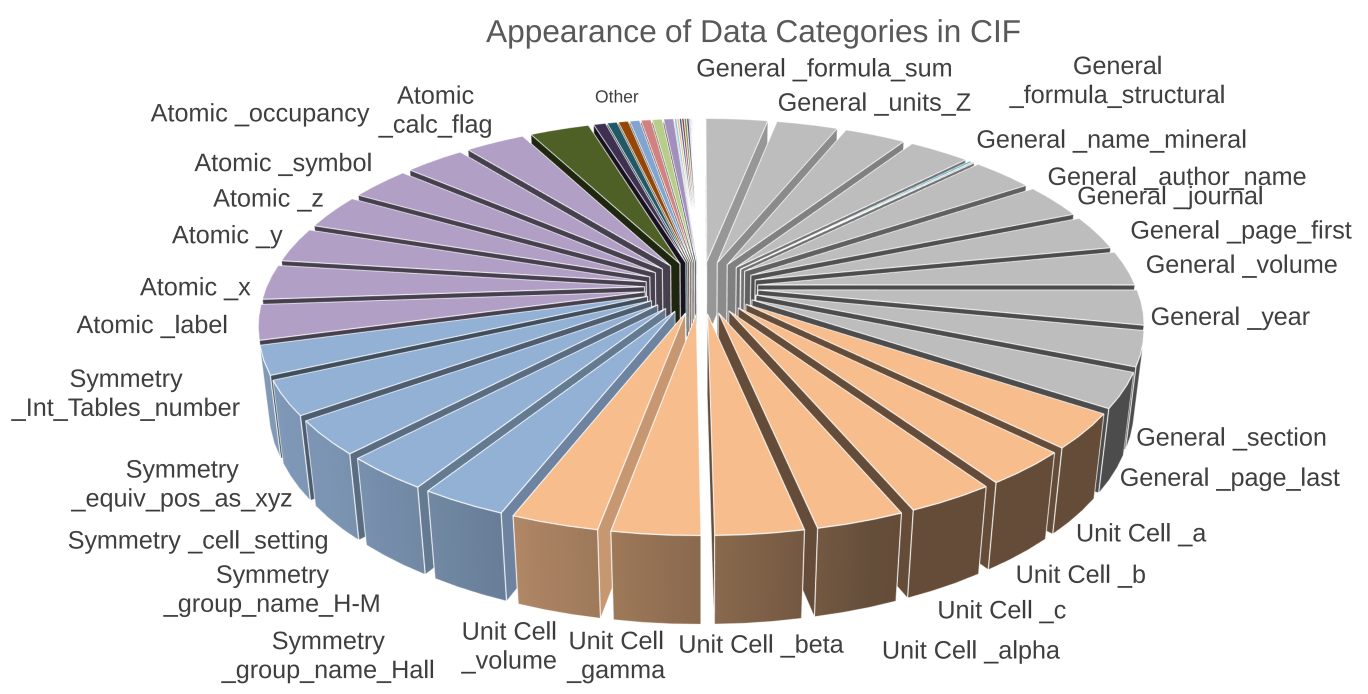
Fast and efficient access to machine-readable crystal data is a vital step in global integration as part of TWA, and it provides a connection between crystal databases and modern research.



Kondinski et al. *Acc. Chem. Res. 2023, 56, 2, 128–139.v*

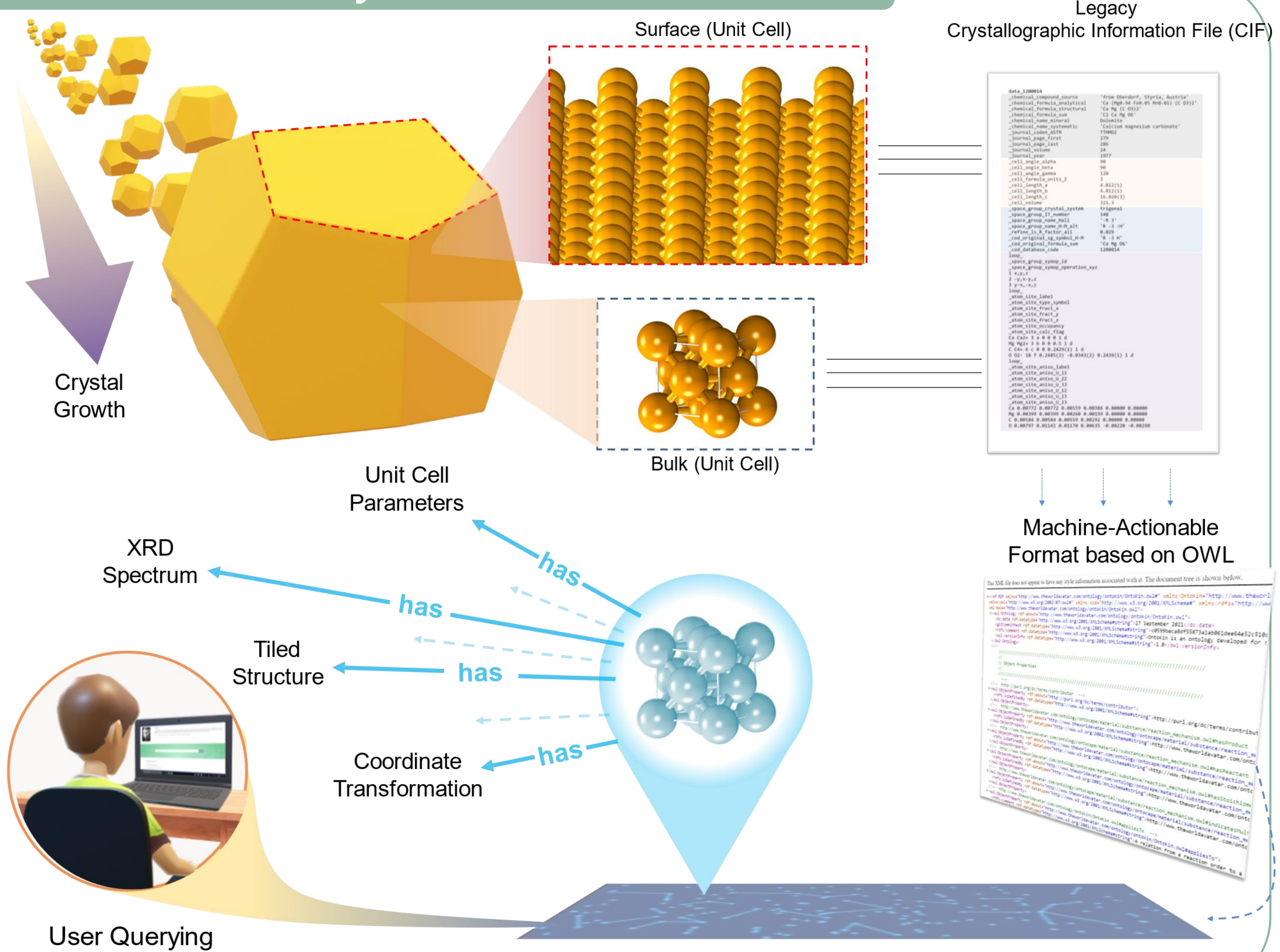
Ontological Representation of Crystalline Information

Crystallographic Information File (CIF)
- *De-facto* standard for data in crystallography
- CIF is a text file with keyword-value pairs
- The standard contains over 3500 keywords
- Main keyword categories: publication, crystal unit cell, atomic structure, symmetry



OntoCrystal ontology:
- Contains 108 Classes and Properties
- Covers the most used CIF inputs
- X-Ray Diffraction (XRD) spectra
- Zeolite-specific information

Work in preparation.



