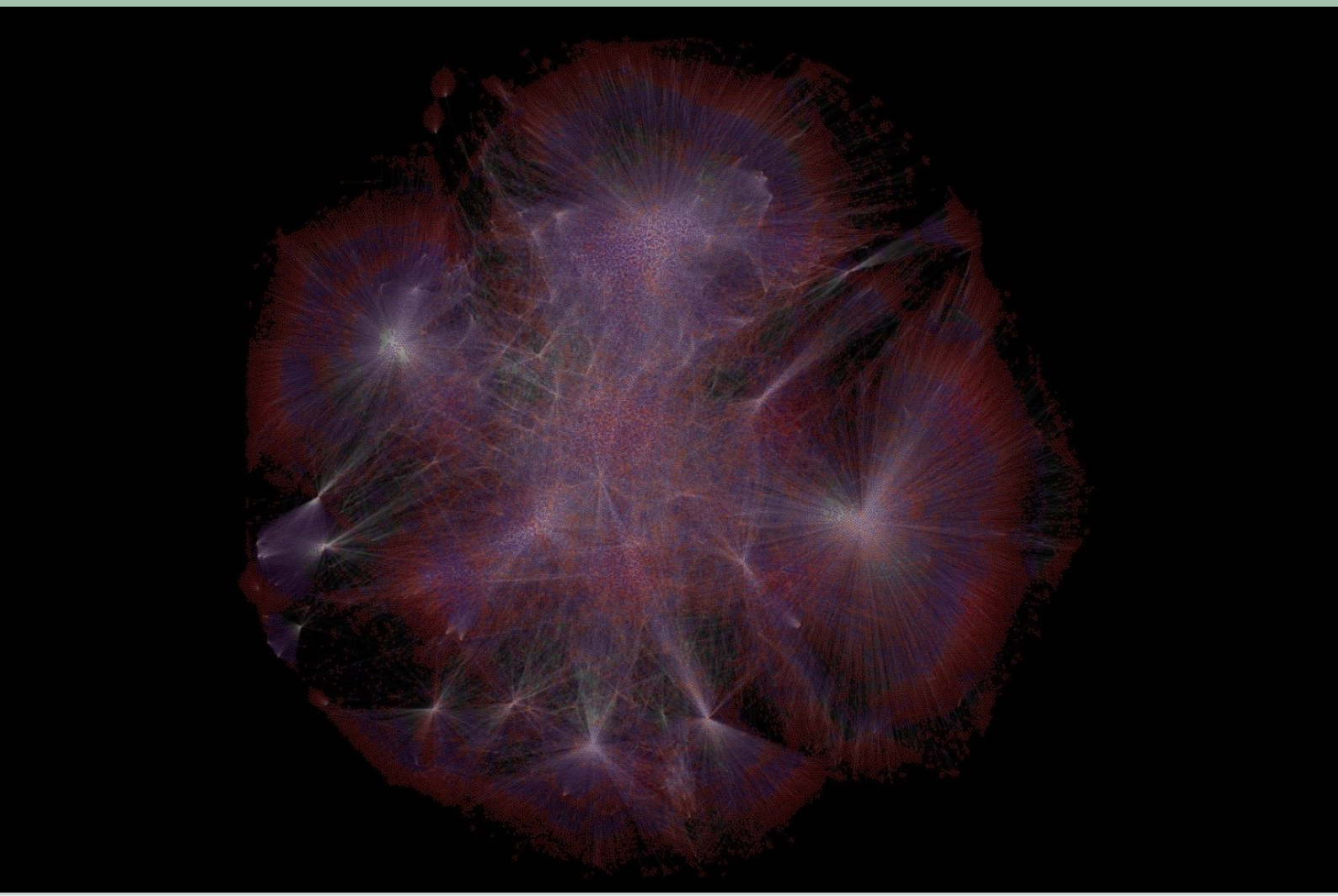
CAMBRIDGE **CARES**

A COLLABORATION BETWEEN THE UNIVERSITY OF CAMBRIDGE,
NANYANG TECHNOLOGICAL UNIVERSITY & NATIONAL UNIVERSITY OF SINGAPORE



Biannual Research Report

April - September 2023

CAMBRIDGE
CARES

CAMBRIDGE CENTRE
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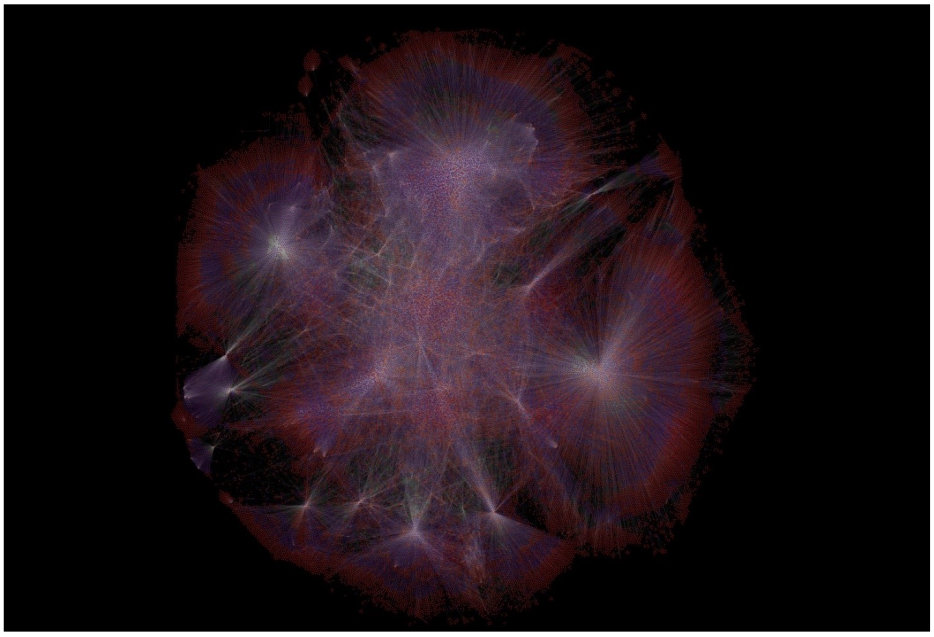
Cover image



A reaction network containing 39,000 chemical reactions (highlighted as purple nodes) and 28,000 chemicals (highlighted as red nodes). Each chemical reaction node in the network has a link (connection) from a chemical reactant and a link to the generated chemical product.

Image by Mr Adarsh ARUN (PhD student, CARES, IRP 1). See more on page 28.

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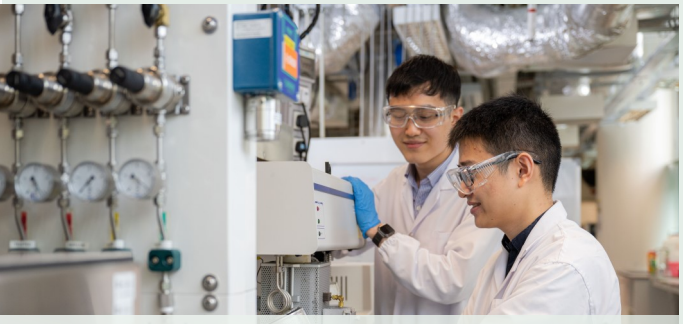
Focus on Fundamental Science



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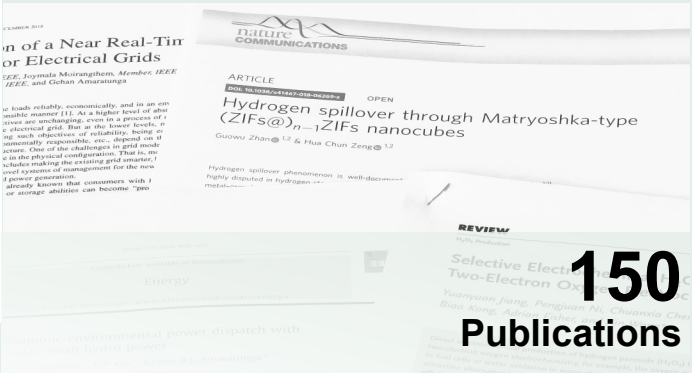

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FOREWORD

The past six months have been exciting ones – the Centre for Lifelong Learning and Individualised Cognition (CLIC) was awarded a further three-year grant by NRF CREATE and the Centre for Carbon Reduction in Chemical Technologies (C4T2) has been extended for two additional years. Both programmes have been enjoying active engagements with local and international stakeholders, including government agencies, policymakers, and relevant industry. The CARES-Singapore ETH Centre (SEC) Intra-CREATE project, Cities Knowledge Graph, came to its conclusion in September and held a successful project completion event to disseminate its findings to relevant parties, including the Singapore Land Transport Authority and the Urban Redevelopment Authority.

CARES drone at the world's first methanol bunkering operation

In a brilliant crossover of academic work and industrial objectives, a drone carrying emissions measurement technology developed in C4T was used to monitor for methanol leaks during the world's first ship-to-containership methanol bunkering operation in August 2023. The Maritime & Port Authority of Singapore coordinated this operation, having first encountered the CARES technology at our public presentation in April. With Singapore driving key activities in the transition to low/zero carbon fuels, I am enthusiastic our proximity to partners in the region will enable further collaboration.

New Pharma Innovation Programme Singapore (PIPS) projects

As our PIPS Pfizer project nears completion, we are moving forward with two new projects within the PIPS public-private partnership framework. CARES will host a project on digital twins for plant operations and another on rapid assessment of the environmental impacts of pharma processes with predictive tools. The PIPS projects will bring CARES research to bear on problem statements of importance to the PIPS pharma industry member companies. The C4T spin-off Chemical Data Intelligence Pte Ltd will also partner with CARES for one of the projects.

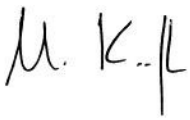
CLIC policy workshop and Brainiverse events

The CLIC programme coordinated a number of public impact events for government agency stakeholders and the Singaporean public in August and September 2023. The policy workshop welcomed staff from Ministry of Education and the Ministry of Social and Family Development and more than 1500 members of the public enjoyed exploring the brain's capabilities in two Brainiverse events at the Singapore ArtScience Museum.

CARES 10th anniversary Scientific Showcase

We are very much looking forward to welcoming several hundred guests both locally and overseas to the culmination of our 10th anniversary year with a Scientific Showcase in December (https://www.cares.cam.ac.uk/10anniversary/). The event will showcase the past decade of our outstanding research science, including our spin-off companies and emerging technologies – I hope to see you there!

Professor Markus Kraft, CARES Director
March 2023



ABOUT US

Cambridge CARES is the University of Cambridge's presence in Singapore

The Cambridge Centre for Advanced Research and Education in Singapore (CARES) is a wholly-owned subsidiary of the University of Cambridge. Cambridge CARES is funded by the National Research Foundation as part of CREATE (Campus for Research Excellence and Technological Enterprise). We have a number of research collaborations between the University of Cambridge, Nanyang Technological University, the National University of Singapore and industrial partners.

The first programme administered by CARES is the Cambridge Centre for Carbon Reduction in Chemical Technology (C4T). The C4T programme is a world-leading partnership between Cambridge and Singapore, set up to tackle the environmentally relevant and complex problem of assessing and reducing the carbon footprint of the integrated petro-chemical plants on Singapore's Jurong Island. It brings together researchers from chemical engineering, biotechnology, chemistry, biochemistry, information engineering, electrical engineering, materials science and metallurgy.

The motivation for the C4T project is to provide a rich pipeline of scientific insight and technological innovation with high potential for positive results within the decarbonisation agenda if deployed by appropriate industry and government parties. Our six collaborative Interdisciplinary Research Programmes (IRPs) combine state-of-the-art experimental analysis with advanced modelling research from Cambridge and Singapore. Whilst each IRP has clearly defined milestones and deliverables, denoted as work packages (WPs), there is significant interaction between the IRPs.

The first five-year research phase of C4T came to an end in October 2018. The programme received a further five years of funding for Phase 2, which commenced in November 2018 and has recently been further extended to 2025.

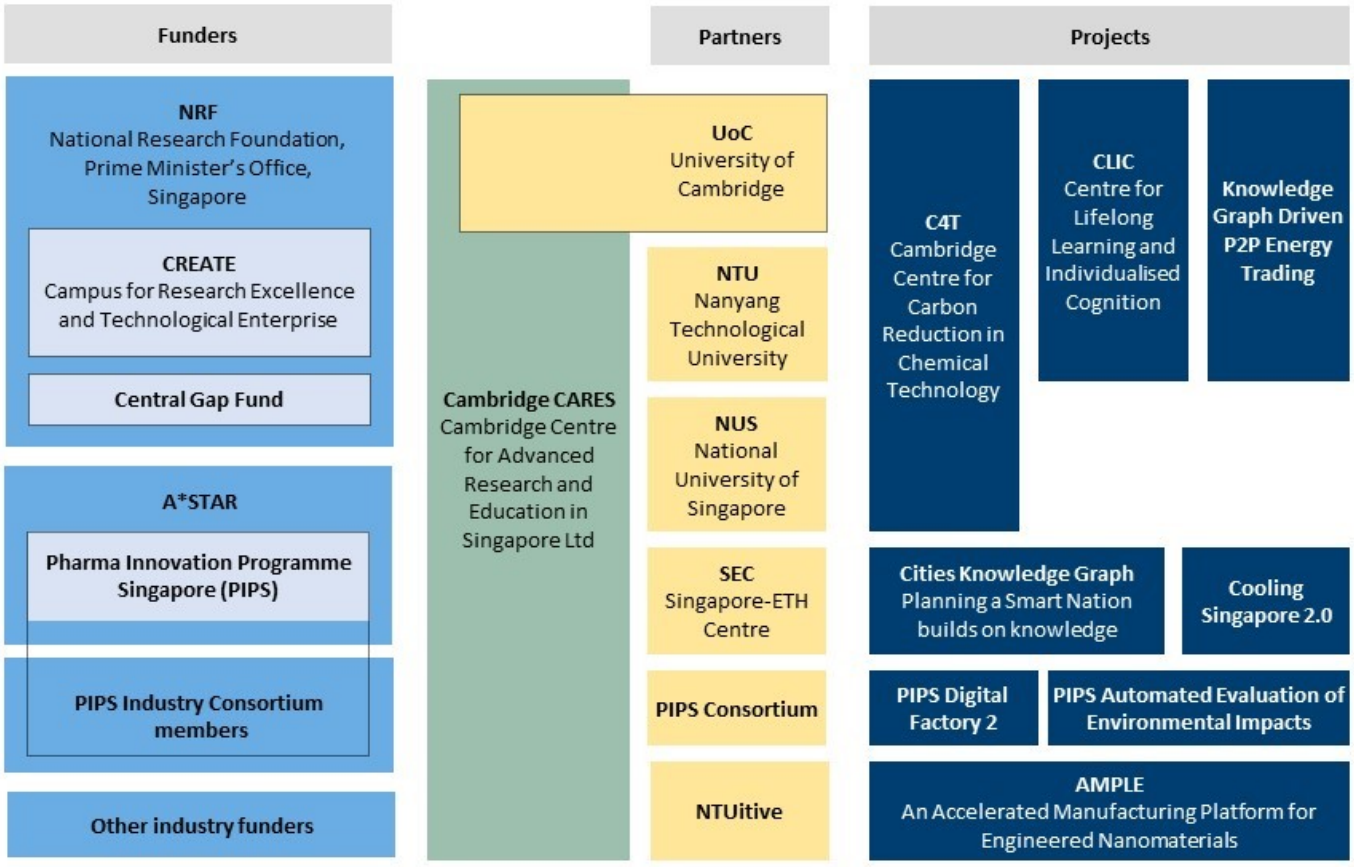
A second large CREATE-funded programme, the Centre for Lifelong Learning and Individualised Cognition (CLIC), began in October 2020. CLIC is a collaboration between University of Cambridge and NTU and focuses on the neuroscience of learning, a new research area for CARES. CLIC has recently received confirmation of a further three years of funding, extending the programme to September 2026.

In April 2020, CARES was awarded a further Intra-CREATE large grant for Cities Knowledge Graph, which brings together researchers from

University of Cambridge and ETH Zürich to harness rapidly growing and diversifying data streams to improve the planning and design of cities. A digital platform was developed in the form of a dynamic knowledge graph which combines multi-domain data to share knowledge about cities. These research findings were disseminated at a lecture and interactive demonstration event during the recent Cities Knowledge Graph completion event.

As well as this large Intra-CREATE grant, CARES is hosting AMPLE (An Accelerated Manufacturing Platform for Engineered Nanomaterials), funded by the Central Gap Fund. There are several smaller projects and spin-offs ongoing: The Intra-CREATE seed funded Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables, and currently three ongoing streams under the Pharmaceutical Innovation Programme Singapore (PIPS); one stream involves industry funding with Pfizer. CARES also takes part in the Cooling Singapore 2.0 programme hosted by the Singapore-ETH Centre. Details and updates for these smaller projects can be found on page 130.

This report is a summary of our last half-year of research progress. It includes scientific updates from each of our researchers, along with abstracts and figures from our recent publications. There are also several articles that explain the fundamental science behind some of our work, and the impact this can have to our society.



HIGHLIGHTS

OUTSTANDING WORK FROM THE LAST SIX MONTHS OF CAMBRIDGE CARES RESEARCH

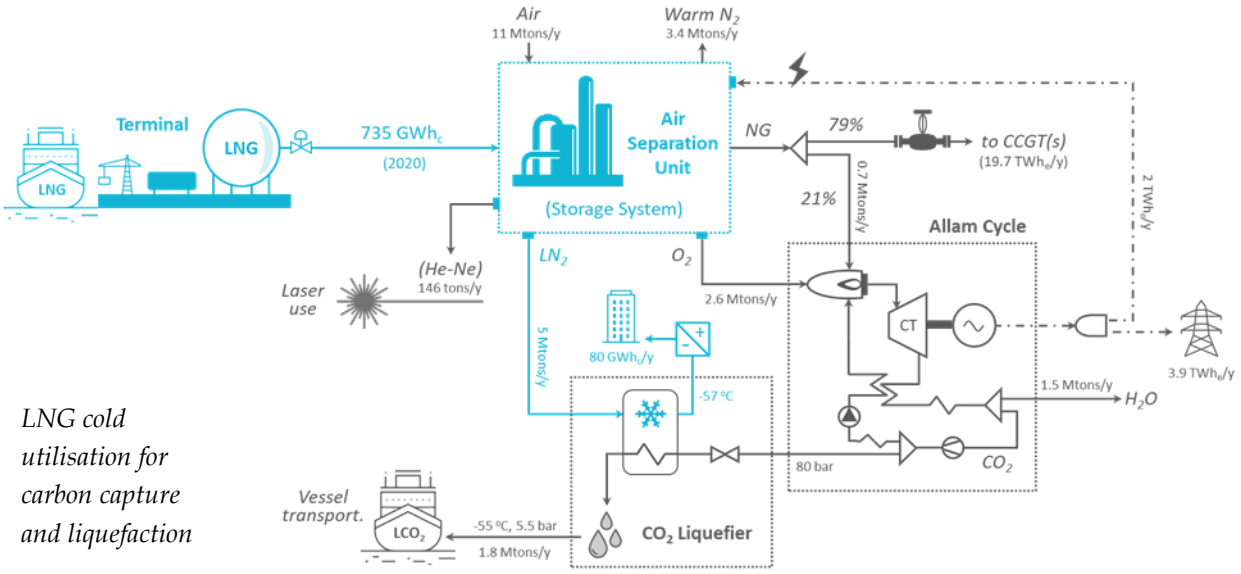
Development and assessment of LNG and LH_2 cold utilisation strategies for Singapore

Dr Mohamed Fadhel AYACHI, Senior Research Fellow, C4T IRP 4

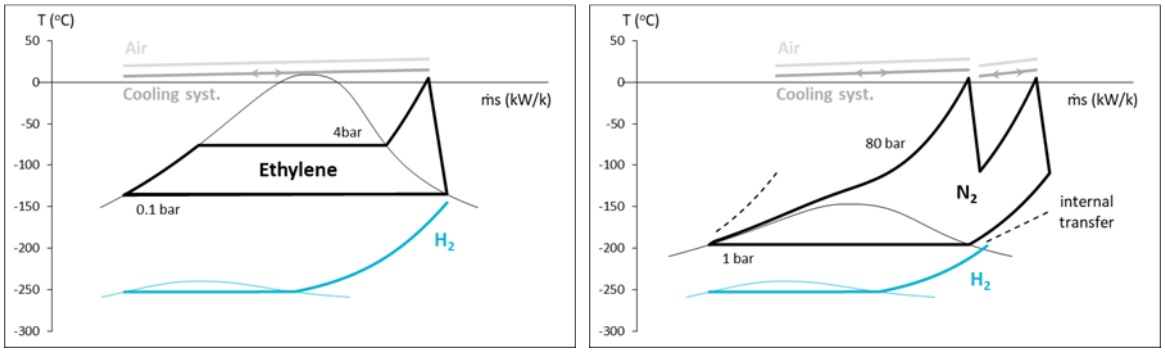
To date, Singapore is heavily reliant on natural gas imports for electricity generation, representing 95% of the fuel mix. With the opening of the SLNG terminal in 2013, LNG imports have growth to reach 35% of total natural gas imports in 2020 and 2021. This LNG imported at -162°C is also a potential source of cold energy. It is estimated that about 735 GWh of LNG cold energy was wasted in 2020.