Ontological Representation of Zeolitic Materials

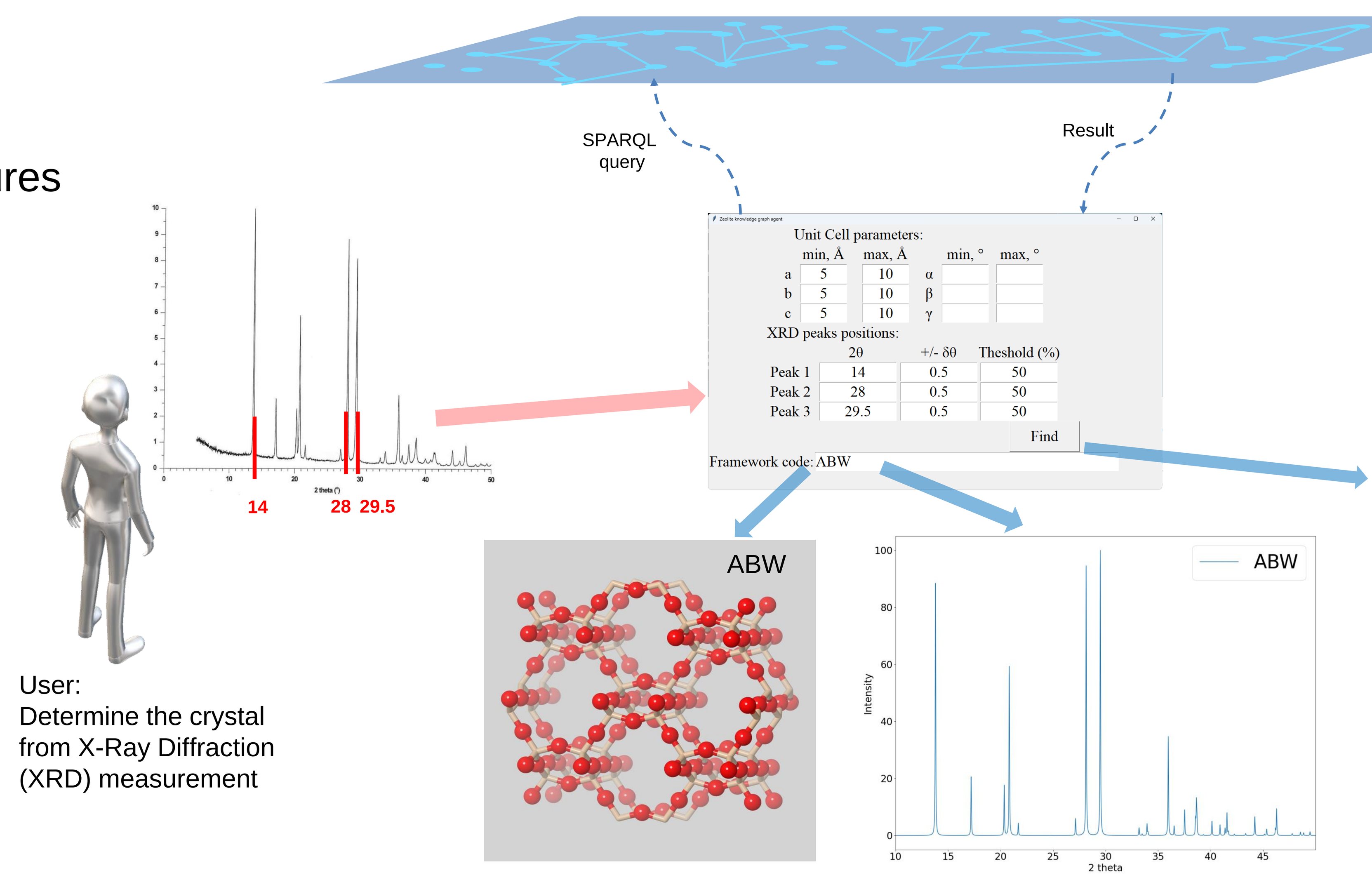
Zeolites are crystalline materials with pores

World production ~3 million tons per year

Over 250 known frameworks and millions of hypothetical structures

Key properties:
- High surface area and variety of guest atoms for catalysts
- Carrier of guest molecules for detergent
- Unique pore size for water or gas purification

User-friendly Zeolite Agent to access the Knowledge Graph
- Crystal lattice parameters
- Up to 3 prominent peaks from the XRD spectrum
- Get the full information about the crystalline material
- Variety of export formats



Lattice (ABW)	
a	9.873 Å
b	5.254 Å
c	8.770 Å
α	90°
β	90°
γ	90°
Symmetry	Ortho-rhombic

[1] CARES, Cambridge Centre for Advanced Research and Education in Singapore; [2] Department of Chemical Engineering and Biotechnology, University of Cambridge;
[3] School of Chemical and Biomedical Engineering, Nanyang Technological University; [4] CMCL Innovations, Cambridge; [5] The Alan Turing Institute, London; Email: mk306@cam.ac.uk