The figure below illustrates one potential business case for Singapore in today's context; it meets energy savings strategies that seek to exploit the LNG cold energy content and environmentally friendly objectives that support carbon capture and storage. The LNG cold energy is mainly utilised to (i) produce oxygen for an Allam cycle that is able to burn up to 21% of the regasified natural gas and (ii) liquefy the resulting CO_2 capture (up to 1.8 million tons per year) for maritime transportation.

On the other hand, Singapore strives to develop a hydrogen economy within the first half of this century. Hydrogen will complement and diversify its power mix alongside solar, imported electricity, and other potential low-carbon energy sources. Depending on technological developments and the development of other energy sources, hydrogen could supply up to half of Singapore's power needs by 2050 and would play an important role in decarbonising its industry. In other regards, the potential import of Liquid Hydrogen (LH_2) to tropical countries, such as Singapore, will bring an available high-grade cold energy content that far exceeds the LNG cold energy content. This LH_2 high-grade cold available at -253°C can be subject to Cold Energy Storage using Phase Change Materials (PCM) as it can be more efficiently exploited for the combined generation of cooling and power.



LNG cold utilisation for carbon capture and liquefaction



Entropy diagrams referred to 1000-tpd LH_2 terminal. (left) Very-low-boiling point ORC [5 – 7.8 MW_e / < 45 MW_c], (right) NTU's IP cryo-cogenerator [15.7 MW_e / 50 MW_c]

The figure above shows two entropy diagrams of two high-grade cold recovery systems using a LH_2 terminal capacity of 1 kiloton per day. Using the same x-axis scale, we compare an Organic Rankine Cycle (ORC) using a very-low-boiling point fluid such as Acetylene (Ethyne) or Ethylene (Ethene) with a conceptual cryo-cogeneration energy system. The figure shows the downside of using an ORC for the recovery of the high-grade cold energy from LH_2 regasification (i.e., high exergy destruction in the evaporator and in the condenser). Conversely, an LH_2-driven cryo-cogeneration system that uses Nitrogen as a working fluid in a multistage cryogenic closed cycle appears to have the adequate properties for a combined generation of cooling and power from LH_2 regasification. It would be able to deliver a continuous cold energy supply to refrigerated warehouses or district cooling systems in warm climates of up to 50 MW_c and appears capable to deliver twice the power output of an organic Rankine cycle (i.e., 15.7 MW_e). This represents a potential recovery of up to 10% of the liquefaction energy consumed prior to shipment, which could represent a possible economic upside in the hydrogen supply chain.

More information on IRP 4's work can be found on page 57 of the report.

Dr Mohamed Fadhel Ayachi is a Senior Research Fellow at NTU. He joined the Energy Research Institute @NTU and the Thermal Energy Systems Lab @NTU in 2017; he has been working on a novel zero-emission concept of cryo-cogeneration system for cooling and power applications, in particular data centres. In 2022, he carried out a heat integration and optimisation study that explored the different solutions that can be undertaken in the city state of Singapore to minimise the energy consumption of the conceptual SPERA-based Hydrogen production facility. In March 2023 he joined CARES with Prof Alessandro Romagnoli as his PI.

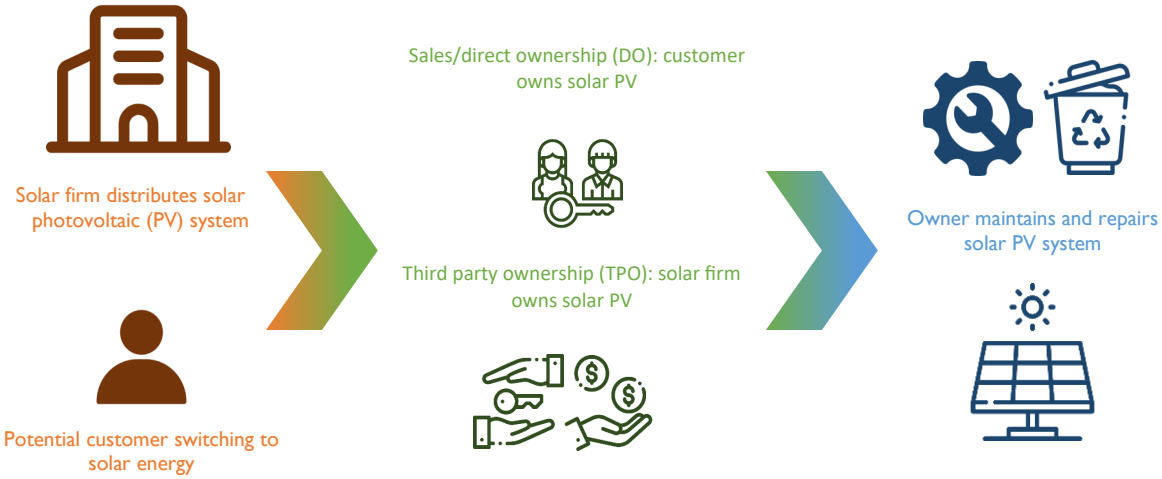
Economics of the energy transition: business models for green technology adoption and carbon utilisation methods

Dr Lemy MARTIN, Research Fellow, C4T IRP BB

Singapore's commitment to achieving net zero emissions by 2050 is emblematic of a global sustainability shift. This target requires adopting multiple decarbonisation pathways that may take years to fully mature or exhibit investment returns. In CARES, the IRP BB team works at the intersection of sustainability and business to balance the transition towards sustainable technologies and ensure economic viability for all stakeholders.

Key to achieving net zero is the energy transition, as shifting to renewables like solar will significantly reduce carbon emissions. For potential solar customers, the difficulty of shifting lies in the investment – notably, the high cost of installing and maintaining rooftop solar power systems. While these installations arguably pay for themselves in the long run, the lengthy payback period and maintenance concerns can function as deterrents towards adoption.

To innovate, some solar power firms offer an alternative called third-party ownership (TPO), wherein the firm funds the system installation and maintenance costs while the rooftop owner pays the firm for the right to use the generated electricity. This payment can be a fixed periodic lease payment or per unit of consumption (e.g., a power purchasing agreement (PPA)). Our research uses game theory to model how the firm and its customers interact under this menu of business models and determine when a particular model is preferred over the rest. We find that customers prefer to buy and maintain their own systems when their risk appetites are high or transaction costs (e.g., maintenance and disposal)



An outline of the firm-customer interaction in rooftop solar adoption.

are lower versus under TPOs. We also find that if customers have different generating capacities and/or electricity demand, at least one customer will prefer leasing whereas another will prefer PPA. We develop pricing algorithms for these models and even consider hybrid pricing wherein customers pay a fixed amount alongside a payment per unit consumption with lower rates compared to the full leasing or PPA prices.

While the world transitions away from fossil fuels, some sectors may find this difficult. For instance, the aviation sector is likely to continue relying on jet fuel. The focus now shifts upstream towards low carbon alternatives such as synthetic fuel (synfuel), wherein green hydrogen is combined with captured carbon from industrial processes to produce fuel. While more expensive to produce versus crude oil-based fuel, the added cost can be viewed as the price of abating the captured carbon for a cycle and avoiding the fossil fuel-based production emissions. We call this the consequential carbon utilization price (CCUP). Our research compares the CCUP of producing synfuel locally using green hydrogen imports versus exporting captured carbon for overseas production. We find that overseas production is more economically viable compared to local production due to the high cost of importing hydrogen. However, other factors such as economies of scale, subsidies, and maturing technologies can reduce the CCUP further or even close the gap to make local production competitive.

Many difficulties lie ahead as Singapore and the rest of the world move towards a net zero future. Ensuring that everyone can transition towards more sustainable technologies creates new opportunities that can birth innovative methods and synergies across stakeholders and industries.

More information on IRP BB's work can be found on page 71 of the report.

Dr J. Lemuel Martin is a Research Fellow at CARES and the Energy Research Institute at NTU (ERI@N) where his work centers on the development of business models for green technologies and analysis of decarbonisation pathways. He earned his PhD in Operations Management from Nanyang Business School in Singapore, focusing on the use of operations management methods to assess and provide actionable insights on humanitarian-related issues with prominent behavioural components, such as in-kind donations management, panic buying, and ad-hoc disaster response. His work has employed the use of game theory, inventory theory, stochastic processes, optimisation, economics, heuristics, and simulation.

Highlighted research outputs from April - September 2023

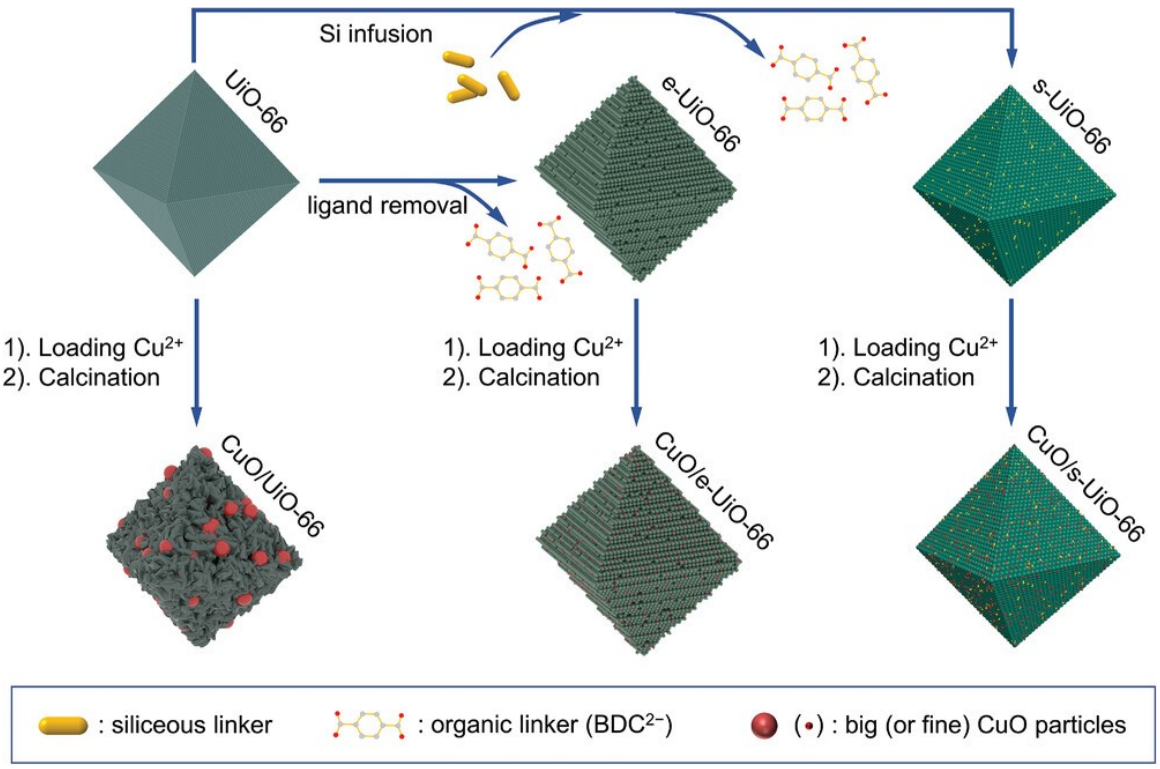
A selection of publications from across our programmes.

C4T IRP 1: Uniform Si-Infused UiO-66 as a Robust Catalyst Host for Efficient CO_2 Hydrogenation to Methanol

Chao Wang, Mohammadreza Kosari, Shibo Xi, and Hua Chun Zeng , *Advanced Functional Materials*

DOI: 10.1002/adfm.202212478

Abstract: Due to the weak nature of organic coordination bonds, metal–organic frameworks (MOFs) can hardly retain their intrinsic physicochemical properties and structural integrity when functioning in harsh heterogeneous reactions. Herein, a post-synthetic strategy to reinforce the MOF structure by inserting siliceous linkers inside is proposed, according to which a Si-infused UiO-66 (s-UiO-66) with well-developed porosity and exceptional thermal/structural stability is fabricated. This monodispersed Si-infused matrix with enlarged nanopores is then utilized as the catalyst host, and is highly conductive to confining ultrafine CuO nanoparticles with uniform dispersion. Targeting CO_2 hydrogenation to methanol reaction, the Cu-loaded s-UiO-66 (CuO/s-UiO-66) delivers a remarkable and efficient methanol production rate outperforming other Cu/ZrO2-based catalysts and the commercial catalyst. Moreover, the robust structure of CuO/s-UiO-66 prevents both copper phase and host material from aggregation during the catalyst preparation procedure and the reaction. In addition to material-oriented studies, in situ characterization techniques are employed to identify the active Cu component and key intermediates formed during the CO_2 hydrogenation reaction, separately. It is envisioned that this Si infusion strategy can be applied to construct stable host materials with boundary-defined structures from the pristine MOFs for broadened applications under extreme circumstances.

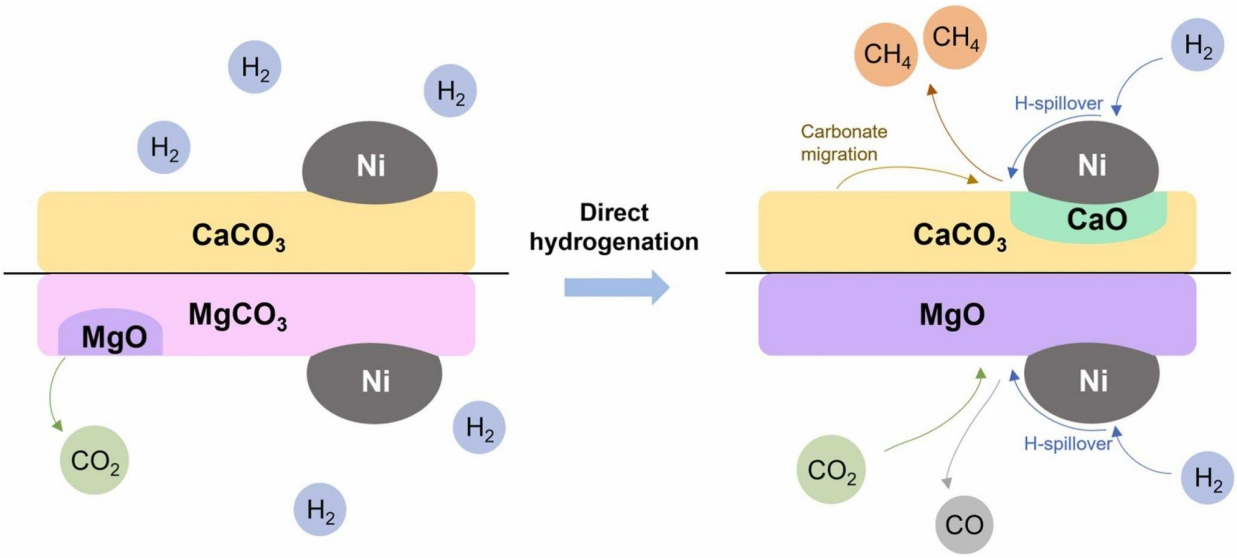


C4T IRP 1: An investigation of the Ni/carbonate interfaces on dual function materials in integrated CO_2 capture and utilisation cycles

Xianyue Wu, Ribooga Chang, Mingwu Tan, Longgang Tao, Qianwenhao Fan, Xiaochun Hu, Hui Ling Tan, Michelle Åhlén, Ocean Cheung, and Wen Liu, *Applied Catalysis B: Environmental*

DOI: 10.1016/j.apcatb.2023.123053

Abstract: CO_2 capture and utilisation (CCU) is a promising strategy to effectively mitigate the adverse greenhouse effects caused by CO_2 emissions at an industrial scale. Through a process intensification strategy known as integrated CO_2 capture and utilisation (ICCU), CO_2 capture and catalytic CO_2 conversion can be achieved in a single process with the use of dual function materials (DFMs), which are both CO_2 sorbents and CO_2 conversion catalysts. Given the significantly different operating conditions of ICCU from conventional catalytic CO_2 hydrogenation, the catalytic mechanism of DFMs, especially during CO_2 hydrogenation, needs to be thoroughly investigated. In this study, the relationship between the nature of the Ni/carbonate interfaces and the performance of Ni-based DFMs over ICCU cycles is systematically investigated. A series of Ni/alkaline earth carbonate DFMs were synthesised with varying Ca:Mg ratios to simulate different metal-carbonate model interfaces. At 400 °C, CH_4 formation with nearly 100% CH_4 selectivity was achieved on Ni/$CaCO_3$ over 15 ICCU cycles. In general, Ni/$CaCO_3$ interfaces correspond to higher CO_2 conversion and higher CH_4 selectivity than Ni/$MgCO_3$ interfaces. Such trend may be attributed to the higher surface basicity of CaO and the higher thermal stability of $CaCO_3$. As a consequence, the hydrogenation of the Ni/$CaCO_3$ interface proceed via the formate pathway, in which carbonates are consecutively converted to surface formates, methoxyl, methyl species and eventually desorb as methane. This reaction model is applicable to the hydrogenation of both surface carbonate and bulk carbonates, although the former proceeds with much faster kinetics. On the weakly alkaline Ni/$MgCO_3$ interface, $MgCO_3$ preferentially decomposes to form gaseous CO_2, which is subsequently hydrogenated via the reverse-water-gas-shift pathway, with CO as the key reaction intermediate. Interestingly, in situ infrared spectroscopy shows similar surface significant species during the direct hydrogenation of DFMs and during the conventional catalytic hydrogenation of molecular CO_2, suggesting that the catalytic mechanisms during the two operating regimes are highly correlated.



C4T IRP 1: Three-Dimensional Assemblages of Metal Silicate for Catalytic CO_2 Conversion to Methanol and Adsorptive Pollutant Removal

Bo Sun, Alvin M. H. Lim, and Hua Chun Zeng, *ACS Sustainable Chemistry & Engineering*

DOI: 10.1021/acssuschemeng.3c00960

Abstract: Morphological transformation was performed on Stöber silica nanospheres (ca. 270 nm in diameter) and transmuted into either ZnSiO (zinc silicate) nanoflowers or MgSiO (magnesium silicate) nanoflowers (600–800 nm in diameter) through a facile hydrothermal process. The zinc silicate materials were then chosen for incipient wetness impregnation to imbue them with different levels of Cu and Zn doping due to the well-established elemental synergy of Cu and Zn toward methanol synthesis via CO_2 hydrogenation. Characterization results concur that zinc silicate nanoflowers loaded with copper(II) oxide were formed after incipient wetness impregnation. Three as-synthesized catalyst candidates with different copper loadings were then evaluated for CO_2 hydrogenation and compared against an industrial catalyst. After the reaction, high-resolution transmission electron microscopy (HRTEM) with energy-dispersive X-ray (EDX) elemental mapping reveal that petite Cu nanoparticles formed on the petals of the impregnated zinc silicate nanoflowers. Experimental results show that all catalyst materials have an exceptional high methanol selectivity, with overall performance exceeding that of the industrial catalyst at per Cu basis. Both ZnSiO and MgSiO were also evaluated through a simple methylene blue adsorption test. Hence, through deliberate morphological control and chemical transformation, superficially inert Stöber silica nanospheres were functionalized into transition- and earth-alkaline metal silicates, which exhibit catalytic and adsorptive properties with a nanoflower morphology that prevents interstacking of nanosheets.

C4T IRP 1: Strained few-layer MoS_2 with atomic copper and selectively exposed in-plane sulfur vacancies for CO_2 hydrogenation to methanol

Shenghui Zhou, Wenrui Ma, Uzma Anjum, Mohammadreza Kosari, Shibo Xi, Sergey M. Kozlov, and Hua Chun Zeng, *Nature Communications*

DOI: 10.1038/s41467-023-41362-y

Abstract: In-plane sulfur vacancies (Sv) in molybdenum disulfide (MoS_2) were newly unveiled for CO_2 hydrogenation to methanol, whereas edge Sv were found to facilitate methane formation. Thus, selective exposure and activation of basal plane is crucial for methanol synthesis. Here, we report a mesoporous silica-encapsulated MoS_2 catalysts with fullerene-like structure and atomic copper ($Cu/MoS_2@SiO_2$). The main approach is based on a physically constrained topologic conversion of molybdenum dioxide (MoO_2) to MoS_2 within silica. The spherical curvature enables the generation of strain and Sv in inert basal plane. More importantly, fullerene-like structure of few-layer MoS_2 can selectively expose in-plane Sv and reduce the exposure of edge Sv. After promotion by atomic copper, the resultant $Cu/MoS_2@SiO_2$ exhibits stable specific methanol yield of 6.11 $mol_{MeOH}\ mol_{Mo}^{-1}\ h^{-1}$ with methanol selectivity of 72.5% at 260 °C, much superior to its counterparts lacking the fullerene-like structure and copper decoration. The reaction mechanism and promoting role of copper are investigated by in-situ DRIFTS and in-situ XAS. Theoretical calculations demonstrate that the compressive strain facilitates Sv formation and CO_2 hydrogenation, while tensile strain accelerates the regeneration of active sites, rationalizing the critical role of strain.

C4T IRP 2: The origin of magnetization-caused increment in water oxidation

Xiao Ren, Tianze Wu, Zizhao Gong, Lulu Pan, Jianling Meng, Haitao Yang, Freyja Bjork Dagbjartsdottir, Adrian Fisher, Hong-Jun Gao, and Zhichuan J. Xu, *Nature Communications*

DOI: 10.1038/s41467-023-38212-2

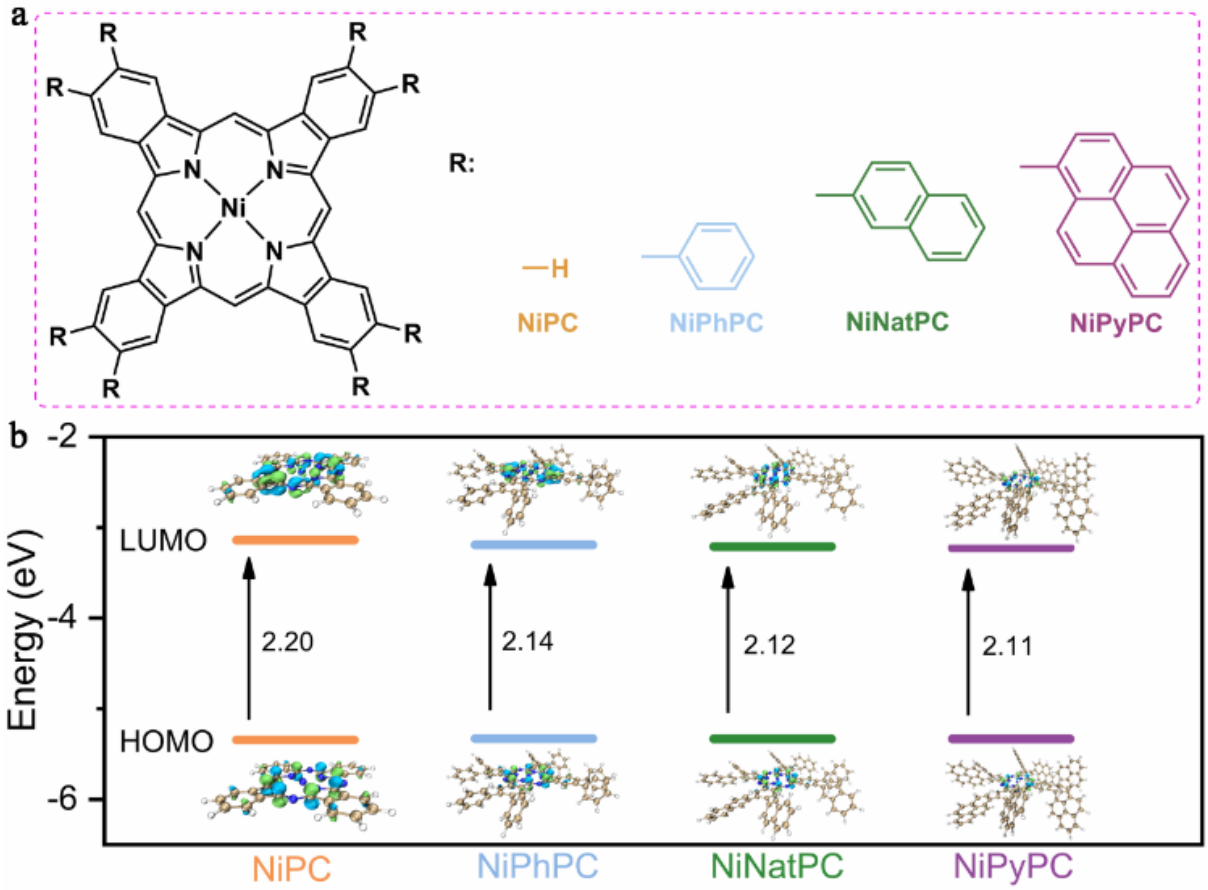
Abstract: Magnetization promoted activity of magnetic catalysts towards the oxygen evolution reaction (OER) has attracted great attention, but remains a puzzle where the increment comes from. Magnetization of a ferromagnetic material only changes its magnetic domain structure. It does not directly change the spin orientation of unpaired electrons in the material. The confusion is that each magnetic domain is a small magnet and theoretically the spin-polarization promoted OER already occurs on these magnetic domains, and thus the enhancement should have been achieved without magnetization. Here, we demonstrate that the enhancement comes from the disappeared domain wall upon magnetization. Magnetization leads to the evolution of the magnetic domain structure, from a multi-domain one to a single domain one, in which the domain wall disappears. The surface occupied by the domain wall is reformatted into one by a single domain, on which the OER follows the spin-facilitated pathways and thus the overall increment on the electrode occurs. This study fills the missing gap for understanding the spin-polarized OER and it further explains the type of ferromagnetic catalysts which can give increment by magnetization.

C4T IRP 2: Conjugated Nickel Phthalocyanine Derivatives for Heterogeneous Electrocatalytic H_2O_2 Synthesis

Libo Sun, Xindie Jin, Tan Su, Adrian C. Fisher, and Xin Wang, *Advanced Materials*

DOI: 10.1002/adma.202306336

Abstract: Electrocatalytic H_2O_2 production has emerged as a promising alternative to the chemical method currently used in industry, due to its environmentally friendly conditions and potential for higher activity and selectivity. Heterogeneous molecular catalysts are promising in this regard, as their active site configurations could be judiciously designed, modified and tailored with diverse functional groups, thereby tuning the activity and selectivity of the active sites. In this work, nickel phthalocyanine derivatives with various conjugation degrees were synthesized and identified as effective pH-universal electrocatalysts for H_2O_2 production after heterogenized on nitrogen-decorated carbon, with increased conjugation degrees leading to boosted selectivity. This is explained by the regulated d-band center, which optimized the binding energy of the reaction intermediate, reducing the energy barrier for oxygen reduction and leading to optimized H_2O_2 selectivity. The best catalyst, NiPyCN/CN, exhibits a high H_2O_2 electrosynthesis activity with nearly 95% of H_2O_2 faradic efficiency in an alkaline medium, demonstrating its potential for H_2O_2 production.



C4T IRP 3: Carbon conversion by Methanococcus maripaludis S2 under diazotrophy and a revised genome-scale metabolic model

Chi Hung Vo, Nishu Goyal, Markus Kraft, and Iftekhar A. Karimi, *Chemical Engineering Science*

DOI: 10.1016/j.ces.2023.118910

Abstract: *Methanococcus maripaludis* can utilize CO_2 as the sole carbon source. Since N_2 is a major component of most flue gases, understanding its impact on the cellular behaviours of *M. maripaludis* is critical. Here, we studied CO_2 conversion by *M. maripaludis* S2 in minimal media with ammonium or N_2 as the sole nitrogen source. N_2-grown cultures exhibited a long lag phase, prolonged growth phase, and lower cell density compared to ammonium. At any specific growth rate, the CO_2 intake and CH_4 evolution fluxes were higher for N_2 than ammonium, suggesting that N_2 is a better nitrogen source for carbon conversion to CH_4. The flux measurements were used to improve a genome-scale metabolic model existing in the literature. The revised model *i*MR557 has a coverage of 32% open reading frames and includes new pathways. *i*MR557 was used to illustrate flux distributions under different conditions and successfully replicate the previously reported acetate dissimilation.

C4T IRP BB: Feasibility of Green Hydrogen-Based Synthetic Fuel as a Carbon Utilization Option: An Economic Analysis

J. Lemuel Martin and S. Viswanathan, *Energies*

DOI: 10.3390/en16176399

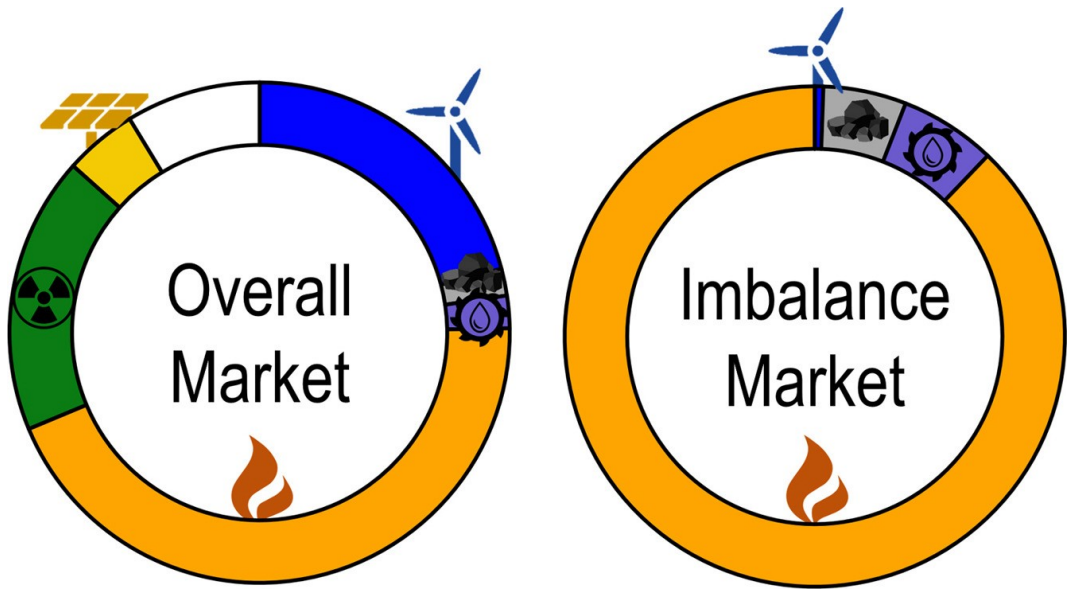
Abstract: Singapore has committed to achieving net zero emissions by 2050, which requires the pursuit of multiple decarbonization pathways. CO_2 utilization methods such as fuel production may provide a fast interim solution for carbon abatement. This paper evaluates the feasibility of green hydrogen-based synthetic fuel (synfuel) production as a method for utilizing captured CO_2. We consider several scenarios: a baseline scenario with no changes, local production of synfuel with hydrogen imports, and overseas production of synfuel with CO_2 exports. This paper aims to determine a CO_2 price for synfuel production, evaluate the economic viability of local versus overseas production, and investigate the effect of different cost parameters on economic viability. Using the current literature, we estimate the associated production and transport costs under each scenario. We introduce a CO_2 utilization price (CUP) that estimates the price of utilizing captured CO_2 to produce synfuel, and an adjusted CO_2 utilization price (CCUP) that takes into account the avoided emissions from crude oil-based fuel production. We find that overseas production is more economically viable compared to local production, with the best case CCUP bounds giving a range of 142 –148 $\$/tCO_2$ in 2050 if CO_2 transport and fuel shipping costs are low. This is primarily due to the high cost of hydrogen feedstock, especially the transport cost, which can offset the combined costs of CO_2 transport and fuel shipping. In general, we find that any increase in the hydrogen feedstock cost can significantly affect the CCUP for local production. Sensitivity analysis reveals that hydrogen transport cost has a significant impact on the viability of local production and if this cost is reduced significantly, local production can be cheaper than overseas production. The same is true if the economies of scale for local production is significantly better than overseas production. A significantly lower carbon capture cost can also the reduce the CCUP significantly.

C4T IRP JPS: British imbalance market paradox: Variable renewable energy penetration in energy markets

John Atherton, Markus Hofmeister, Sebastian Mosbach, Jethro Akroyd, Feroz Farazi, and Markus Kraft,
Renewable and Sustainable Energy Reviews

DOI: 10.1016/j.rser.2023.113591

Abstract: The expansion of variable renewable energy (VRE) generation propagates numerous challenges for national energy systems. Despite recent years of VRE expansion and declining coal utilisation in the overall market profile, coal energy generation has maintained and grown its position as a marginal seller in the imbalance market. Coal's disproportionate resurgence as a bidder of later resort in the imbalance market also represents a shift in its bidding behaviour. A comparative breakdown of Britain's overall market with that of Germany, followed by a specific investigation of Britain's imbalance market provides insight into changing roles of VRE, fossil fuelled energy, and compensation technologies. Historically, VRE trends in the British and German markets have been broadly consistent. Recently, increasing distress in Britain's overall market is found to result in the increased use of high pollution technologies to meet imbalances. As a result, the composition of the overall and imbalance markets have increasingly diverged, and although the dominance of gas in the latter is expected, the resurgence of coal energy is more remarkable. Thus, while the proportion of generation by renewables has continued to increase, fossil fuelled (notably including coal) capacity, and its associated infrastructure costs and influence as the price setting marginal seller, remains dominant in the imbalance market.

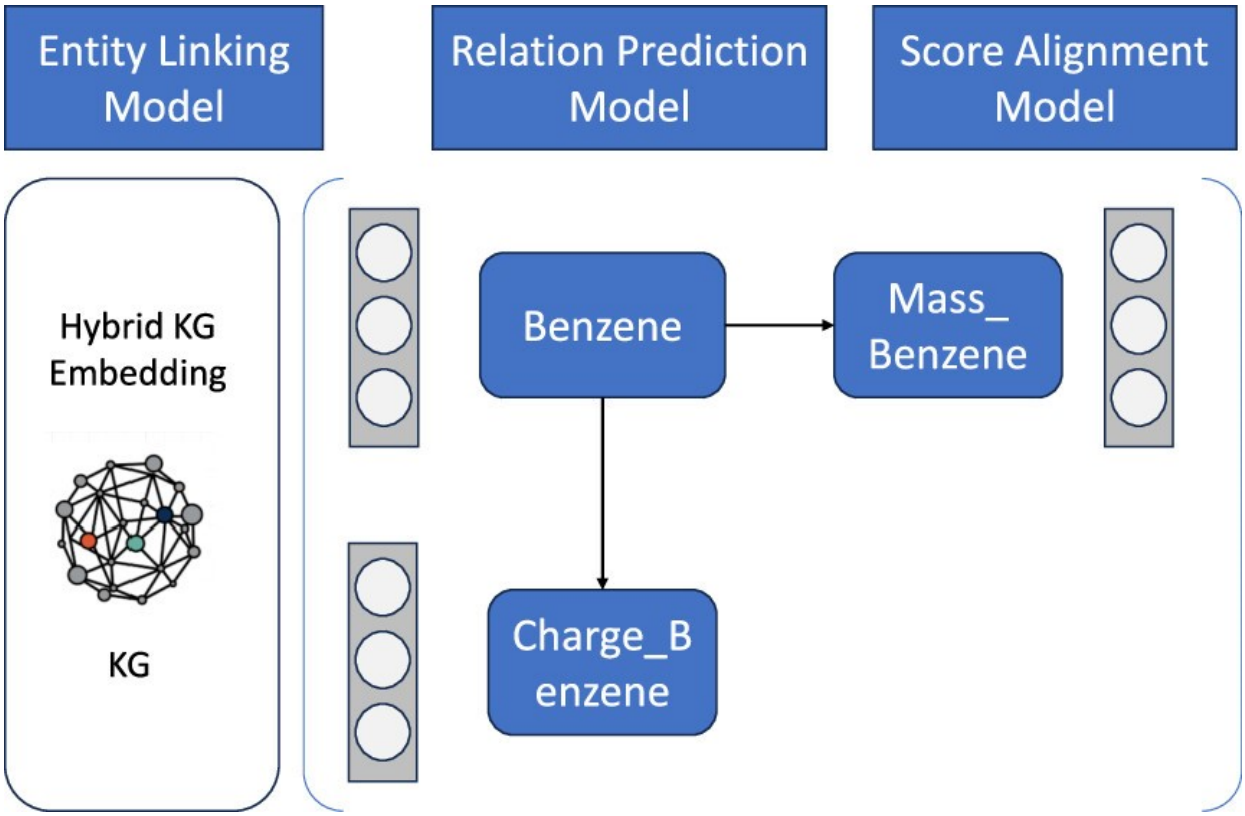


C4T IRP JPS: Marie and BERT—A Knowledge Graph Embedding Based Question Answering System for Chemistry

Xiaochi Zhou, Shaocong Zhang, Mehal Agarwal, Jethro Akroyd, Sebastian Mosbach, and Markus Kraft, *ACS Omega*

DOI: 10.1021/acsomega.3c05114

Abstract: This paper presents a novel knowledge graph question answering (KGQA) system for chemistry, which is implemented on hybrid knowledge graph embeddings, aiming to provide fact-oriented information retrieval for chemistry-related research and industrial applications. Unlike other existing designs, the system operates on multiple embedding spaces, which use various embedding methods and queries the embedding spaces in parallel. With the answers returned from multiple embedding spaces, the system leverages a score alignment model to adjust the answer scores and rerank the answers. Further, the system implements an algorithm to derive implicit multihop relations to handle the complexities of deep ontologies and improve multihop question answering. The system also implements a BERT-based bidirectional entity-linking model to enhance the robustness and accuracy of the entity-linking module. The system uses a joint numerical embedding model to efficiently handle numerical filtering questions. Further, it can invoke semantic agents to perform dynamic calculations autonomously. Finally, the KGQA system handles numerous chemical reaction mechanisms using semantic parsing supported by a Linked Data Fragment server. This paper evaluates the accuracy of each module within the KGQA system with a chemistry question data set.

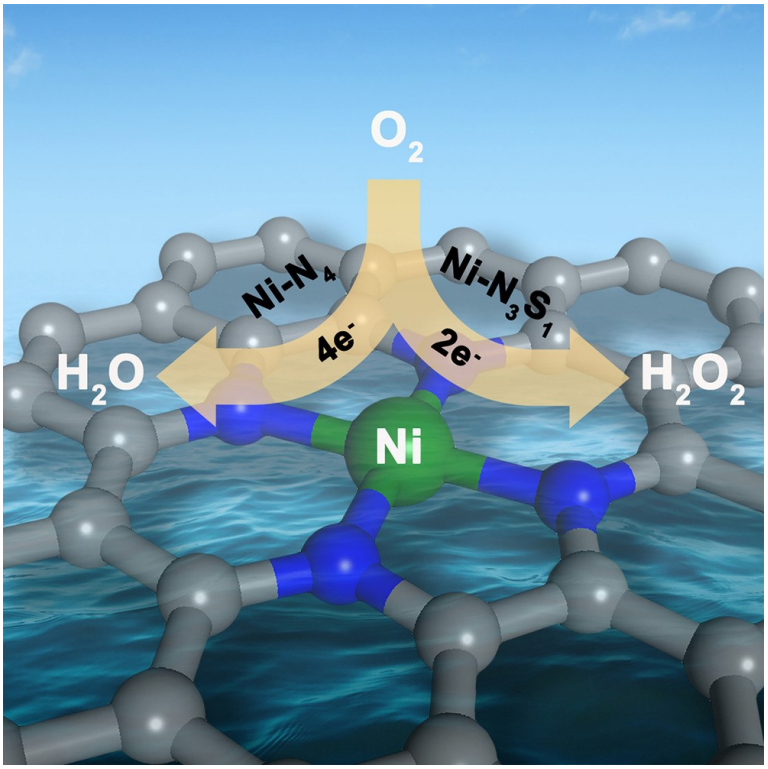


C4T IRP 1 and IRP 2: Sulfur-modulated isolated NiNx sites toward electrocatalytic hydrogen peroxide generation

Xiaogang Li, Wenjie Xu, Luan Q. Le, Shuangming Chen, Li Song, Tej S. Choksi, and Xin Wang , *Chem Catalysis*

DOI: 10.1016/j.checat.2023.100724

Abstract: Achieving hydrogen peroxide (H_2O_2) production through the electrocatalytic two-electron (2e−) oxygen reduction reaction (ORR) is a crucial alternative to the energy-intensive anthraquinone process. The competitive four-electron (4e−) ORR pathway, however, limits the selectivity to H_2O_2. Here, we report the rational design of isolated NiN3S moieties by introducing one sulfur atom into NiNx sites embedded in carbon supports. The sulfur-modified active sites yield a selectivity of nearly 90% for H_2O_2 generation. Density functional theory calculations indicate that incorporation of sulfur in Ni's coordination environment, together with oxidation of the active-site motif, weakens the adsorption energy of OOH∗. This weakening of adsorption strengths for a key reaction intermediate in the 2e− pathway increases selectivity toward H_2O_2. This work provides a promising approach to direct the selectivity of oxygen reduction by modulating the local structure of isolated metal sites.