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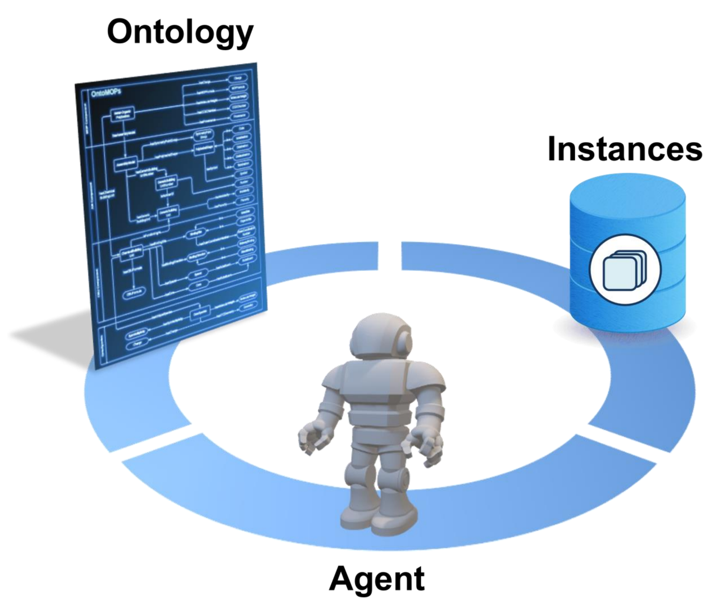
Knowledge Engineering of Reticular Materials

Aleksandar Kondinski,[1] Feroz Farazi,[2] Sebastian Mosbach,[1,2,4] Jethro Akroyd,[1,2,4] Markus Kraft[1,2,3,4,5]

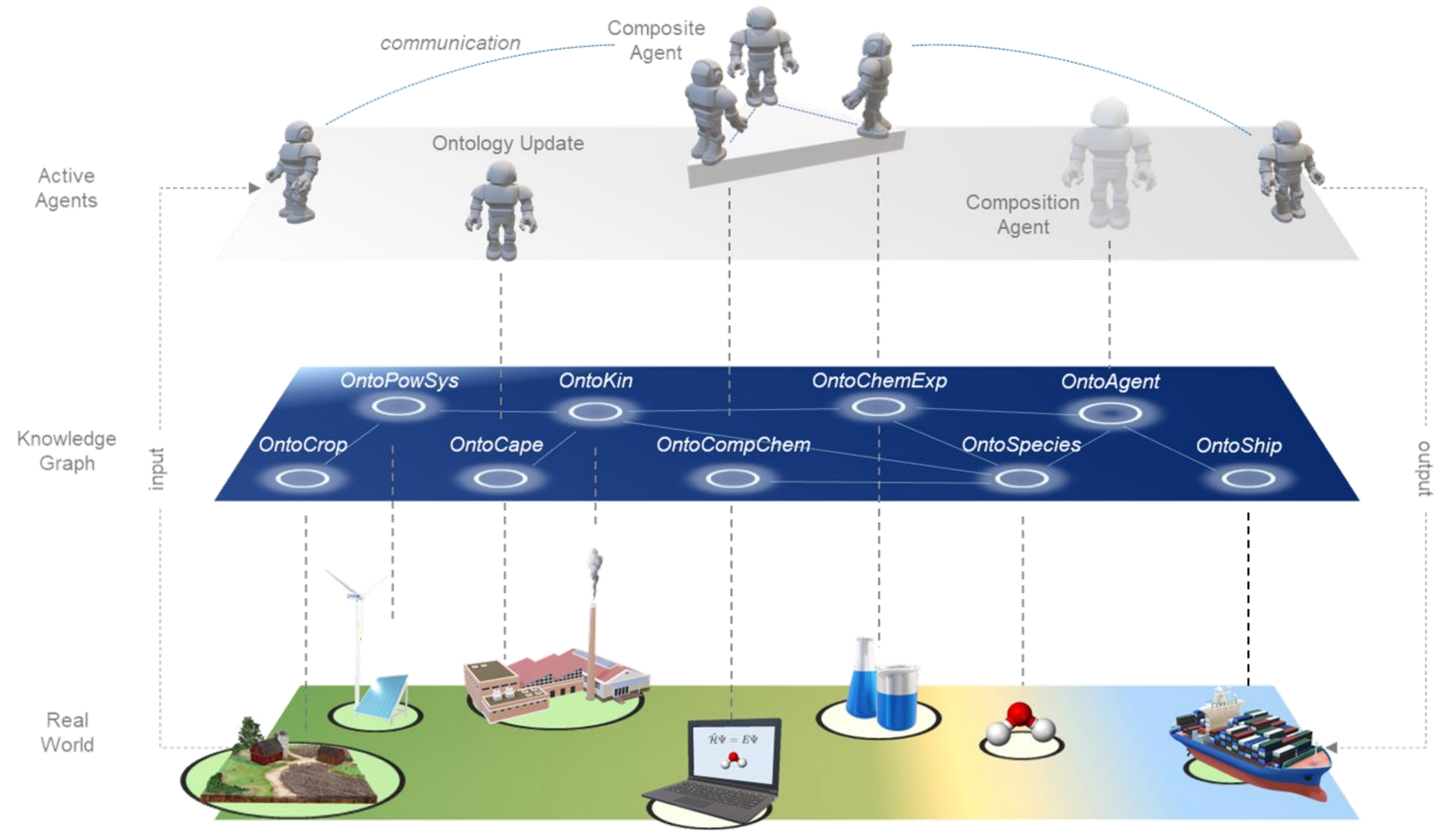
The World Avatar (TWA)

TWA aims to create a digital 'avatar' of the real world. It uses a **dynamic knowledge graph** based on an ontological representation of physical entities and interoperable computational agents, offering **cross-domain interoperability**. It can describe the state and behaviour of physical systems and, in this sense, acts as a **universal digital twin**.



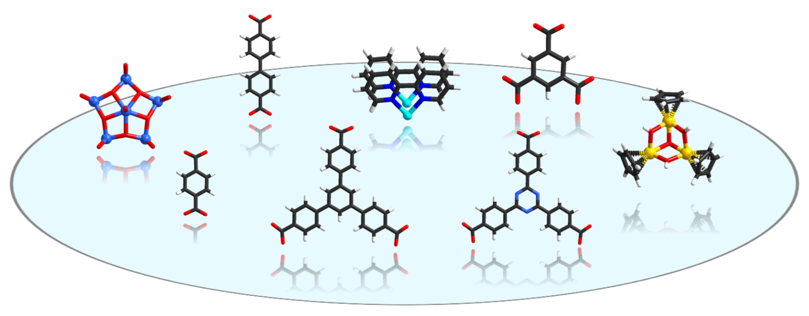
Knowledge engineering is a subfield of artificial intelligence that emulates the decision-making processes of human experts. TWA applies a knowledge engineering approach to solve problems in chemistry, making use of ontologies, instantiated knowledge and autonomous agents.

Using the search engine ***Marie***, TWA can answer complex chemical questions using natural language queries.