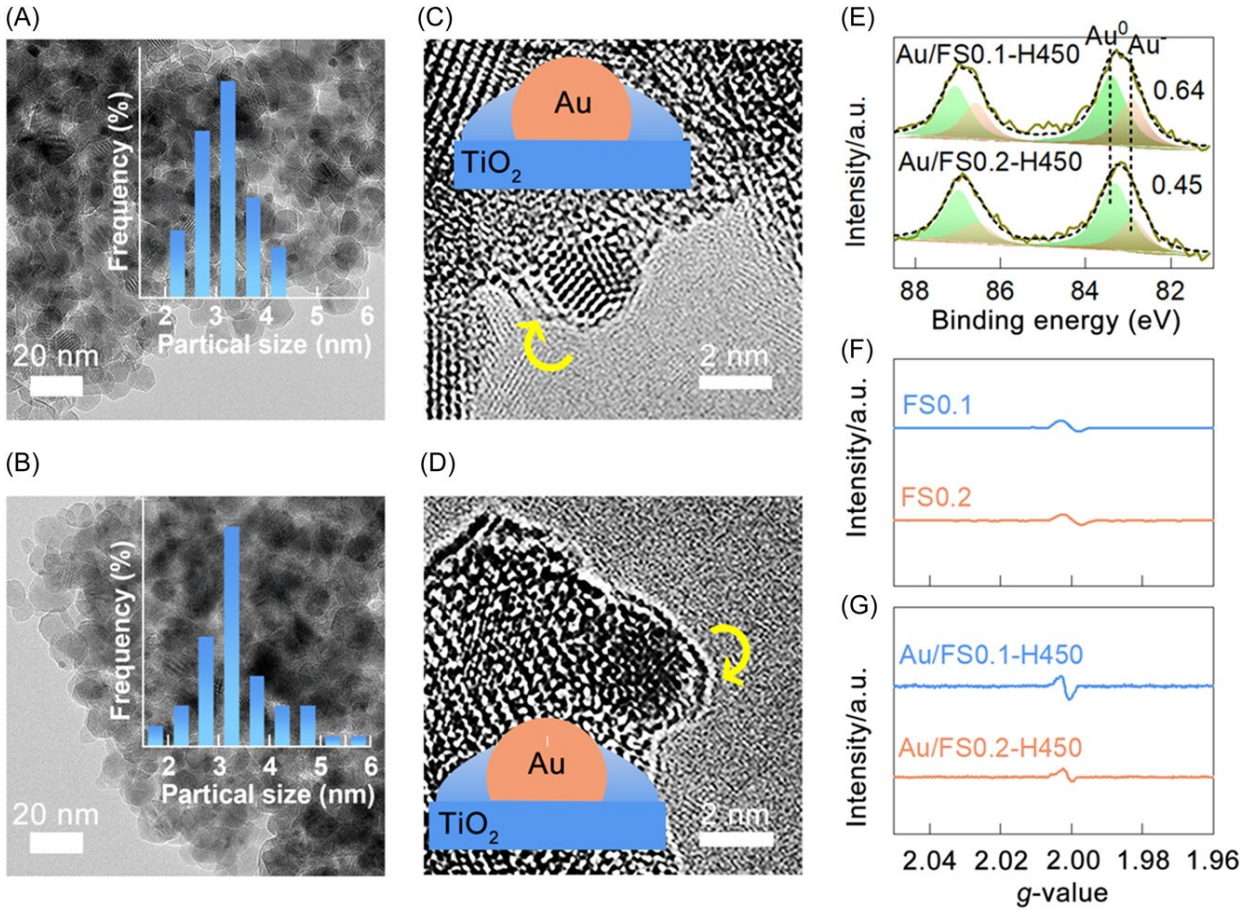


C4T IRP 1 and IRP 3: Investigating the impact of dynamic structural changes of Au/rutile catalysts on the catalytic activity of CO oxidation

Xiaochun Hu, Qianwenhao Fan, Mingwu Tan, Yuqing Luo, Xianyue Wu, Manoel Y. Manuputty, Jie Ding, Tej S. Choksi, Markus Kraft, Rong Xu, Zhiqiang Sun, and Wen Liu, *Carbon Energy*

DOI: 10.1002/cey2.412

Abstract: The surface properties of oxidic supports and their interaction with the supported metals play critical roles in governing the catalytic activities of oxide-supported metal catalysts. When metals are supported on reducible oxides, dynamic surface reconstruction phenomena, including strong metal–support interaction (SMSI) and oxygen vacancy formation, complicate the determination of the structural–functional relationship at the active sites. Here, we performed a systematic investigation of the dynamic behavior of Au nanocatalysts supported on flame-synthesized TiO_2, which takes predominantly a rutile phase, using CO oxidation above room temperature as a probe reaction. Our analysis conclusively elucidated a negative correlation between the catalytic activity of Au/TiO_2 and the oxygen vacancy at the Au/TiO_2 interface. Although the reversible formation and retracting of SMSI overlayers have been ubiquitously observed on Au/TiO_2 samples, the catalytic consequence of SMSI remains inconclusive. Density functional theory suggests that the electron transfer from TiO_2 to Au is correlated to the presence of the interfacial oxygen vacancies, retarding the catalytic activation of CO oxidation.

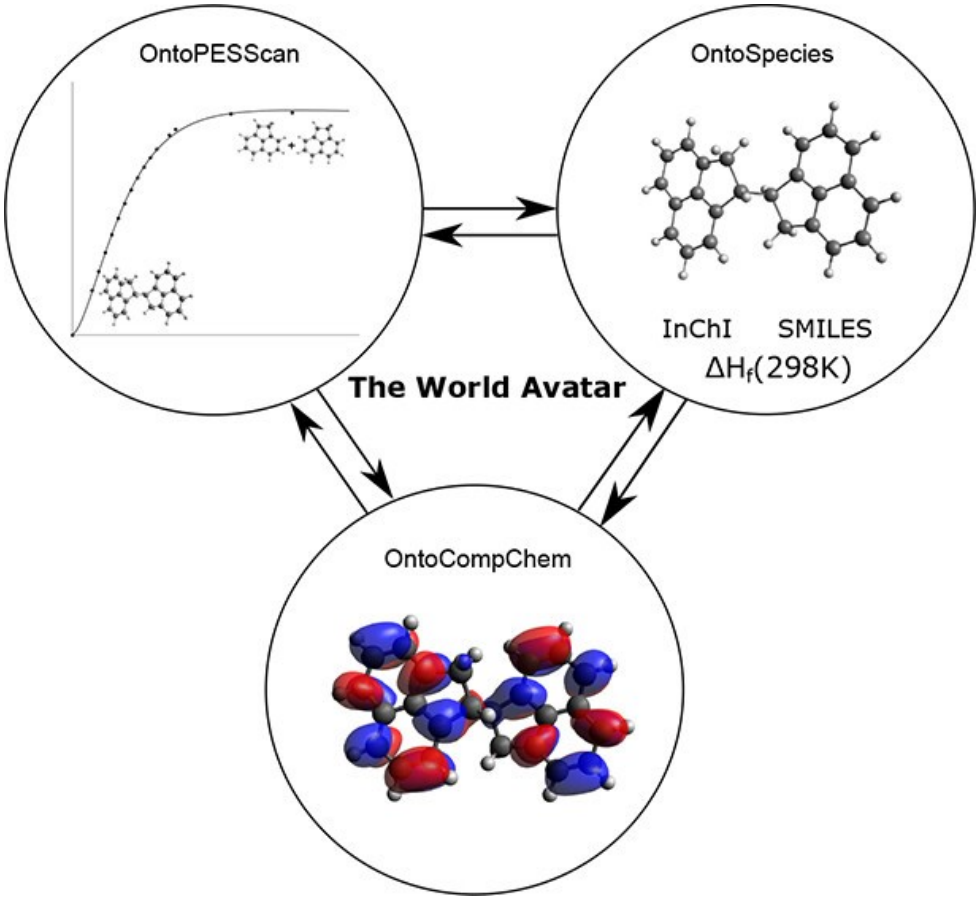


C4T IRP 3 and IRP JPS: OntoPESScan: An Ontology for Potential Energy Surface Scans

Angiras Menon, Laura Pascazio, Daniel Nurkowski, Feroz Farazi, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *ACS Omega*

DOI: 10.1021/acsomega.2c06948

Abstract: In this work, a new OntoPESScan ontology is developed for the semantic representation of one-dimensional potential energy surface (PES) scans, a central concept in computational chemistry. This ontology is developed in line with knowledge graph principles and The World Avatar (TWA) project. OntoPESScan is linked to other ontologies for chemistry in TWA, including OntoSpecies, which helps uniquely identify species along the PES and access their properties, and OntoCompChem, which allows the association of potential energy surfaces with quantum chemical calculations and the concepts used to derive them. A force-field fitting agent is also developed that makes use of the information in the OntoPESScan ontology to fit force fields to reactive surfaces of interest on the fly by making use of the empirical valence bond methodology. This agent is demonstrated to successfully parametrize two cases, namely, a PES scan on ethanol and a PES scan on a localized π-radical PAH hypothesized to play a role in soot formation during combustion. OntoPESScan is an extension to the capabilities of TWA and, in conjunction with potential further ontological support for molecular dynamics and reactions, will further progress toward an open, continuous, and self-growing knowledge graph for chemistry.



C4T IRP 3 and eCO$_2$EP: Selective and Stable CO_2 Electroreduction to CH_4 via Electronic Metal–Support Interaction upon Decomposition/Redeposition of MOF

Guanyu Liu, Quang Thang Trinh, Haojing Wang, Shuyang Wu, Juan Manuel Arce-Ramos, Michael B. Sullivan, Markus Kraft, Joel W. Ager, Jia Zhang, and Rong Xu, *Small*

DOI: 10.1002/smll.202301379

Abstract: The CO_2 electroreduction to fuels is a feasible approach to provide renewable energy sources. Therefore, it is necessary to conduct experimental and theoretical investigations on various catalyst design strategies, such as electronic metal–support interaction, to improve the catalytic selectivity. Here a solvent-free synthesis method is reported to prepare a copper (Cu)-based metal–organic framework (MOF) as the precursor. Upon electrochemical CO_2 reduction in aqueous electrolyte, it undergoes in situ decomposition/redeposition processes to form abundant interfaces between Cu nanoparticles and amorphous carbon supports. This Cu/C catalyst favors the selective and stable production of CH_4 with a Faradaic efficiency of ≈55% at −1.4 V versus reversible hydrogen electrode (RHE) for 12.5 h. The density functional theory calculation reveals the crucial role of interfacial sites between Cu and amorphous carbon support in stabilizing the key intermediates for CO_2 reduction to CH_4. The adsorption of COOH* and CHO* at the Cu/C interface is up to 0.86 eV stronger than that on Cu(111), thus promoting the formation of CH_4. Therefore, it is envisioned that the strategy of regulating electronic metal–support interaction can improve the selectivity and stability of catalyst toward a specific product upon electrochemical CO_2 reduction.

CITIES: Semantic 3D city interfaces—Intelligent interactions on dynamic geospatial knowledge graphs

Arkadiusz Chadzynski, Shiying Li, Ayda Grišiūtė, Jefferson Chua, Markus Hofmeister, Jingya Yan, Huay Yi Tai, Emily Lloyd, Yi Kai Tsai, Mehal Agarwal, Jethro Akroyd, Pieter Herthogs, and Markus Kraft, *Data-Centric Engineering*

DOI: 10.1017/dce.2023.14

Abstract: This article presents a system architecture and a set of interfaces that can build scalable information systems capable of large city modeling based on dynamic geospatial knowledge graphs to avoid pitfalls of Web 2.0 applications while blending artificial and human intelligence during the knowledge enhancement processes. We designed and developed a GeoSpatial Processor, an SQL2SPARQL Transformer, and a geospatial tiles ordering tasks and integrated them into a City Export Agent to visualize and interact with city models on an augmented 3D web client. We designed a Thematic Surface Discovery Agent to automatically upgrade the model's level of detail to interact with thematic parts of city objects by other agents. We developed a City Information Agent to help retrieve contextual information, provide data concerning city regulations, and work with a City Energy Analyst Agent that automatically estimates the energy demands for city model members. We designed a Distance Agent to track the interactions with the model members on the web, calculate distances between objects of interest, and add new knowledge to the Cities Knowledge Graph. The logical foundations and CityGML-based conceptual schema used to describe cities in terms of the OntoCityGML ontology, together with the system of intelligent autonomous agents based on the J-Park Simulator Agent Framework, make such systems capable of assessing and maintaining ground truths with certainty. This new era of GeoWeb 2.5 systems lowers the risk of deliberate misinformation within geography web systems used for modeling critical infrastructures.

IRP 1

SUSTAINABLE REACTION ENGINEERING FOR CARBON NEUTRAL INDUSTRY

IRP 1 is focused on chemical technologies that allow rapid decarbonisation of the chemical industry and the chemical supply chain. Our target is to deliver innovative solutions to direct utilisation of carbon dioxide as a feedstock, as well as to significantly increase the efficiency in conversion of methane to bulk intermediates. We are also exploring the options for the emerging circular economy, by developing new transformations of molecules available in different bio-waste resources into high-value functional molecules. Potential impact on carbon emissions reduction is evaluated by life cycle assessment tools.

IRP 1 Principal Investigators:

Professor Alexei LAPKIN
University of Cambridge

Asst Professor Paul LIU Wen
Nanyang Technological University

Assoc Professor YAN Ning
National University of Singapore

OVERVIEW

In the last quarter IPR1 was preparing for the transition to the no-cost extension of the C4T Phase 2 grant, primarily in transforming the on-going projects into the collaborative impact-focused projects in the no-cost extension period. This involved preliminary work on the set-up of the case studies for the bio-based chemical synthesis project, identification of the end-points for the catalyst development projects, and the policy-oriented process studies. In the meantime, significant portions of work were completed, such as the generation of a large data set by Mr Aniket Chitre for his work on formulations design and the catalysts development work by Dr Zhou Shenghui which will soon be published as a high-profile paper, among many others.

Professor Alexei Lapkin, PI
University of Cambridge

Update on work package 1.1

Design of nano-structured catalysts

Dr Quan ZHANG (Research Fellow, NUS) continues his investigation into the mechanism for the outstanding ammonia decomposition catalytic performance for the novel Co-CoMgOx catalyst that he discovered. Various characterisations have been performed, such as H_2 TPR, H_2 TPD, N_2 TPD, CO_2 TPD, NH_3 TPD, and in situ IR. The results indicated that the CoMgOx support with a solid-solution structure is crucial for high performance because this structure can accelerate the H_2 and N_2 desorption from the surface of the catalyst. However, only a small percentage of Co can be included in the support in order to maintain the solid-solution structure due to the poor thermal stability with higher Co content. With increasing the content of Co, the best performance sample should have the highest amount of active sites. In addition, the stability of the catalyst for ammonia decomposition has also been studied. The catalyst shows almost no degradation during the 100 h test at 500°C indicating good catalytic stability.

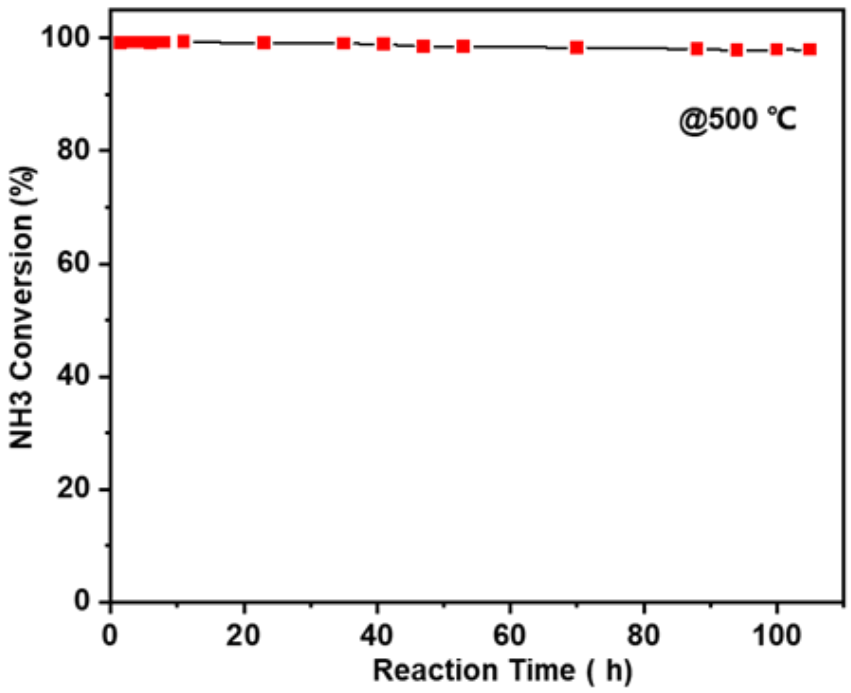


Figure 1.1: Catalytic stability measurement of the Co-CoMgOx catalyst

Dr Quan ZHANG

Update on work package 1.2

Novel reactions and functional molecules

Guided by **Prof Alexei LAPKIN (PI, CAM)**, **Dr Zhen GUO (Senior Research Fellow, CARES)** has been closely collaborating with **Prof Ning YAN (PI, NUS)** on the valorisation of chemicals originated from chitin as a biowaste. Searching for new reaction routes from these renewable chemicals to value-added chemicals was conducted by employing an organic synthesis planner (CASP system). This work has been summarised in a paper which has been submitted to *ChemSusChem*. Separately, Dr Guo is also working with **Mr Adash ARUN (PhD student, CAM)** and Dr Bing LI (non-C4T Research Fellow, NUS) to investigate how to optimise the production of fine chemicals through synchronisation of each other's knowledge across ontology of biowastes, reaction network, and organic synthesis.

Targeting current issues in the chemical industry, Dr Guo has also been working on gathering data on biodegradability, toxicity, and developing tools for the prediction of molecular properties using machine learning algorithms.

Next, Dr Guo will continue developing the tools for molecular analysis and searching for chemical routes, aiming at transforming the fossil-fuel chemical industry into a sustainable one.

Mr Aniket CHITRE'S (PhD student, CAM) has continued to use his semi-automated high-throughput liquid formulations workflow as described in the last reporting to generate a dataset of over 800 formulations including phase stability, turbidity, and rheology experiments. This is the first-such dataset in the community and will enable the training of ML models for liquid formulations property prediction. This work is being written up now. Additionally, he has recently submitted a paper on the pHbot he developed. This is a fully-automated titration robot driven by a physics-informed ML algorithm. Mr Chitre has been presenting his workflow at international conferences and published an application note with Opentrons on retrofitting their liquid handling robot to pipette viscous fluids. Finally, Mr Chitre attended a summer school in the UK on molecular simulation methods to deepen his understanding of MD and its potential application to his project.