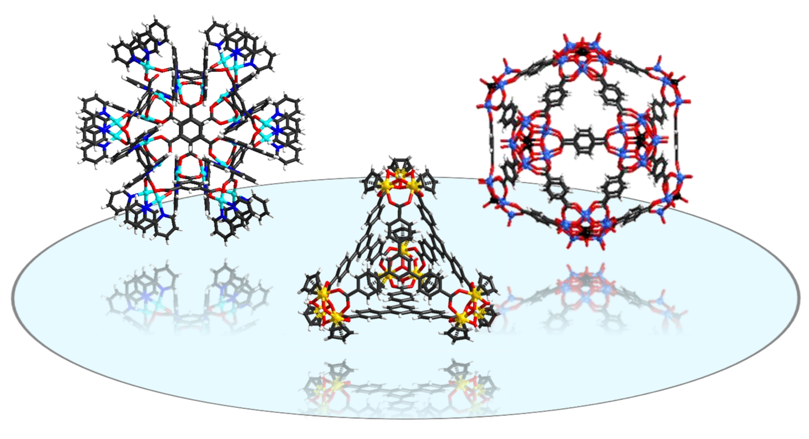
Kondinski et al. *Acc. Chem. Res.* 2023, 56, 2, 128–139.

AUTOMATED RATIONAL DESIGN OF MOPs



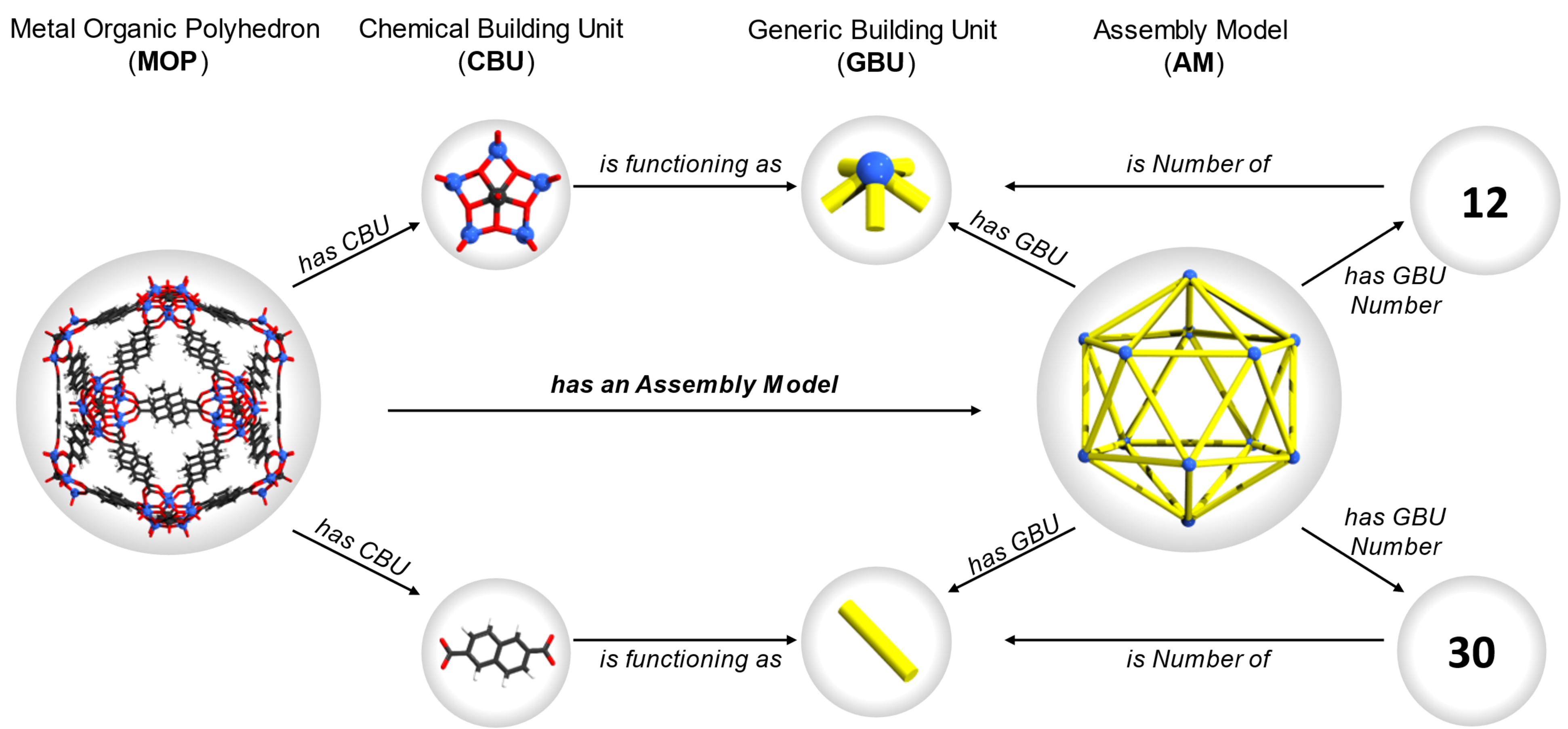
137 CBUs

MOPs are symmetrical molecular hybrids of inorganic and organic **chemical building units** (CBUs).

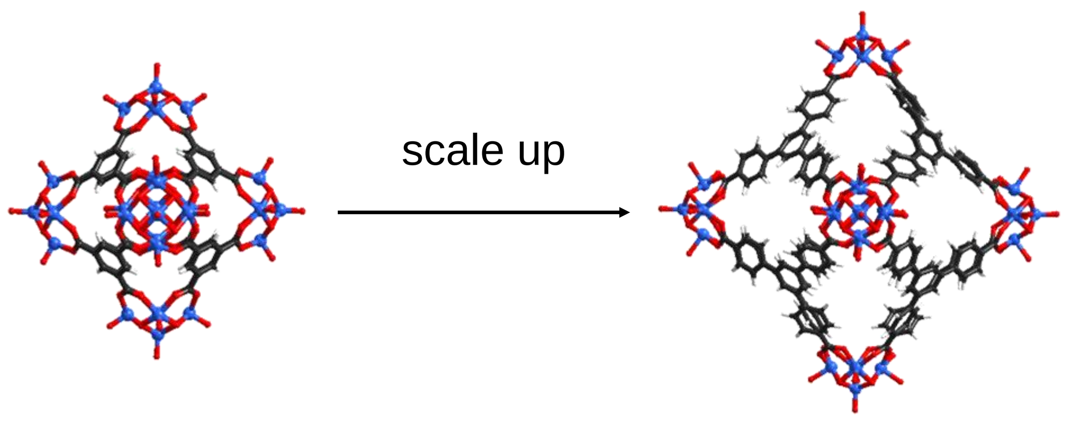


151 MOPs

The recent literature suggests that many more MOPs can be made based on the available CBUs.



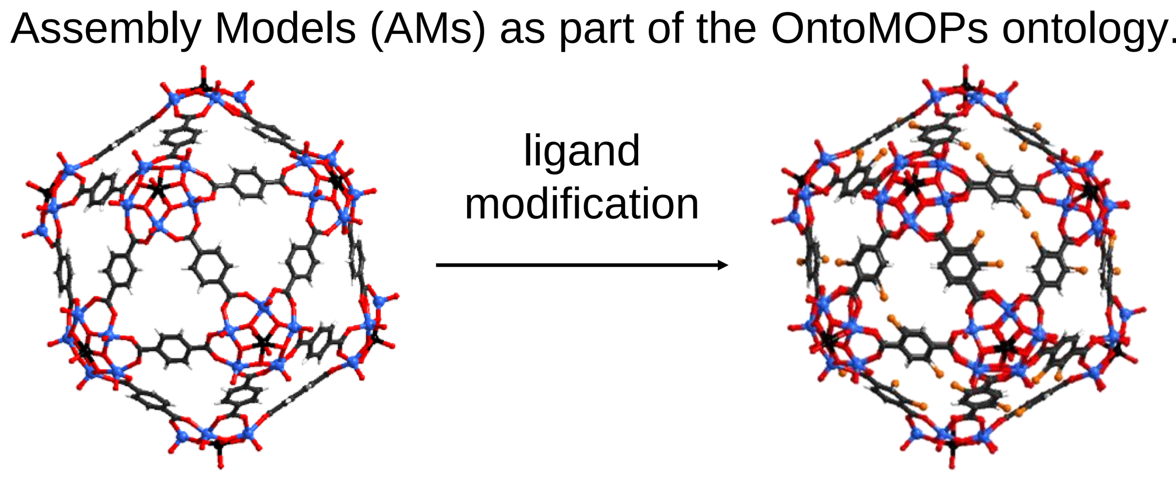
To mimic the cognitive process behind the rational design of MOPs, we introduced the concepts of Generic Building Units (GBUs) and Assembly Models (AMs) as part of the OntoMOPs ontology.



10.1039/C3SC53099J

"new instance"

Using inductive reasoning, a **MOP Discovery Agent** automatically identifies new MOPs. Based on 137 CBUs, up to 1418 new MOP instances can be rationally designed. Typical suggestions are formal substitution of CBUs and ligand modification.



10.1021/jacs.8b10866

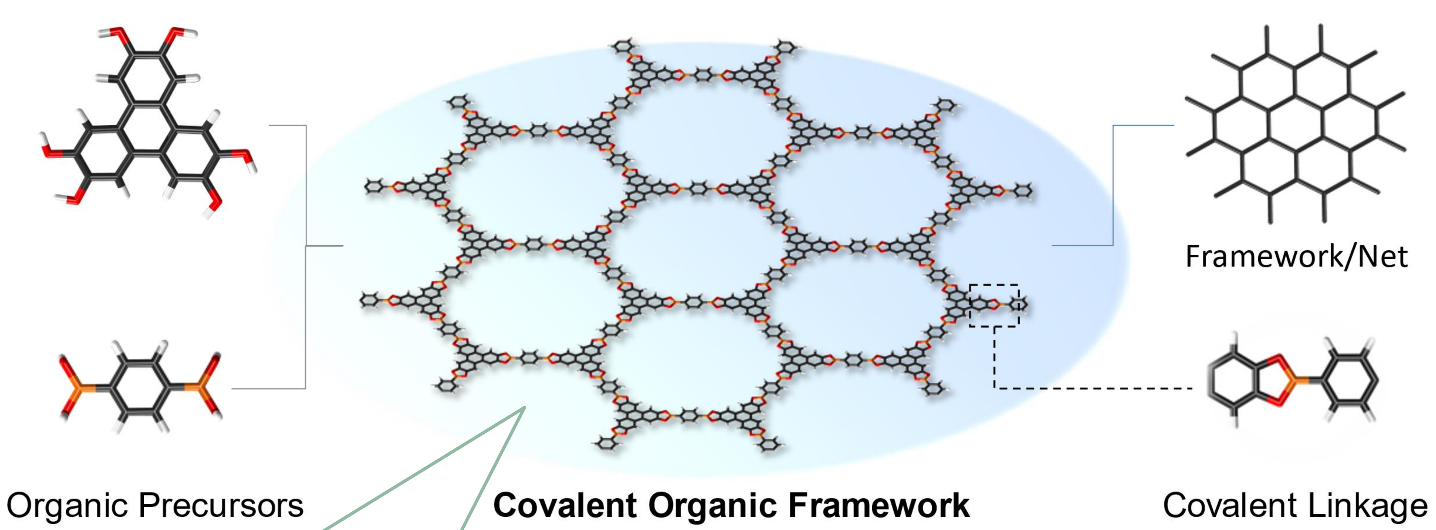
"new instance"

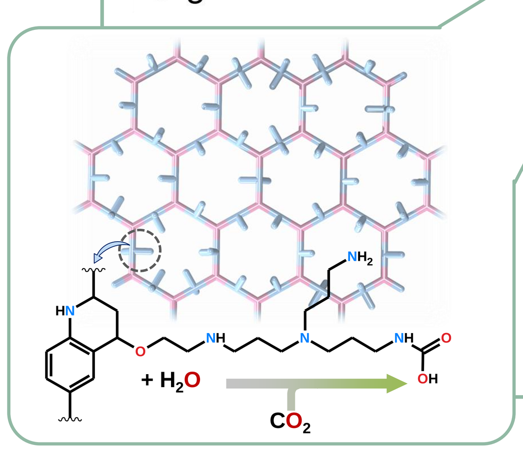
Kondinski et al. *J. Am. Chem. Soc.* 2022, 144, 26, 11713–11728.

AUTOMATED RATIONAL DESIGN OF COFs

COFs are porous, crystalline polymers depicting the topology of continuous frameworks.

COFs are made of organic precursors that undergo different linkage formation reactions.





COFs show promising applications as printable electronics, nanofilters and carbon capture materials.