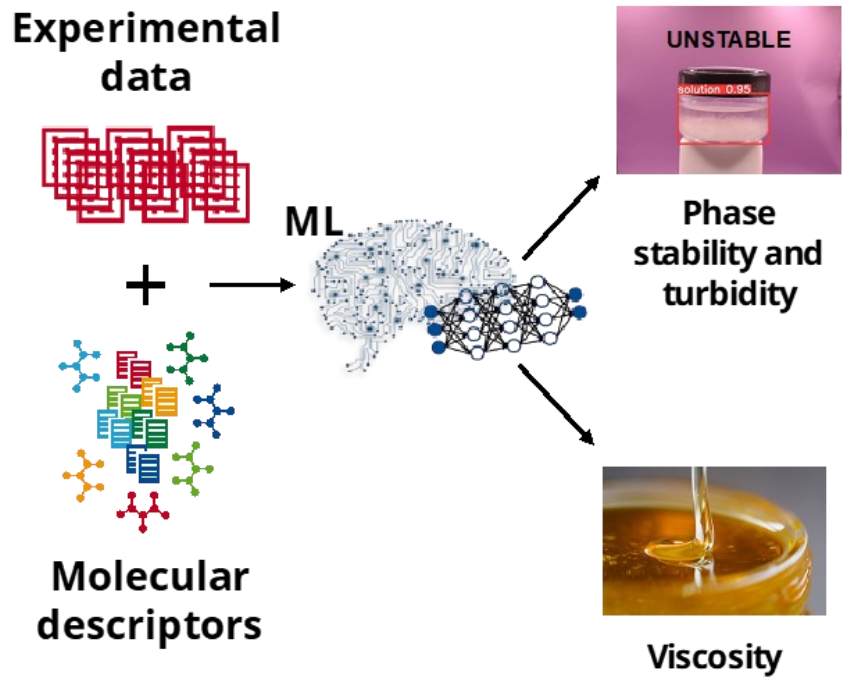


Figure 1.2: Machine learning over the collected experimental dataset will enable a forward model (formulation – property relationships) to be developed, which can be used to accelerate the design of (ultimately, greener) liquid formulated products, e.g., shampoo or detergent.

Mr Aniket CHITRE

Mr Adarsh ARUN (PhD student, CAM) commenced his PhD in January 2021 and focuses mainly on identifying sustainable routes from biowaste to value-added chemicals using networks and knowledge graphs (KGs). He has completed development of an early-stage ontology/ schema to represent the required data, integrating a variety of existing ontologies and data sources from a variety of domains (location, biowaste sources, biowaste taxonomy, biowaste feedstocks, processes, chemical reactions, chemical species). Over the past several months, he has been populating a preliminary knowledge graph based on literature on common biowaste sources in Asia, including pretreatment processes to isolate key feedstocks from biowaste. He has also integrated large language models (GPT 3.5) to automate the knowledge extraction and text mining from these literature sources.

The knowledge graph currently has ~60 biomass samples (across 16 types), ~40 pretreatment processes (across 7 types) and ~120 biowaste feedstocks. It also contains ~20,000 chemical reactions from biowaste feedstocks to value-added chemicals, mined from the Reaxys database. He is now looking to integrate open-source process simulators with the knowledge graph for the calculation of sustainability metrics to evaluate pathways in the knowledge graph. Concurrently, he is also investigating machine learning methods for link prediction to infer missing biowaste properties.

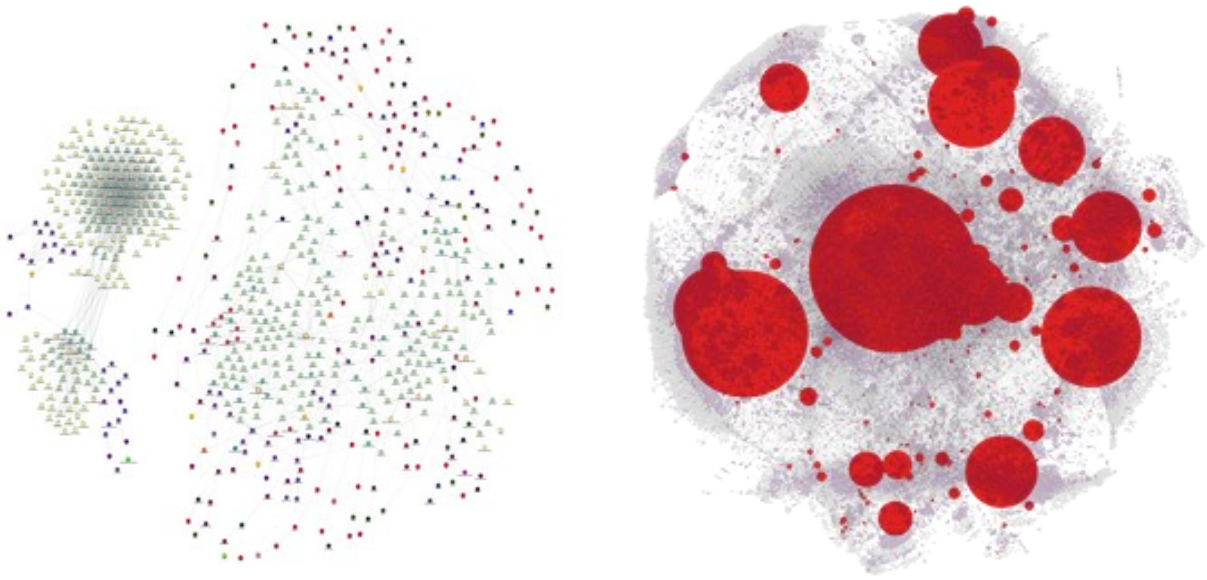


Figure 1.3: (left) Knowledge graph of locations, biowaste sources, biowaste taxonomies, biowaste feedstocks, and pre-treatment processes and (right) knowledge graph of chemical reactions from biowaste feedstocks to value-added chemicals.

Mr Adarsh ARUN

Update on work package 1.3

Novel reactors and process technology

Dr Yu SHAO (Research Fellow, NTU) has been working on the chemical looping–dry reforming of methane (CL–DRM) process, enabled by a novel high entropy oxide (HEO) catalyst (Figure 1.4). As illustrated, the CL–DRM technique breaks down the overall methane dry reforming reaction ($CH_4 + CO_2 \rightarrow 2CO + 2H_2$) into two sub-reactions (Figure 1.4a). Compared to conventional DRM processes, the separation of the reforming and regeneration stages not only overcomes the thermodynamic limitations on equilibrium conversion, but also avoids undesired side reactions (e.g., $CO_2 + H_2 \rightarrow CO + H_2O$) since CO_2 and the product H_2 stream are not in contact. The HEO catalyst exhibits a homogeneous distribution of the constituent metal elements, manifesting a solid-solution behaviour (Figure 1.4b). During the CL–DRM application, HEO's well-documented structural robustness facilitates the exsolution and dissolution of metallic nanoparticles over the repeated reduction–oxidation cycles, hence demonstrating superior catalyst stability compared to benchmark $NiFeAlO_x$ and $NiFeZrO_x$ materials (Figure 1.4c). The former has an established performance in the chemical looping–steam reforming of the methane process. Moreover, the oxygen-carrying ability of our HEO catalysts favours the conversion via the partial oxidation of methane rather than the methane cracking route. Overall, the transition metal-based HEOs are competent candidates for industrial applications, owing to their low cost, simple synthesis, decent performance and stability, and structural robustness.

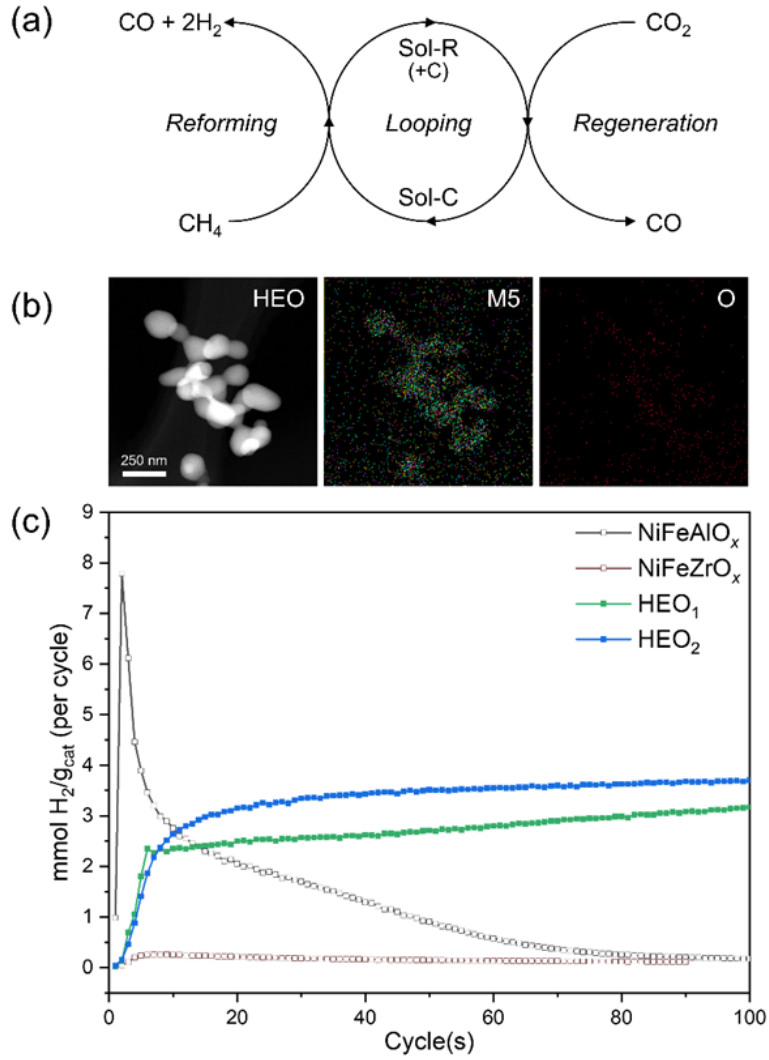


Figure 1.4: (a) Schematic illustration of the CL–DRM process. (b) HAADF image and EDS elemental mapping of the HEO catalyst. (c) CL–DRM performance of the HEO catalysts over 100 cycles.

Dr Yu SHAO

Dr Yao SHENG's (Research Fellow, NTU) main research interest lies in the development of CO_2 capture and in-situ hydrogenation process using dual-function materials (DFMs). Recently, she has been focusing on writing a manuscript titled "A Review of Mechanistic Insights into CO_2 Reduction to Higher Alcohols for Rational Catalyst Design". After several rounds of revisions, this manuscript has been submitted to the journal *Applied Catalysis B: Environmental*. This review performed a critical and comprehensive analysis of the previous mechanistic studies of CO_2 reduction to higher alcohols (Figure 1.5) and formulated feasible strategies for further development and optimisation of the catalysts for this reaction. In particular, the review paper discussed in detail various ways to facilitate the elementary steps limiting the catalysts' activity in CO_2 reduction, i.e., CO_2 and H_2 activation, and selectivity, i.e., C-C coupling. Depending on the nature of the catalyst, the latter process involves CO, CH_x, CH_xO, HCOO, and other species, which offers very rich chemistry and many opportunities for reaction engineering. We conclude this review by outlining future directions in experimental and computational research on higher alcohol synthesis that are likely to produce breakthrough results in the near future.

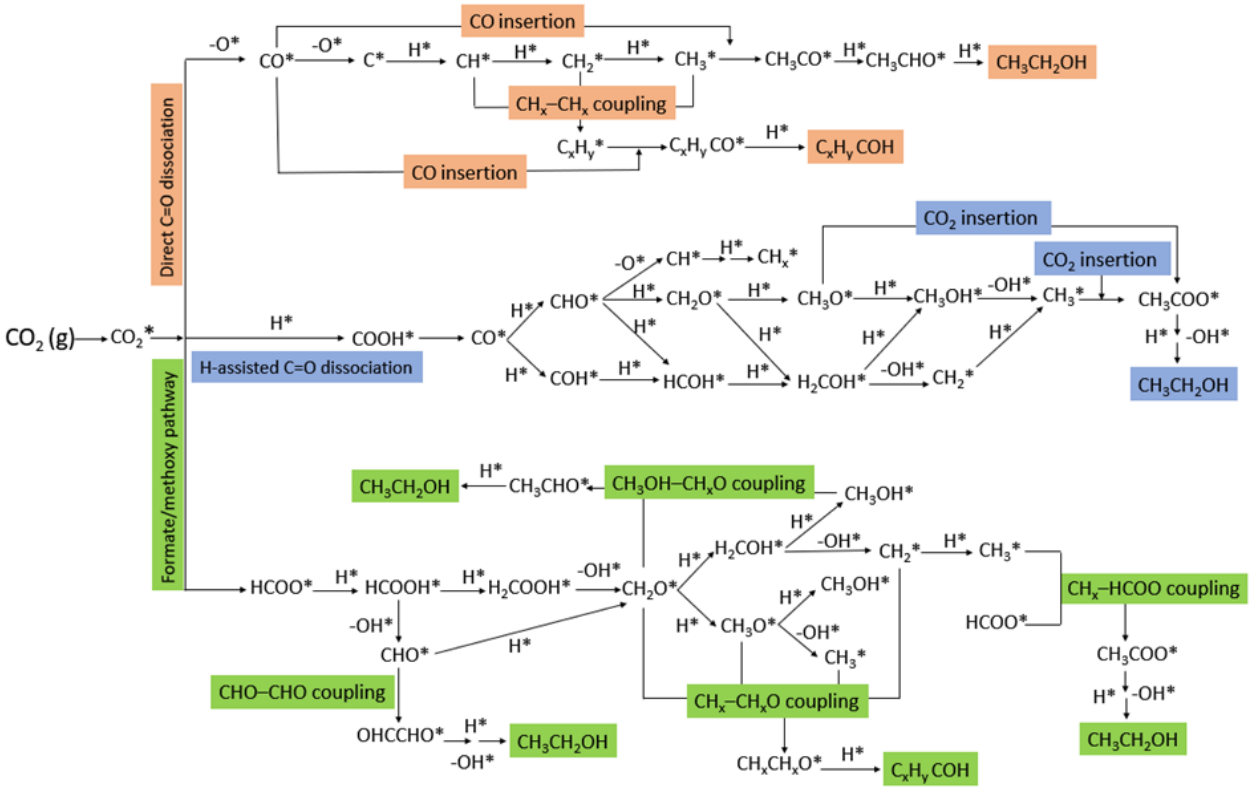


*Figure 1.5: Summary of possible pathways of CO_2 hydrogenation to higher alcohols. * indicates adsorbed species.*

Dr Yao SHENG

Ms Xianyue WU (CARES Visitor, NTU) has been actively working on the development of CO_2 capture and in-situ hydrogenation process using Ni/alkaline earth metal carbonate dual-function materials(DFMs). She has finished her first research work on integrated CO_2 capture and hydrogenation on Ni/$CaCO_3$ and Ni/$MgCO_3$ DFMs. In this work, she studied reaction pathways on Ni/$CaCO_3$ and Ni/$MgCO_3$ DFMs during the direct hydrogenation scheme using in situ DRIFT. By analysing the key surface intermediate species, she suggested that the hydrogenation step on Ni/$CaCO_3$ mainly undergoes formate reaction pathway while that on Ni/$MgCO_3$ undergoes reverse-water-gas-shift pathway (Figure 1.6). Recently, she is working

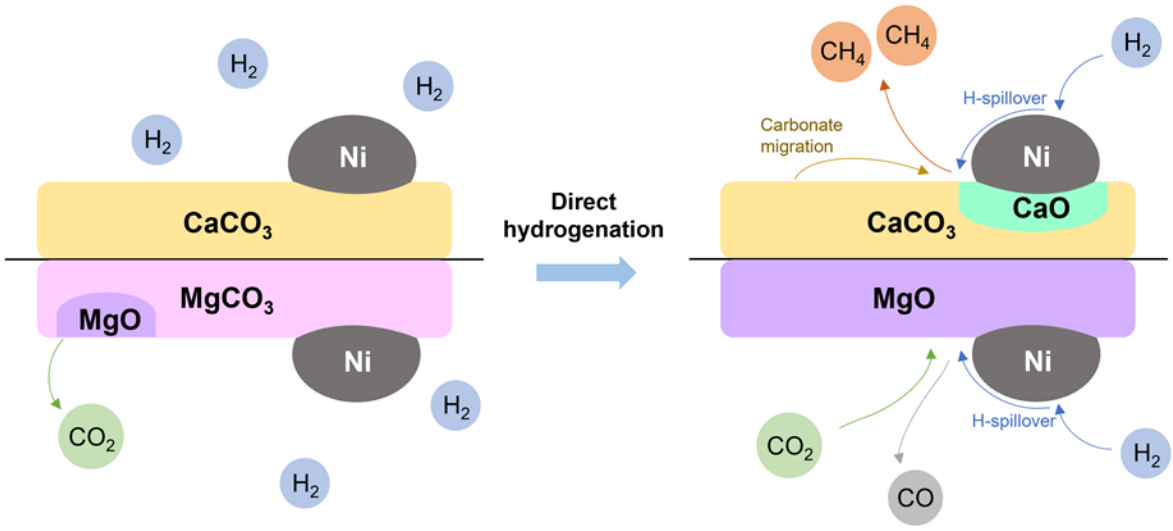


Figure 1.6: Schematic illustration showing the different reaction pathways on Ni/$CaCO_3$ and Ni/$MgCO_3$ dual functional materials for integrated CO_2 capture and conversion to produce CO and CH_4.

Ms Xianyue WU

on a new research project to investigate the particle size and dispersion effects of Ni-based DFMs on their CO_2 capture and in-situ hydrogenation performance. She is now adapting ethylene glycol (EG) and oleylamine method to synthesise Ni or NiO nanoparticles with different sizes.

Asst Prof Tej CHOKSI's (Co-PI, NTU) group is part of IRP 1 and is funded by an Emerging Opportunities Fund grant. The objective of this grant is to design supported metal catalysts that enable CO_2 conversion and formic acid chemistry using first-principles methods. In the last six months, this group has made progress with three of the project aims: (1) predicting catalytic stability, (2) understanding the selectivity trends among CO_2 reduction catalysts and formic acid decomposition, and (3) designing energy-efficient reactors for unconventional processes. The group leveraged a linear model to estimate adhesion energies of gold films on carbide and nitride supports, to determine sintering temperatures. After screening > 6000 gold/support combinations, the group identified an order of 100+ gold/carbide systems that maximise the sintering temperature. Such insights are vital in any high temperature CO_2 conversion catalysed by gold where sintering has been a perennial problem and has not yet been integrated into catalyst design.

Dr Shenghui ZHOU (Research Fellow, NUS) and **Prof Hua Chun ZENG's (Co-PI, NUS)** conducted a series of advanced characterisations on the structure and physicochemical properties of the previously synthesised catalyst with fullerene -like MoS_2 structure (MoS_2@SiO_2 and Cu/MoS_2@SiO_2). XRD analysis (Figure 1.7a) revealed that the MoS_2 in the synthesised catalyst exhibited a few-layered structure. N_2 physisorption analysis (Figure 1.7b) indicated that Cu/MoS_2@SiO_2 had a type IV physisorption isotherm with a type H4 hysteresis loop, a characteristic feature of mesoporous silica. This sample exhibited a BET surface area of 98.1 m^2/g, a pore volume of 0.15 cm^3/g, and a pore size range from 2.0 to ~18 nm, thus affirming the existence of mesopores. Electron paramagnetic resonance (Figure 1.7c) measurements showed that Cu/MoS_2@SiO_2 displayed a significantly higher peak intensity than other samples, implying a higher concentration of sulfur vacancies in Cu/MoS_2@SiO_2. Synchrotron-radiation-based X-ray absorption spectra (Figure 1.7d-f) and the wavelet transforms analysis (Figure 1.7g) of Cu K-edge EXAFS oscillations further suggested the total absence of metallic Cu and atomic dispersion of Cu species in Cu/MoS_2@SiO_2. In addition, over the past six months, we have also completed the catalytic performance tests and the writing and submission of the corresponding paper.