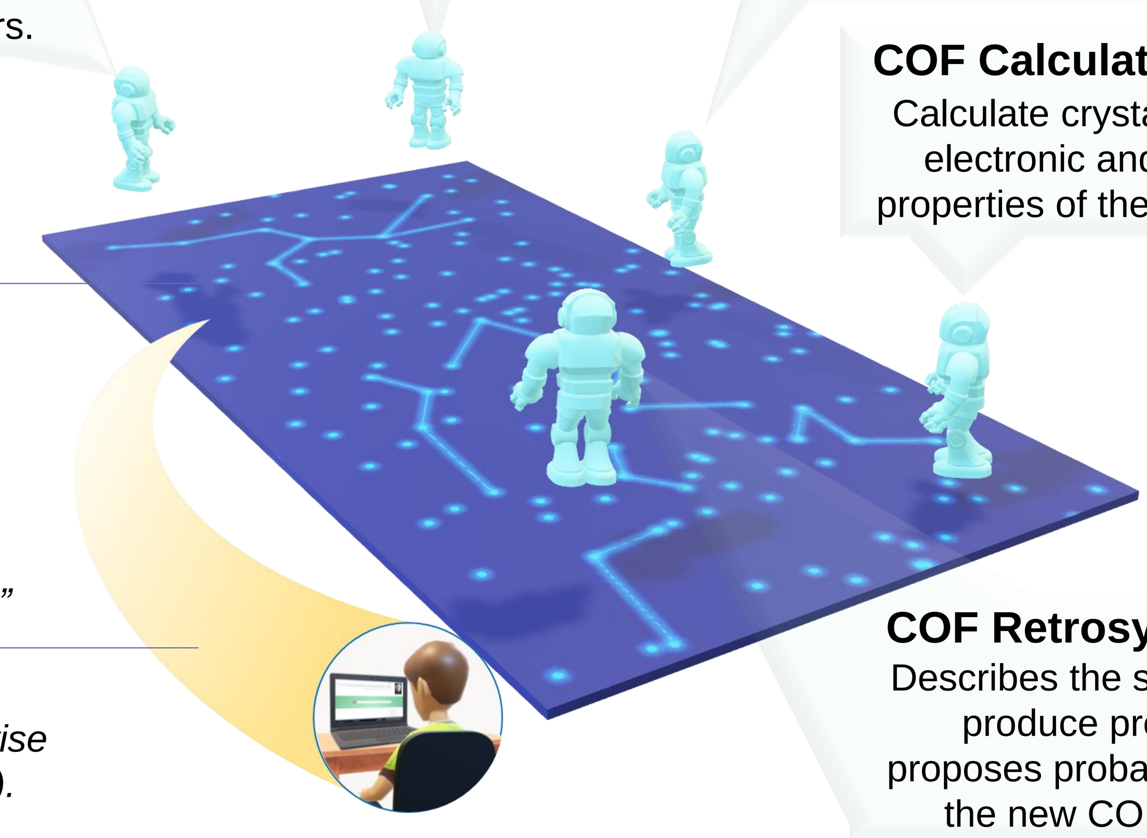
work in preparation

COF Discovery Agent
A composite agent exploring new COF formulations based on known precursors.

COF Drawing Agent
Facilitates communication with chemists and external cheminformatic resources.

COF Constructing Agent
Creates spatial models of new COFs by stitching molecular (CBU) fragments.

COF Calculation Agent
Calculate crystallographic, electronic and porosity properties of the new COFs.



Knowledge graph interconnecting instances of COFs, precursors, reactions, crystal materials and calculated properties.

User querying "reversed" molecular design (e.g. given a particular porosity, show me a stepwise synthesis of the material).

COF Retrosynthesis Agent
Describes the synthesis steps to produce precursors and proposes probable conditions for the new COF preparation.

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Estimating anthropogenic heat and pollution impacts from heavy industrial activities using dynamic knowledge graphs

Kok Foong Lee[1], Karthik Nagarajan[1], Srishti Ganguly[1], Hou Yee Quek[1] and Markus Kraft[1,2,3,4,5]

Background

Jurong Island is the heartbeat of Singapore's industrial might, vital for energy security and export revenue. Yet, little is known about the magnitude and geographical reach of their heat and pollutant emissions' impacts on our quality of life. One notable gap in assessing these impacts stems from the lack of **inclusive data access**, namely from fragmented, incomplete data and limited organisational / institutional resources.

Figure 1. 3D CityGML representation of structures on Jurong Island in The World Avatar.