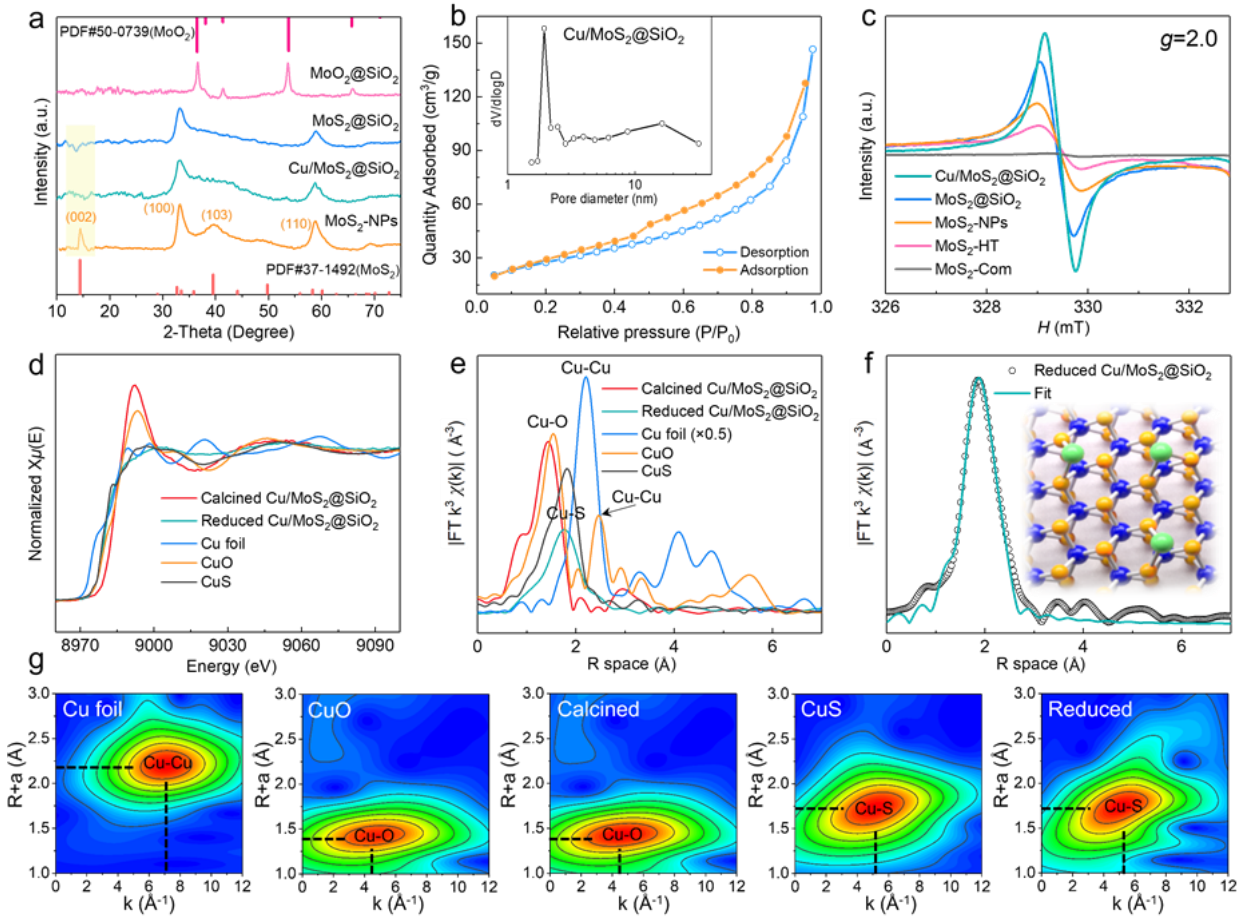


Figure 1.7: Characterisation of different catalysts. (a) XRD patterns, (b) Nitrogen sorption isotherms and the corresponding pore-size distribution, and (c) EPR spectra of different samples. (d) d,e, Cu K-edge normalised XANES spectra, and (e) FT k³-weighted Cu K-edge EXAFS spectra of calcined and reduced $Cu/MoS_2@SiO_2$ and the references. (f) Corresponding FT-EXAFS fitting curves of reduced $Cu/MoS_2@SiO_2$ in R space. (g) WT-EXAFS plots of calcined and reduced $Cu/MoS_2@SiO_2$ and the references.

Dr Shenghui ZHOU

Dr Nicholas JOSE (Research Fellow, CARES) has developed the third iteration of FLAB, an open-source Python platform for automating laboratories, which is intended to decrease the time and cost of digitising laboratories. This work was recently presented at a conference in Cambridge and will also be shared at the Continuous Flow Reactor Technology Conference in Ireland in September. He has also worked with **Dr Dogancan KARAN (Research Fellow, CARES)** from the PIPS project to create new drivers for equipment in the CARES lab, including the Polar Bear Reactor, Harvard Syringe Pumps and Vici Pumps, which are available for CARES use.

Scientific output

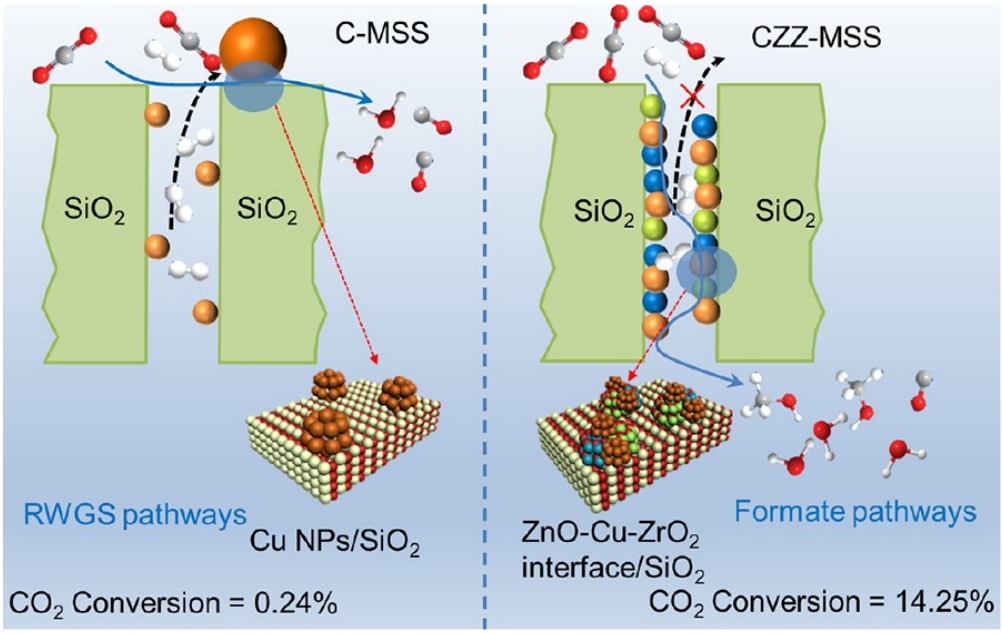
The following are the CREATE-acknowledged publications generated by IRP 1 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Optimizing the Interfacial Environment of Triphasic ZnO-Cu-ZrO_2 Confined inside Mesoporous Silica Spheres for Enhancing CO_2 Hydrogenation to Methanol

Changwei Chen, Mohammadreza Kosari, Shibo Xi, Alvin M.H. Lim, Chi He, and Hua Chun Zeng, *ACS ES&T Engineering*

DOI: 10.1021/acsestengg.2c00371

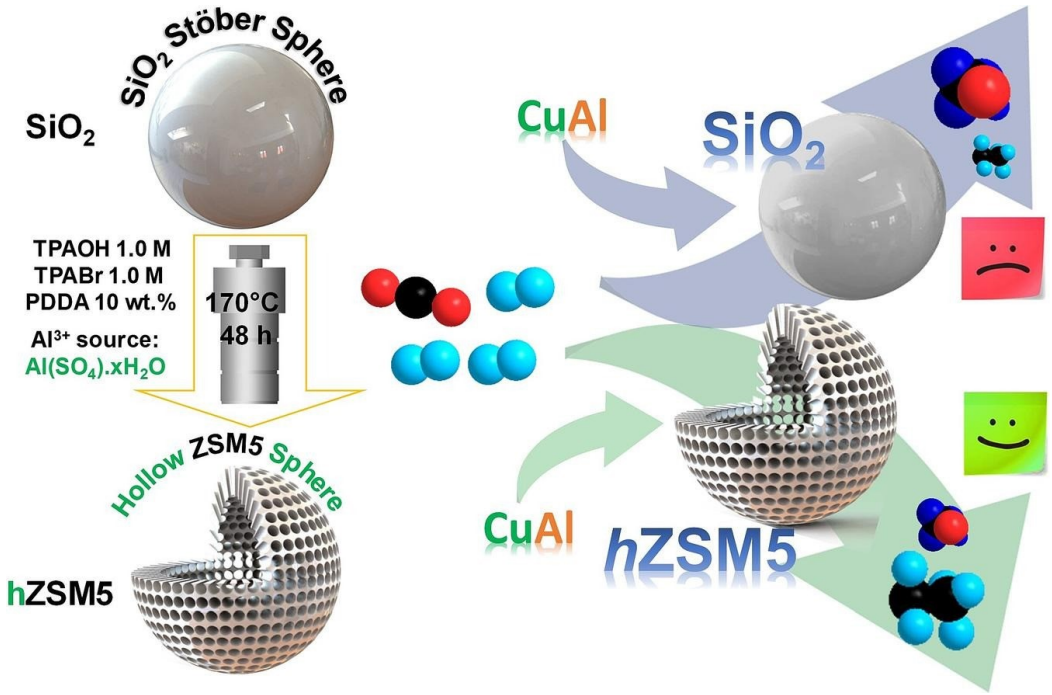
Abstract: Achieving the desired catalytic activity and selectivity in CO_2 hydrogenation to methanol remains a grand challenge using nonprecious metals. Herein, the well-known ternary Cu-ZnO-ZrO_2 (CZZ) was spatially sequestered as fine, uniformly dispersed active interfaces onto an engineered mesoporous silica sphere (MSS), giving rise to Cu-ZnO-ZrO_2/MSS (CZZ-MSS) with confined binary Cu-ZnO/Cu-ZrO_2 and ternary interfaces that fostered methanol production under moderate conditions (30 bar and 200–280 °C). By systematically investigating the CZZ-MSS performance, we show that spatial confinement and optimization of the interfacial environment of the catalytically active interfaces inside well-fabricated mesoporous silica deliver a markedly enhanced specific methanol yield (2211 $g_{MEOH} \cdot kg_{Cu}^{-1} \cdot h^{-1}$) compared to conventional supported catalysts including an industrial catalyst (368 $g_{MEOH} \cdot kg_{Cu}^{-1} \cdot h^{-1}$) and a vast majority of reported catalysts. Besides, the strong metal–support interaction arising from interacting metallic Cu and metal oxides (ZnO and ZrO_2) within the confined, ultrasmall nanoparticles (<3.0 nm) demotes the sintering of Cu NPs while retaining their H_2 dissociation strength, resulting in superior and prolonged catalytic stability over 100 h. In situ DRIFTS of confined catalysts with monophasic, biphasic, and triphasic interfaces expectedly suggests the occurrence of different CO_2 hydrogenation reaction paths over triphasic Cu-ZnO-ZrO_2/MSS (formate pathway) compared to monophasic Cu/MSS (reverse water–gas shift (RWGS) pathway) and biphasic ZnO-ZrO_2/MSS. From the appreciable insights gained herein, the rational support synthesis bringing the confinement effect to the robust ZnO-Cu-ZrO_2 interface is the rationale behind the higher rate of methanol synthesis observed in the CO_2 hydrogenation.



Optimizing hollow ZSM-5 spheres (hZSM5) morphology and its intrinsic acidity for hydrogenation of CO_2 to DME with copper–aluminum

Mohammadreza Kosari, Kyungho Lee, Chao Wang, Sajjad Rimaz, Shenghui Zhou, Emmerson Hondo, Shibo Xi, Abdul Majeed Seayad, Hua Chun Zeng, and Armando Borgna, *Chemical Engineering Journal*
DOI: 10.1016/j.cej.2023.144196

Abstract: Hollow zeolites are normally made by synthesizing parent rigid zeolites form soluble silica-alumina suspension followed by removal of the aluminum-deficient centers, during which the uniformity of hollow zeolites is compromised. Herein, two uniform spherical hollow ZSM-5 (hZSM5) with distinct morphologies, monodispersed (mhZSM5) and networked (nhZSM5), were hydrothermally synthesized using premade Stöber SiO_2 spheres along with structure directing agents with and without aluminum. Subsequently, both mhZSM5 and nhZSM5 supports were impregnated with mono- and multimetallic Cu-based catalysts to investigate CO_2 hydrogenation with in-depth catalyst characterizations (HRTEM-EDX, Pyridine-FTIR, H_2-TPR, XPS, XANES, and DRIFTS). It was evidenced that uniform and decent morphology of mhZSM5 spheres arises from the existence of framework-intrinsic Al^{3+}. Besides, it was revealed that mhZSM5-AlCu containing both framework-intrinsic Al^{3+} and catalyst-extrinsic Al^{3+} promoter leads to an optimal DME production (33.5 $mg_{DME} \cdot g_{cat.}^{-1} \cdot h^{-1}$), which is comparable or even higher to the ones reported in several published works. Not only was mhZSM5-AlCu activity even better, but also it showed a prolonged stability compared to comZSM5-AlCu and nsZSM5-AlCu samples that were derived using commercial ZSM-5 supports with better physiochemical properties. Based on our *in-situ* DRIFTS, a stepwise mechanistic pathway of DME formation over mhZSM5-AlCu was proposed, assuming that the hollow ZSM-5 shell framework dehydrates methanol that is formed *in-situ* via CO_2 hydrogenation.



Phase Segregation in PdCu Alloy Nanoparticles During CO Oxidation Reaction at Atmospheric Pressure

Yingying Jiang, Alvin M. H. Lim, Hongwei Yan, Hua Chun Zeng, and Utkur Mirsaidov, *Advanced Science*

DOI: 10.1002/advs.202302663

Abstract: Bimetallic nanoparticle (NP) catalysts are widely used in many heterogeneous gas-based reactions because they often outperform their monometallic counterparts. During these reactions, NPs often undergo structural changes, which impact their catalytic activity. Despite the important role of the structure in the catalytic activity, many aspects of how a reactive gaseous environment affects the structure of bimetallic nanocatalysts are still lacking. Here, using gas-cell transmission electron microscopy (TEM), it is shown that during a CO oxidation reaction over PdCu alloy NPs, the selective oxidation of Cu causes the segregation of Cu and transforms the NPs into Pd–CuO NPs. The segregated NPs are very stable and have high activity for the conversion of CO into CO2. Based on the observations, the segregation of Cu from Cu-based alloys during a redox reaction is likely to be general and may have a positive impact on the catalytic activity. Hence, it is believed that similar insights based on direct observation of the reactions under relevant reactive conditions are critical both for understanding and designing high-performance catalysts.

Other activities and achievements

Asst Prof Tej CHOKSI's (Co-PI, NTU) group gave two in-person presentations at the 28th North American Catalysis Society Meeting in Providence, USA from 18 – 23 June 2023. These were "Supported Metal Catalysts Circumvent Limitations in Reactivity for Oxygen Electrocatalysis" and "Interfacial Engineering of Metal/ Mxene Heterostructures for Electrochemical CO_2 Reduction to C1 Products and Beyond". A poster presentation was given on "Discovering Trends in the Work Function of Mxenes through Machine Learning".

Dr Yu SHAO (Research Fellow, NTU) gave a poster presentation on "Development of Cost-Effective Catalysts and Sorbents for Carbon Capture and Utilisation" at CREATE Symposium 2023 in Singapore on 10 July.

Asst Prof Paul LIU (PI, NTU) gave a poster presentation on the topic "In-situ CO_2 Capture and Catalytic Methanation Using Ni/alkaline Earth Metal Carbonate Dual Function Materials" at Gordon Research Conference on Carbon Capture and Utilisation in Les Diablerets, Switzerland from 28 May – 2 June 2023.

Ms Xianyue WU (CARES Visitor, NTU) gave an oral presentation on the topic "In-situ CO_2 Capture and Catalytic Methanation Using Ni/ alkaline Earth Metal Carbonate Dual Function Materials" at the 27th International Symposium-for Chemical Reaction Engineering (ISCRE) 27 in Quebec City, Canada from 11 - 14 June 2023 and at the 28th North American Catalysis Society Meeting in Providence, USA from 18 – 23 June 2023.

Mr Adarsh ARUN (PhD student, CARES) gave an in-person presentation on "Towards a database of biowaste sources and pretreatment processes: A knowledge graph approach" at the University of Cambridge's Department of Chemical Engineering and Biotechnology (CEB) Annual Research Conference from 22 - 23rd June 2023.

Dr Nicholas JOSE (Research Fellow, CARES) gave a poster presentation, "Accelerating Autonomous Experimentation with Flab" at the 6th Machine Learning and AI Bio(Chemical) Engineering Conference in Cambridge from 6 – 7 July 2023.

Mr Aniket CHITRE (PhD student, CAM) delivered presentations at the conferences below:

- Virtual talk of "Accelerating Formulations Design: Adopting Automation & AI" at the BASF Shanghai, NAO Family Day 2023 on 29 June 2023.
- Poster presentation of "Molecular Modelling for Liquid Formulations Design" at the CCP5 Molecular Simulation Summer School in Durham from 16 – 27 July 2023.
- Poster presentation of "Accelerating Formulations Design: Adopting Automation & AI" at the Accelerate23 conference in Toronto from 22 – 25 August 2023.
- Online webinar of "Opentrons Mass Balance Integration and Developing a Proxy High-throughput Viscometer" on 21 September 2023.

Mr Chitre's PhD is funded by BASF Shanghai and his work is in close collaboration with BASF's Formulations, Molecular Modelling & Digitalisation of R&D groups. He is on exchange in Prof Kedar HIPPALGAONKAR'S (Non-C4T PI, NTU) group at the Institute of Materials Research and Engineering at A*STAR.

IRP 2

ELECTROSYNTHETIC PATHWAYS FOR ADVANCED LOW-CARBON CHEMICAL MANUFACTURING

In IRP 2, low carbon electrosynthetic processes and technologies are developed which target local, on-scale and on-demand conversion of electricity to commodity or specialty chemicals. As the contribution of renewables to the total electricity generation capacity continues to grow, novel technological opportunities arise for direct chemical conversion of the newly available low carbon electrons. This project addresses core challenges to the implementation of low carbon, on-demand driven advanced manufacturing of chemical targets via electrosynthesis.

IRP 2 Principal Investigators:

Professor Adrian FISHER
University of Cambridge

Professor Jason Zhichuan XU
Nanyang Technological University

Asst Professor ZHANG Sui
National University of Singapore

OVERVIEW

The IRP2 is exploring new advanced low-carbon manufacturing routes using electrosynthesis for applications in advanced manufacturing, electro-oxidation, the production of future fuels and clean water treatment methods. In this reporting period, work has delivered new strategies for ammonia synthesis, gas separation paths and molecular catalysts for hydrogen peroxide electrosynthesis.

Dr Chencheng Dai and Dr Libo Sun's research is focused on electrode architectures, catalysis and new low-carbon pathways for chemical manufacturing. In this reporting period, they have been exploring the potential of electro-oxidation reactions in future energy vectors including ammonia and new approaches for electrochemical generation of disinfectants.

The glycerol electro-oxidation reaction (GOR) at industrial-level current density (> 200 mA cm^{-2}) coupled with hydrogen generation for practical application has not been widely studied yet. The electrolysis of widely available glycerol can produce many useful intermediates or valuable fine chemicals, it is also interesting as it could also act as a replacement for the oxygen evolution reaction (OER) in hydrogen production. In this reporting period, we performed systematic investigations of the GOR using a membrane electrolyte assembly (MEA) electrolyser with various configurations.

In parallel with the electro-oxidation activities, work has continued on electrocatalytic nitrate reduction (eNO_3RR) for potential applications in NH_3 production and nitrate pollutant removal under ambient conditions. Our investigations in this reporting period reveal that a molecular catalyst containing a metal centre with an N_2(pyrrole)-N_2(pyridine) configuration demonstrates superior activity than the others. This catalyst exhibits a much lower overpotential for eNO_3RR and delivers high ammonia Faradaic efficiency (FE) of over 90% in the tested range and reaches the highest of ca. 94%.

Asst Prof Sui Zhang's research is focused on the development of (re)active membrane structures, including targets such as self-cleaning, disinfection and gas separation (e.g., H_2). In this reporting period, a unique hierarchical pore structure with multi-level micropores and mesopores has been formed, this favours the adsorption kinetics and diffusion of CO_2 across the membrane. As a result, high CO_2 permeance and selectivity have been achieved.

IRP 2 Singapore-based start-up company Datum ElectroniX has successfully entered Phase 1 of the SMART Innovation Grant 2.0 in early 2023. Through the program, DEX have been focusing extensively on market analysis and product development. This has identified new market niches and customers and DEX is now initiating discussions with potential strategic partners for market positioning.

Professor Adrian Fisher, PI
University of Cambridge

Update on work package 2.1

Advanced electrode architectures

Dr Chencheng DAI (Research Fellow, NTU) is investigating glycerol which is an abundant feedstock from biomass conversion by-product with facile accessibility. The electrochemical valorisation of glycerol can not only produce many useful intermediates or valuable fine chemicals but also replace the oxygen evolution reaction (OER) to reduce the electricity consumption for hydrogen production due to its thermodynamic favour. The development of electrochemical glycerol oxidation reaction (GOR) at industrial-level current density (> 200 mA cm^{-2}) coupled with hydrogen generation for practical application has not been widely studied yet. In this work, we performed the GOR in membrane electrolyte assembly (MEA) electrolyser with various configurations. The influence of the type of ion exchange membrane and electrolyte on the GOR activity, liquid product crossover and selectivity have been studied. In addition, the electrochemical neutralisation energy (ENE) has been harvested in the acid-alkali electrolyser to improve cell performance. Impressively, the AEM-based acid-alkali MEA electrolyser outperforms all other configurations. The decrease in the cell voltage requirement is significant, so that it not only valorises glycerol and produces hydrogen with a current density of 0.2 A cm^{-2} at a whole-cell potential 0.377 V, but also can be used as a fuel cell to generate electricity with a maximum power density of 13.4 mW cm^{-2} at the current density of 71.4 mA cm^{-2}. Moreover, when working as a conventional electrolyser, it possesses a liquid product total FE close to 100% at the current density up to 0.5 A cm^{-2}, which suggest that all electricity consumption can be devoted to hydrogen and value-added product production without carbon emission. This work provides a potential prototype device for highly energy-efficient co-generation of hydrogen and valorised products.

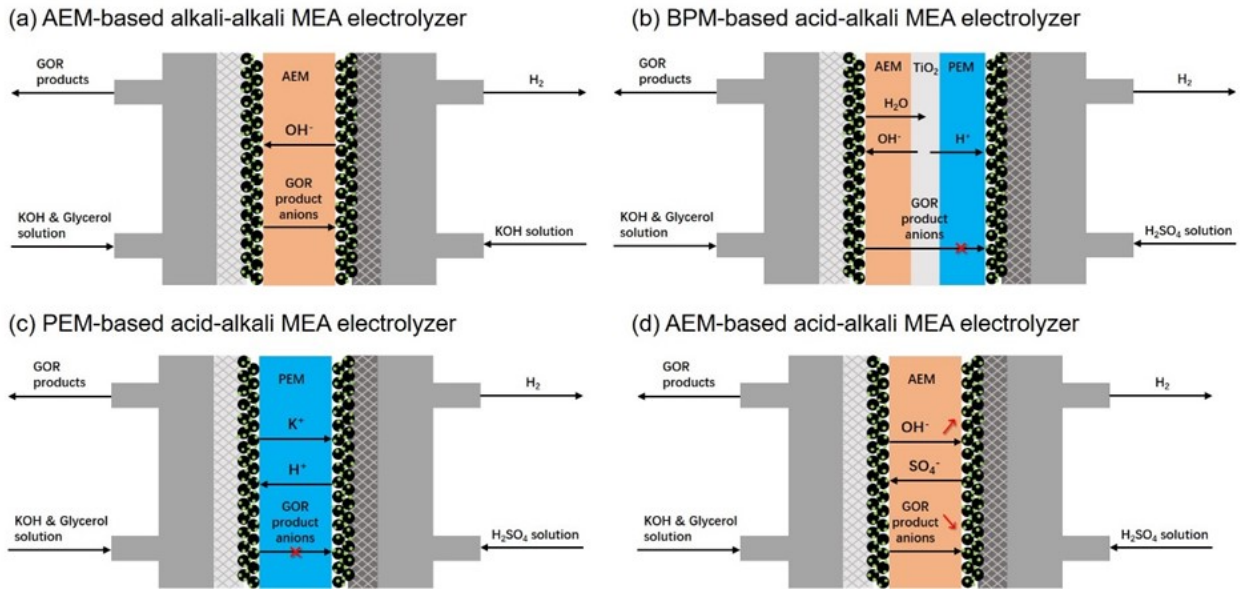


Figure 2.1: Schematic illustration of (a) AEM-based alkali-alkali, (b) BPM-based acid-alkali, (c) PEM-based acid -alkali and (d) AEM-based acid-alkali MEA electrolysers.

Dr Chencheng DAI

Asst Prof Sui ZHANG's (PI, NUS) group reports that conjugated microporous polymers (CMPs), a type of porous material which possesses impressive pore uniformity and superior stability, have emerged as a promising candidate for constructing next-generation membranes for molecular sieving. Chemical polymerisation is a commonly used method to synthesise CMPs materials. However, they are usually complex and time-consuming. In addition, the resulting materials are usually solid powders with low solubility in many solvents, which is not conducive to preparing CMPs materials into films. In recent years, attention has been paid to the preparation of CMPs by electrochemical polymerisation (EP) to obtain high-quality CMPs films. An important feature of EP is that it polymerises on the electrode surface, where organic molecules can be deposited directly to form a thin film.

Following the last report, the group continues to work on conjugated microporous polymer membranes by optimising the electropolymerisation process, and probing the fundamental mechanisms by various characterisations, such as microscopic methods, conductivity measurements, etc. Interestingly, they found that with increasing monomer concentration, polymerisation degree decreases and more mesopores emerge. A unique hierarchical pore structure with multi-level micropores and mesopores is formed, which favours the adsorption kinetics and diffusion of CO_2 across the membrane. As a result, high CO_2 permeance and selectivity have been achieved. Figure 2.2 presents the membrane performances and mechanisms.

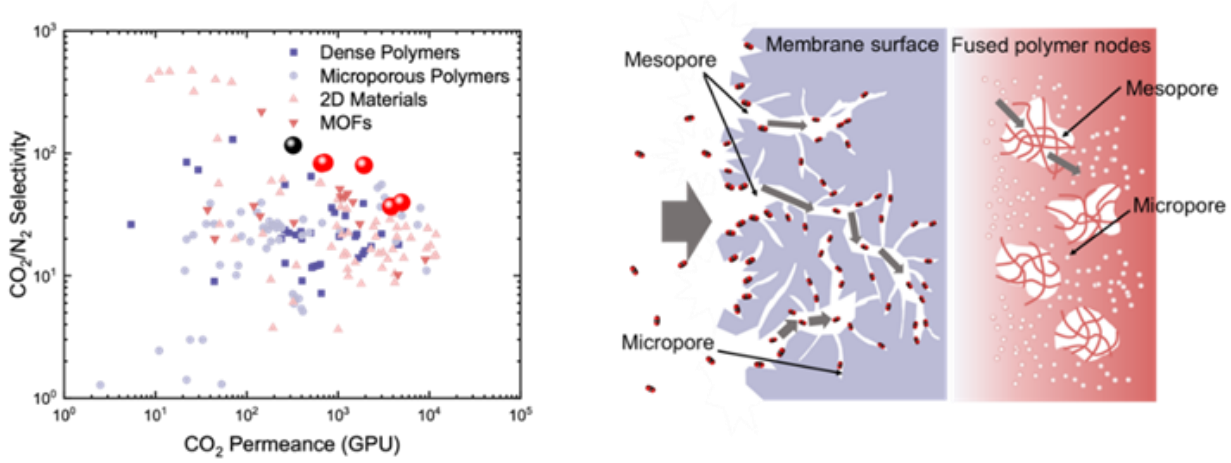


Figure 2.2: (Left) A comparison of the CMP membranes with literature work for CO_2/N_2 separation; and (right) an illustration of the hierarchical pore structure.

Asst Prof Sui ZHANG

Update on work package 2.2

Co-generation and electrolytic synthesis reactor engineering

Dr Libo SUN (Research Fellow, NTU) reports that ammonia plays a vital role in modern industry and represents promising next-generation carbon-free energy carrier. Electrocatalytic nitrate reduction (eNO_3RR) offers a potential solution for NH_3 production and nitrate pollutant removal under ambient conditions. However, the progress of eNO_3RR is hindered by a lack of efficient electrocatalysts with high selectivity, activity, and stability. To address this challenge, we propose the utilisation of molecular catalysts and developed a series of macrocyclic molecular catalysts for heterogeneous eNO_3RR. These molecular catalysts possess different coordination environments around the metal center by decorating surrounding subunits. As a result, the electronic

state of active center can be altered, enabling tunable activity towards eNO_3RR. Our investigation reveals that the metal center with an N_2(pyrrole)-N_2(pyridine) configuration demonstrate superior activity than the others. This catalyst exhibits much lower overpotential for eNO_3RR and delivers high ammonia Faradaic efficiency (FE) of over 90% in the tested range, and reaching the highest of ca. 94%. Furthermore, it achieves a production rate of up to 11.28 mg mg^{-1} h^{-1}, and a turnover frequency of up to 3.28 s^{-1}. Further analysis unveiled a correlation between magnetic moment with turnover frequency and d-band center. This correlation influences the potential of the rate-determining step, thereby optimising the reaction activity. By establishing the relationship between electronic structure, experimental activity, and computational parameters, this work paves the way for exploring effective molecular catalysts for eNO_3RR.

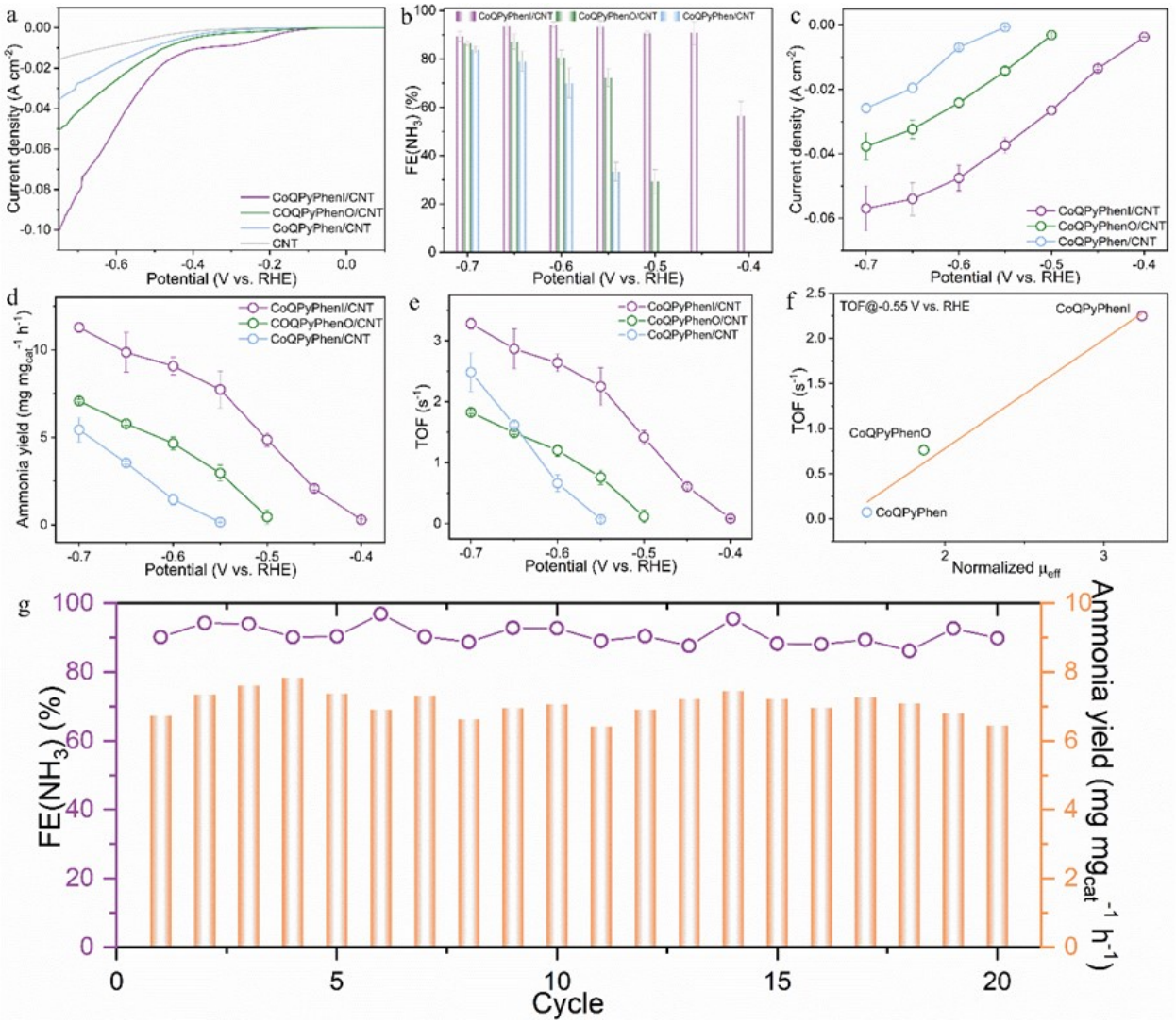


Figure 2.3: a) Polarisation curves of CoQPyPhenI/CNT, CoQPyPhenO/CNT, CoQPyPhen/CNT and bare CNT. b) Comparison of Faradaic efficiency of CoQPyPhenI/CNT, CoQPyPhenO/CNT, and CoQPyPhen/CNT. c) The partial current densities during electrocatalytic nitrate reduction. d) Ammonia yield calculated. e) Turnover frequency calculated. f) The relationship between normalised magnetic effective moment and turnover frequency. g) Cycling test of CoQPyPhenI/CNT at -0.5 V vs. RHE.

Dr Libo SUN

Update on work package 2.3

Micro-variable pressure and temperature electrosynthesis plant

Research interests lie in investigating novel electrochemical systems where a complex relationship exists between chemistry and mass transport. In this reporting period, new studies have explored the use of novel electroanalytical approaches to aid with inline control and feedback for optimisation of electrochemical synthesis reactions. Variational Mode Decomposition (VMD) has been explored as a tool for analysing current-density-time-voltage signals. VMD is a method established in scholarship for successfully decomposing transient signals into subcomponents or Intrinsic Mode Functions (IMFs). The assessment of VMD for the specific application of analysing current-density signals was conducted and the approach was found to show a robust removal of mode-mixing and noise allowed for explicit graphical representations. Through the unique frequencies and shapes of the IMFs and their Hilbert transform, precise information can be conveyed, facilitating a more physically meaningful interpretation of the signal. The method shows considerable promise, and we are exploring opportunities to link this approach to automated control methods for electro-synthesis.

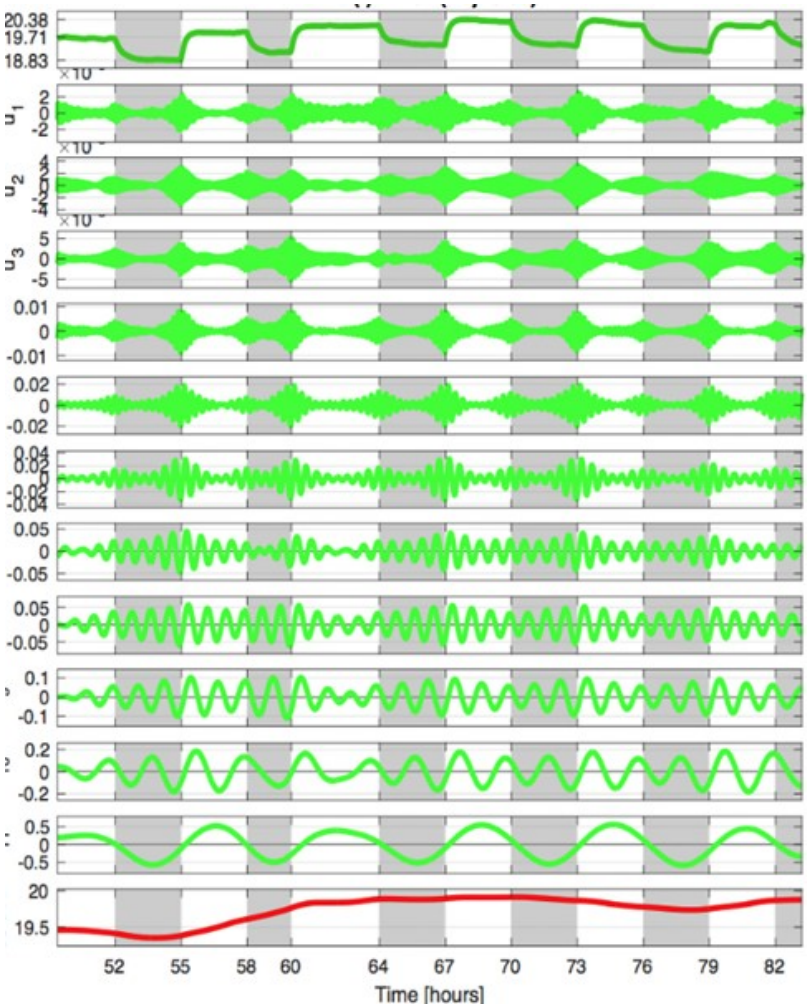


Figure 2.4: Illustration of VMD decomposition of an input current-time-voltage signal (red) and the modes (green) separated by the analysis approach.

Mr Leopold KLOYER (Non-C4T PhD student, CAM) and Ms Elisa SOLVAY (Non-C4T Masters student, CAM)

Ms Freyja DAGBJARTSDÓTTIR (PhD student, CAM) is currently writing their thesis "Developing numerical and analytical descriptions of electrochemical systems that can be used to investigate, design and monitor electrochemical systems" which will be submitted in late-2023.

Scientific output

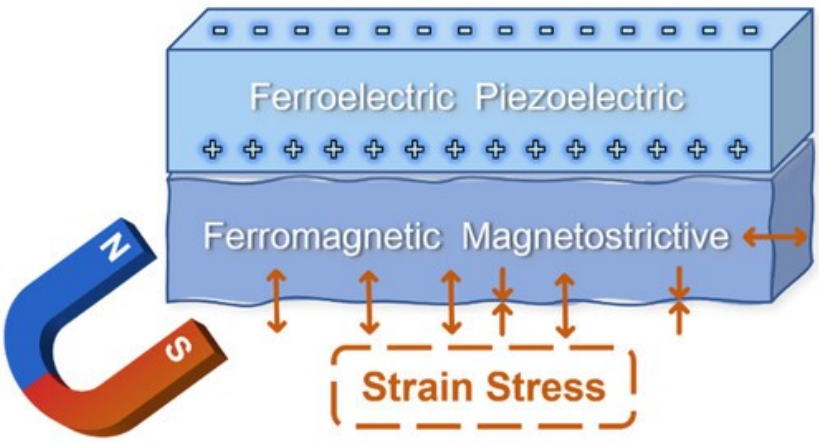
The following are the CREATE-acknowledged publications generated by IRP 2 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Navigating surface reconstruction of spinel oxides for electrochemical water oxidation
Yuanmiao Sun, Jiarui Wang, Shibo Xi, Jingjing Shen, Songzhu Luo, Jingjie Ge, Shengnan Sun, Yubo Chen, John V. Hanna, Shuzhou Li, Xin Wang, and Zhichuan J. Xu, *Nature Communications*
DOI: 10.1038/s41467-023-38017-3

Abstract: Understanding and mastering the structural evolution of water oxidation electrocatalysts lays the foundation to finetune their catalytic activity. Herein, we demonstrate that surface reconstruction of spinel oxides originates from the metal-oxygen covalency polarity in the MT–O–MO backbone. A stronger MO–O covalency relative to MT–O covalency is found beneficial for a more thorough reconstruction towards oxyhydroxides. The structure-reconstruction relationship allows precise prediction of the reconstruction ability of spinel pre-catalysts, based on which the reconstruction degree towards the in situ generated oxyhydroxides can be controlled. The investigations of oxyhydroxides generated from spinel pre-catalysts with the same reconstruction ability provide guidelines to navigate the cation selection in spinel pre-catalysts design. This work reveals the fundamentals for manipulating the surface reconstruction of spinel pre-catalysts for water oxidation.

A Perspective of Magnetoelectric Effect in Electrocatalysis
Dongsheng Shao, Tianze Wu, Xiaoning Li, Xiaoming Ren, and Zhichuan J. Xu, *Small Science*
DOI: 10.1002/smsc.202300065

Abstract: The integration of magnetic fields with magnetoelectric (ME) coupling materials has been recently reported for electrocatalysis applications. Highly efficient energy conversion and storage can be potentially provided by this emerging approach. The ME properties, that is, the coexistence of ferromagnetic (FM) and ferroelectric (FE) ordering in some multiferroic materials, can be manipulated by magnetic or electric fields. The ME coupling can result in unique spin-related physical properties in catalysts, further leading to interesting effects on electrocatalytic reactions. Herein, a discussion on the ME coupling multiferroic materials, as well as their potential opportunities and challenges as electrocatalysts in selected electrochemical reactions, is provided.