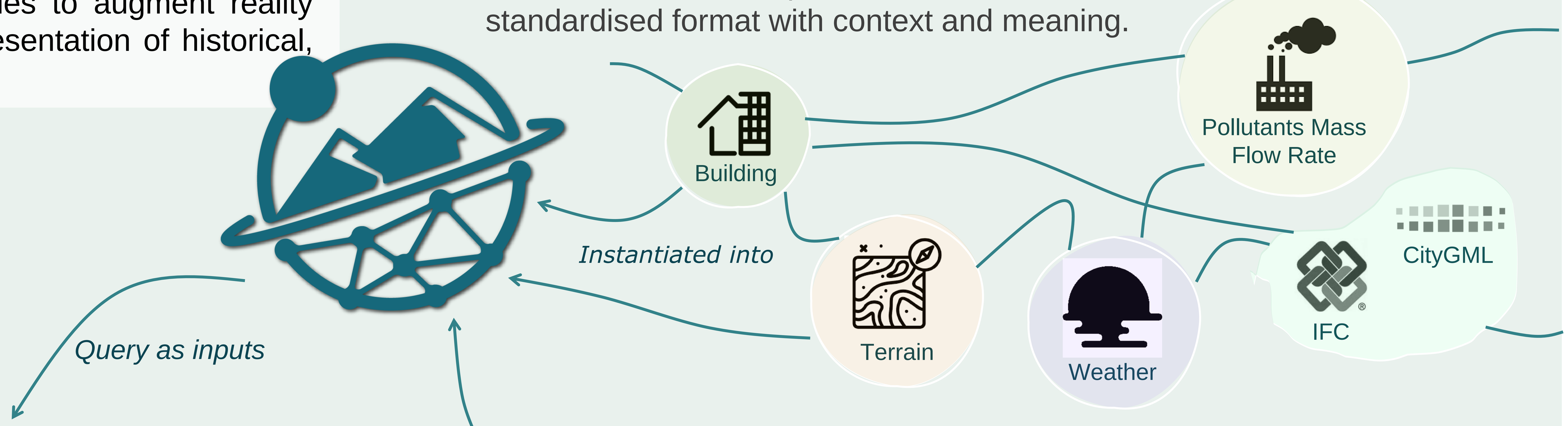
Methods

The World Avatar

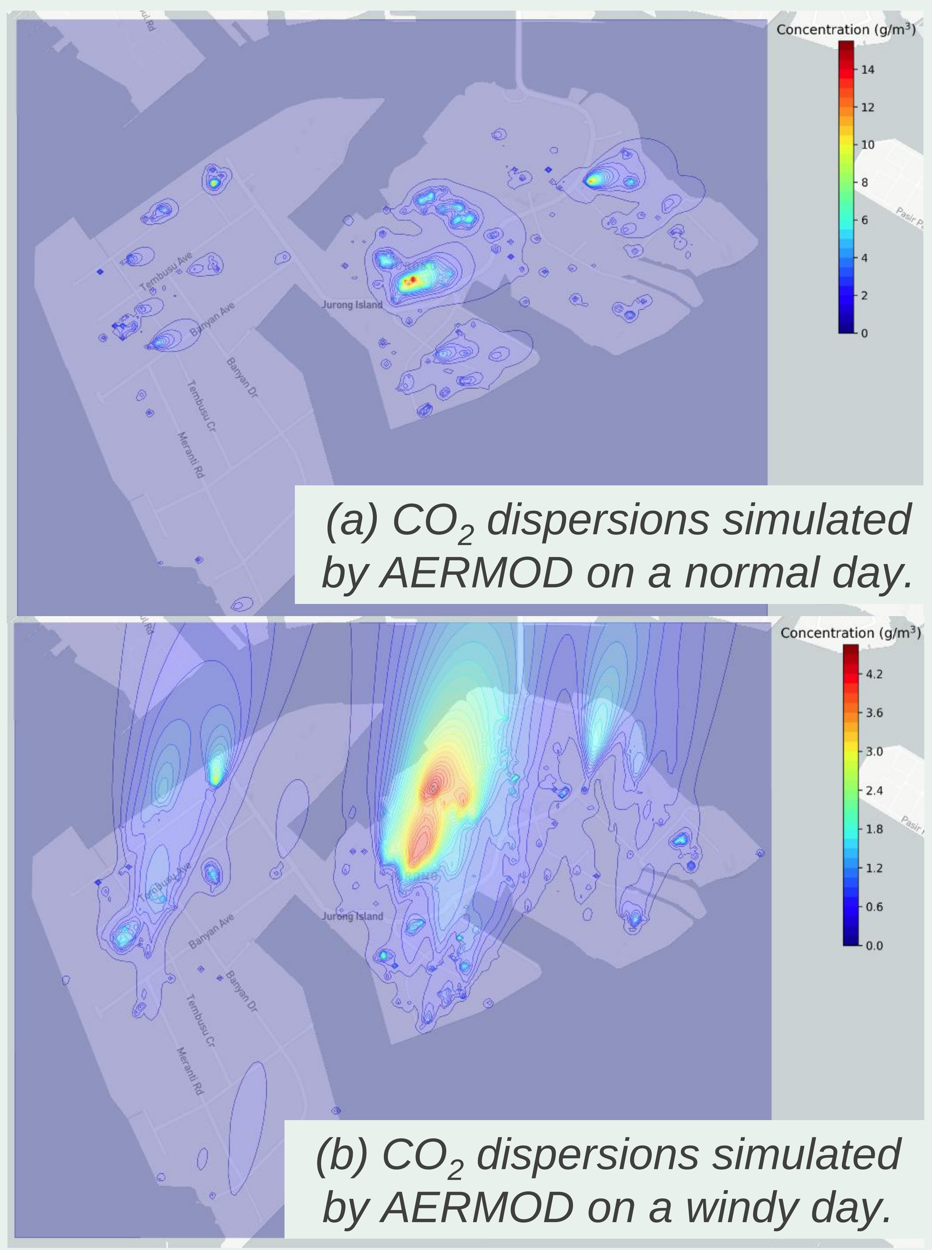
Employs a dynamic knowledge graph approach to ingest, integrate and process data source, software and tool across organisations, geographies and scales to augment reality with a rich interoperable digital representation of historical, current, and future knowledge.

1. LINKING DATA VIA ONTOLOGIES

Ontologies define and structure concepts, entities, and their relationships in a machine-readable standardised format with context and meaning.



2. SIMULATION MODELS



(a) CO_2 dispersions simulated by AERMOD on a normal day.

(b) CO_2 dispersions simulated by AERMOD on a windy day.

Figure 2. CO_2 dispersions on Jurong Island simulated by AERMOD during different weather.

<u>(2.1) American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD)</u>

An atmospheric dispersion modelling system designed to simulate and predict the dispersion of air pollutants emitted from various sources, such as industrial facilities and power plants.

<u>(2.2) Weather Research & Forecasting (WRF)</u>

A numerical weather prediction model designed to simulate atmospheric conditions like temperature and wind speed.

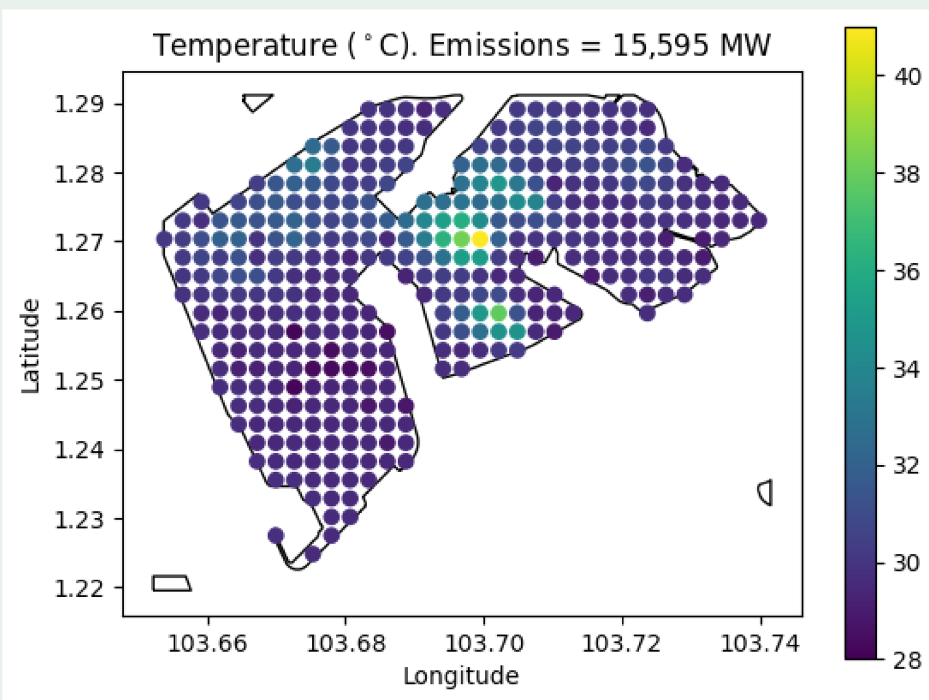


Figure 3. Temperature hotspots on Jurong Island estimated by WRF model based on emission outputs.

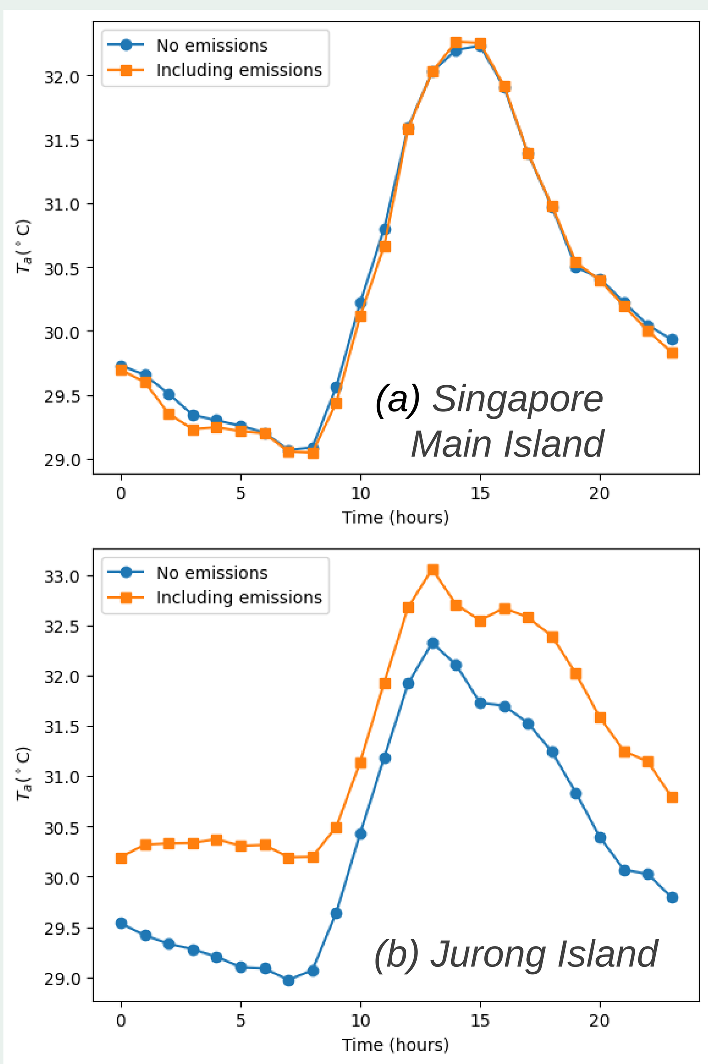


Figure 4. Time evolution comparisons of average temperature with and without emissions. Minimal impact of anthropogenic heat from Jurong Island on main island.

3. VISUALISATION INTERFACE

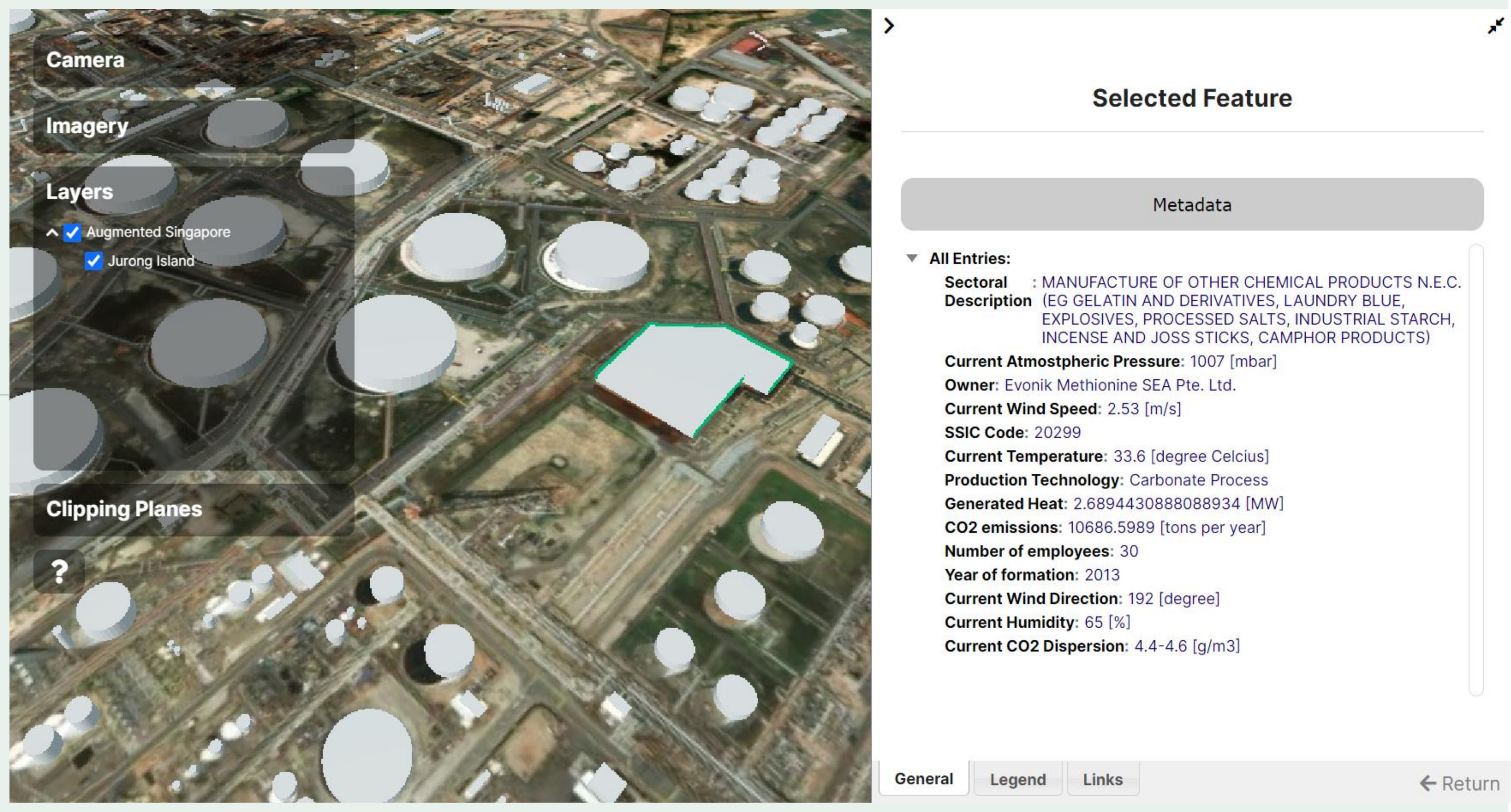


Figure 5. The World Avatar's augmented Jurong Island visualisation on a web browser. Availability of simulation inputs and outputs in one interface for inclusive data access.

Conclusions

Impact of heat and pollutant dispersions

- Negligible impact on mainland Singapore from Jurong Island activities in most weather conditions.

Opportunities of dynamic knowledge graph

- Knowledge graphs offer a rich interoperable knowledge base that can act as inputs for a variety of models.
- Simulation and software can be incorporated through The World Avatar's modular agent architecture.
- Inclusive platform-agnostic visualisation interfaces enable innovative forms of human-machine interactions.

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