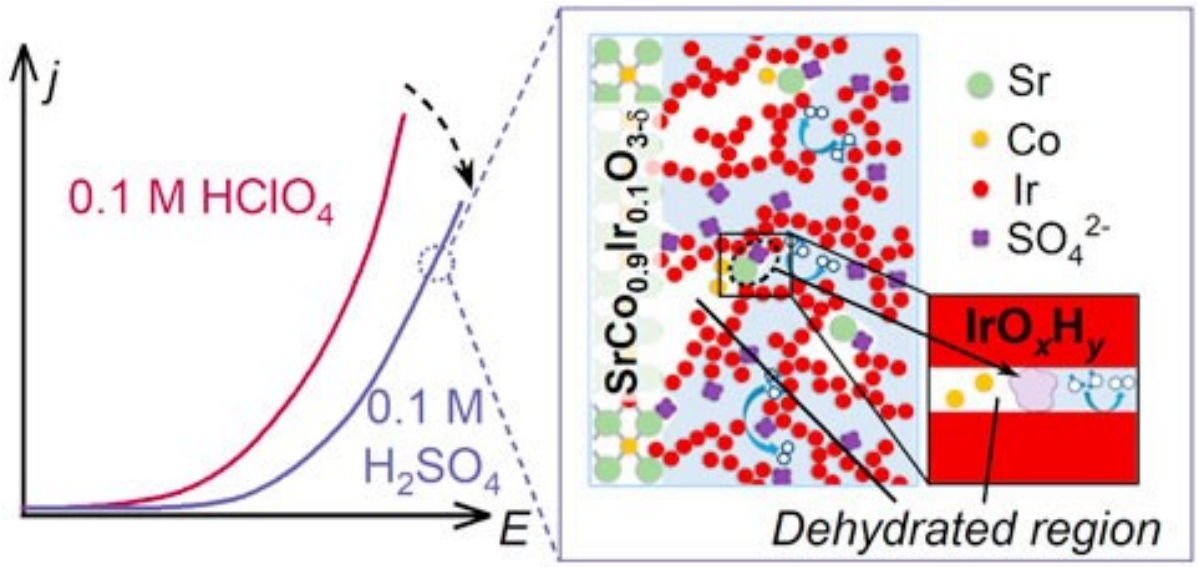


Deciphering the Poisoning Effect of Sulfate on a Perovskite-Derived IrOxHy Catalyst for Water Oxidation in Acid

Justin Zhu Yeow Seow, Yubo Chen, Jingjie Ge, Adrian C. Fisher, and Zhichuan J. Xu, *Journal of The Electrochemical Society*

DOI: 10.1149/1945-7111/accb70

Abstract: A highly efficient and stable oxygen evolution reaction (OER) plays a key role in the commercialization of proton exchange membrane (PEM) water electrolyzers. Perovskite-derived IrO_xH_y catalysts have been demonstrated to be highly catalytically active in a harsh acidic environment. On the other hand, the inevitable degradation of the PEM can induce the release of sulfate ions, which could poison electrocatalysts. Herein, the poisoning effects of sulfate ions on a representative $SrCo_{0.9}Ir_{0.1}O_{3-\delta}$-derived IrO_xH_y catalyst and a standard IrO_2 are studied. It is found that, besides sulfate ion adsorption on Ir active sites impacting both Ir-based catalysts, $SrSO_4$ precipitation is the most prominent cause of activity degradation of IrO_xH_y. This phenomenon is unique to a reconstructed surface undergoing continuous cation leaching from the perovskite-oxyhydroxide interface, in which $SrSO_4$ precipitate blocks electrolyte-accessible IrO_xH_y-walled channels, preventing further Sr and Co ion leaching from the interface and dehydrating the isolated portion of the blocked channels, resulting in a reduction in the number of Ir active sites and causing the catalyst to have an OER performance stability inferior to commercial IrO_2.

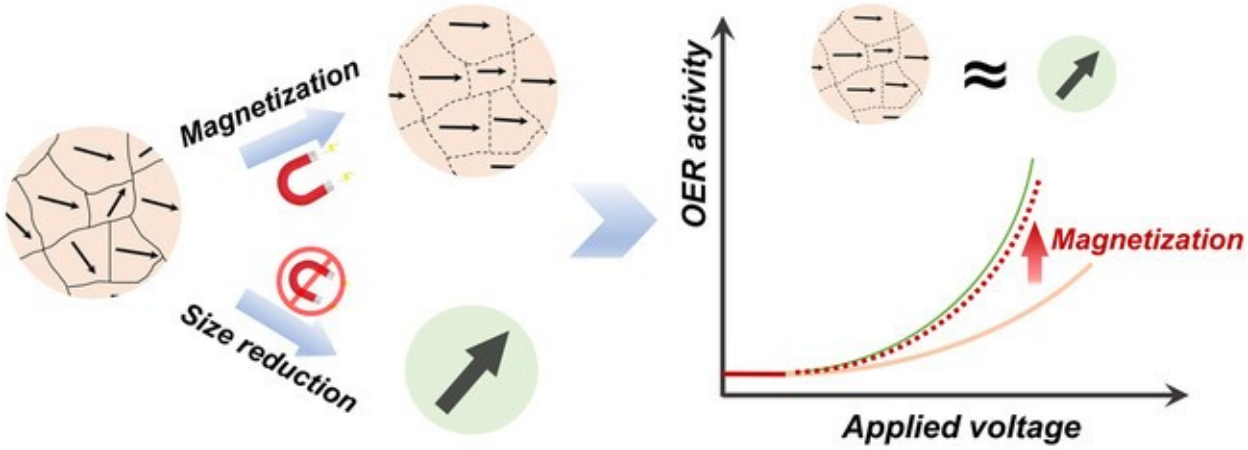


Multi-Domain versus Single-Domain: A Magnetic Field is Not a Must for Promoting Spin-Polarized Water Oxidation

Jingjie Ge, Xiao Ren, Riccardo Ruixi Chen, Yuanmiao Sun, Tianze Wu, Samuel Jun Hoong Ong, and Prof Zhichuan J. Xu, *Angewandte Chemie International Edition*

DOI: 10.1002/anie.202301721

Abstract: The reaction kinetics of spin-polarized oxygen evolution reaction (OER) can be enhanced by ferromagnetic (FM) catalysts under an external magnetic field. However, applying a magnetic field necessitates additional energy consumption and creates design difficulties for OER. Herein, we demonstrate that a single-domain FM catalyst without external magnetic fields exhibits a similar OER increment to its magnetized multi-domain one. The evidence is given by comparing the pH-dependent increment of OER on multi- and single-domain FM catalysts with or without a magnetic field. The intrinsic activity of a single-domain catalyst is higher than that of a multi-domain counterpart. The latter can be promoted to approach the former by the magnetization effect. Reducing the FM catalyst size into the single-domain region, the spin-polarized OER performance can be achieved without a magnetic field, illustrating an external magnetic field is not a requirement to reap the benefits of magnetic catalysts.



Other activities and achievements

Dr Chencheng DAI's (Research Fellow, NTU) technical disclosure for "An MEA electrolyzer for hydrogen production by electrochemical cracking of ammonia" has received a Singapore Patent Application #10202301326Y. The other inventors are **Prof Jason Zhichuan XU (Co-I, NTU), Prof Adrian FISHER (PI, CAM), and Dr Kamal ELOUARZAKI (Co-Founder of Datumelectronix, IRP2 spin-off)**.

Dr Dai also gave a poster presentation on "Ammonia E-Cracking" at CREATE Symposium 2023 in Singapore on 10 July 2023.

The work in IRP 2 aims to develop novel electrocatalytic routes to produce cleaner synthesis of specialty chemicals for the chemical industry.

IRP 3

COMBUSTION FOR CLEANER FUELS AND BETTER CATALYSTS

To formulate the fuel of the future, IRP 3 looks at new molecules that can be produced within the techno-economic constraints of a refinery and that have the potential to reduce pollutant emissions when added to fossil-derived fuels. This research will help to identify the best fuels (or fuel mixtures) for low-emission energy conversion, and to design and manufacture optimised cost-effective nanostructured materials for catalysis.

IRP 3 Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor XU Rong
Nanyang Technological University

Assoc Professor YANG Wenming
National University of Singapore

OVERVIEW

In this reporting period, we have made further strides in expanding the cheminformatics capabilities of our knowledge-graph based digital twin of the world, The World Avatar, in three areas, namely the representation and processing of chemical species, covalent organic frameworks (COFs), and zeolites. Firstly, we have extended our ontology for representing chemical species and their properties such that data from chemistry databases such as PubChem can be retrieved and enhanced using a software agent. This representation enables advanced data analysis and visualisation, including queries to find and compare properties of compounds, and automate data gathering and processing tasks. Secondly, we have continued to refine our toolsets to design COFs as materials with potential for printable electronics and direct air capture of CO_2 and water. Using an ontology we previously developed together with existing cheminformatic libraries, we have created a drawing agent that produces graphical representations of COFs. COFs are now searchable within the knowledge graph based on substructure units and are thus more easily accessible. The ability to semantically represent and depict these materials forms an important basis for addressing the problem of retrosynthetic construction in future. And thirdly, we have been developing an ontology for zeolites. Zeolites are inorganic crystalline materials, which, due to their favourable thermal stability and structural properties, are promising candidates for carbon capture and conversion. Our ontology can represent physico-chemical properties such as structure, rational design, chemical composition, porosity, and synthesis methods. In addition, we have designed it in such a way that it builds upon a more general ontology of crystals which captures unit cells, lattice parameters, atomic arrangements, and spatial categorisation. This kind of representation helps making broader ranges of materials findable and accessible within the knowledge graph.

In the field of electrocatalysis, we have been working both experimentally and computationally. In the lab, we have developed innovative designs for gas diffusion electrodes (GDEs). Our novel designs aim to address issues that negatively affect the efficiency and stability of CO_2-reduction GDEs, in particular under industrially relevant conditions with high current density. Computationally, we have advanced our understanding of the detailed kinetic reaction mechanism of electrocatalytic CO_2 reduction, with a view of more generally probing and isolating kinetic effects in complex heterocatalytic systems.

Professor Markus Kraft, PI
University of Cambridge

Update on work package 3.1

Refinery, fuel and engine of the future — experimental

Properties of surrogate fuels, marine engine after-treatment

Dr Yichen ZONG (Senior Research Fellow, NUS) is currently leading experimental research on future fuels aimed at reducing emissions and decarbonising the environment. This research is being conducted with researchers from NUS and Cambridge. From this study, Dr Zong has investigated a wide range of fuel additives to optimise combustion performance and curb emissions. Dr Zong is also working on a new research project focused on plasma combustion and laser diagnostics. Since 2023, Dr Zong has been building connections with industrial partners, such as City Energy and PS Energy for the utilisation of IRP3 research outcomes and potential commercialisation of the technology.

Update on work package 3.2

Refinery, fuel and engine of the future — modelling

Chemical mechanisms, PAH chemistry, after-treatment

Dr Laura PASCAZIO (Research Fellow, CARES) is working on extending The World Avatar (TWA) capabilities in the chemistry domain. Recently, she has been focusing on extending OntoSpecies, an ontology for the representation of chemical species and their properties. The goal is to enrich the TWA chemistry domain by retrieving data from chemistry databases such as PubChem and store the data in TWA using a software agent. The ontological format permits advanced queries, easy data analysis, and visualisation. This can be used to compare chemical properties of similar compounds, find compounds with required characteristics, and automate laborious data gathering. A paper on this project is in preparation.

Jointly with **Mr Simon RIHM (PhD student, CARES)**, she has started work on the digital representation of chemical laboratories. A paper on this topic was recently published in *Chemie Ingenieur Technik*.

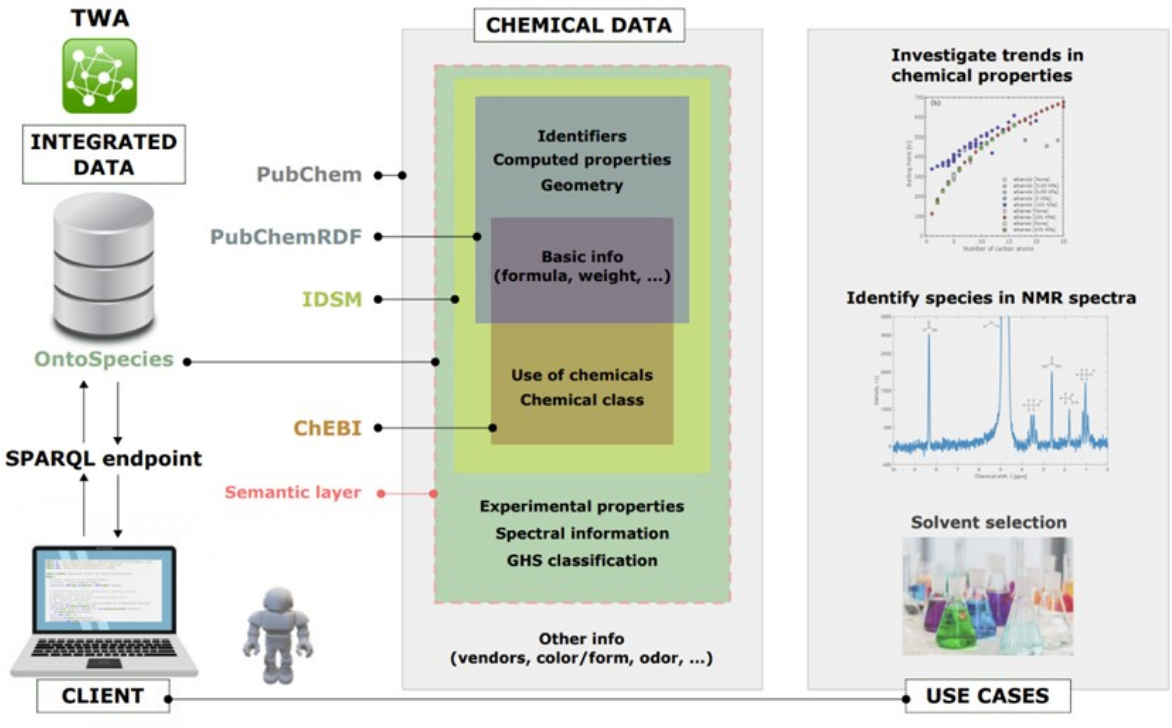


Figure 3.1: A schematic representation of the data flow from various web sources of chemical data, integrated and semantically represented in OntoSpecies Knowledge Graph, which is then accessed via a SPARQL endpoint. Some use cases are depicted to highlight the practical applications and utility of OntoSpecies in scientific research.

Dr Laura PASCAZIO

Update on work package 3.3

Better, cheaper, cleaner nanostructures — experimental

Flame synthesis of thin films of mixed metal oxide nanoparticles

Dr Morteza KOLAEI (Research Fellow, NTU) has recently dedicated his efforts to developing innovative designs for gas diffusion electrodes (GDEs). The issue of flooding is a critical concern that negatively affects the efficiency and stability of CO_2 reduction GDEs, particularly under industrial conditions with high current density, and it requires attention and resolution. To mitigate the problem, Dr Kolaei proposed integrated PTFE membrane-Cu GDE. In this new design, the Cu foam serves a dual purpose. It can be utilised as a substrate for the deposition of catalyst particles using a flame-based process, or it can be directly employed as a catalyst layer positioned on top of the PTFE membrane. Cu foam offers significant advantages as a substrate for catalyst particle deposition, mainly due to its outstanding conductivity and the potential for high-temperature post -treatment of electrodes. In this integrated design, PTFE is utilised as the gas diffusion layer. He has developed a method to perfectly integrate these two separate components, creating a unified GDE. Prototypical electrodes have been successfully created and demonstrated their functionality.

Additionally, in his investigation of alkaline water electrolysis within an industrial condition, employing a full-cell configuration, he has identified the beneficial impact of chromium and iron dissolution within the electrolyte. This presence contributes to the reduction of iron detachment from the anode, ultimately leading to an extended stability for the anode.

Update on work package 3.4

Better, cheaper, cleaner nanostructures — modelling

Gas- and surface-phase kinetics, molecular modelling and reactor optimisation

Mr Simon RIHM (PhD student, CARES) continues his work to advance our understanding of electrocatalytic CO_2 reduction (eCO_2R) - specifically its reaction mechanism. Based on an invited talk he gave at an international research conference and ensuing discussions, he now focuses on the more general problem of probing and isolating kinetic effects in complex heterocatalytic systems (Figure 3.2). Currently, he is participating in an effort to provide a comprehensive review of this topic together with known experts in the field. Furthermore, he initiated further collaboration with **Dr Hangjuan REN (CARES Visiting Scientist, Oxford)** based on their prior work using proton-transfer-reaction mass-spectrometry to characterise eCO_2R products.

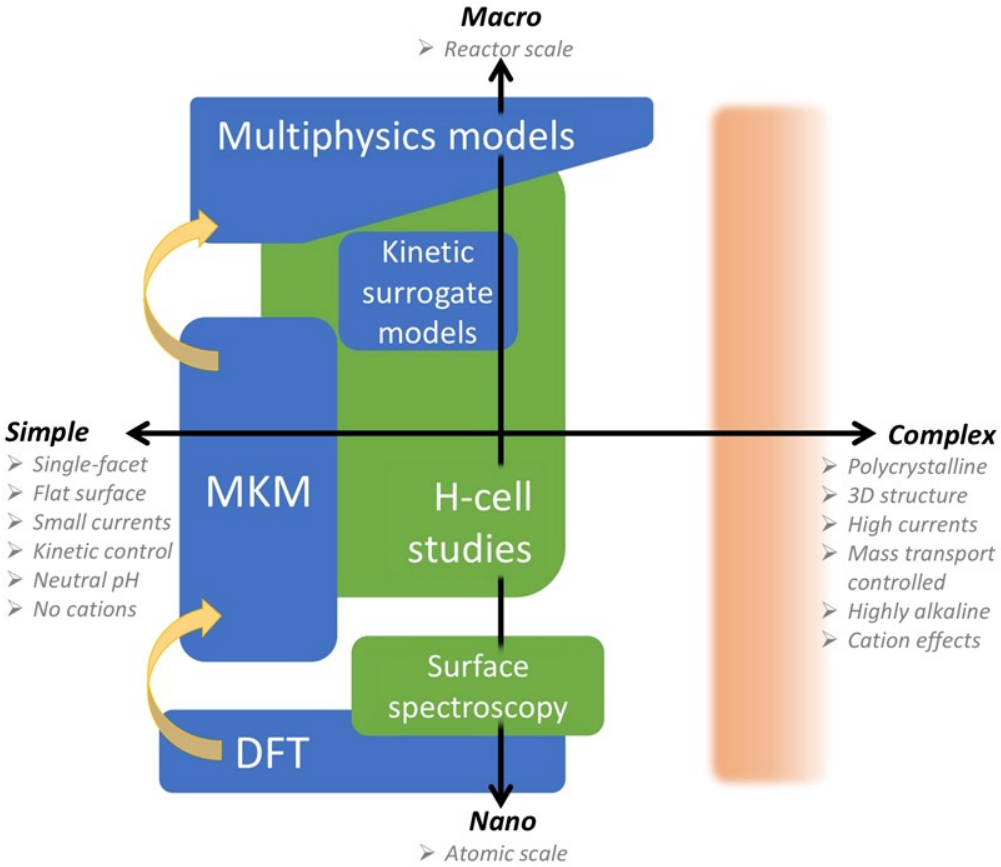


Figure 3.2: Methods of knowledge gain for complex reaction mechanisms of heterocatalysis. Ranging in applicability from simple to complex reactors and in level of mechanistic understanding from nano to macro scale, experimental methods are depicted in green and computational methods in blue. While understanding on a macro scale can theoretically be derived from first principles (see arrows), our understanding for mechanism and kinetics in commercially-relevant reactor types (shown in red) is still lacking.

Mr Simon RIHM

Dr Aleksandar KONDINSKI's (Research Fellow, CARES) develops knowledge-based AI technology tailored to address the automated rational design of porous polymeric materials called covalent organic frameworks (COFs). These COFs are crystalline in nature, and they offer potential in areas such as printable electronics and gas storage, notably capturing CO_2 and water vapour from the air. The study employs chemical knowledge and chemical knowledge processing for molecular and materials engineering.

In this reporting period, Dr Kondinski has worked on the representation of COFs in a graphical format. Using the established ontology as a reference, he incorporated cheminformatic methods to improve the drawing agent. COFs within the knowledge graph are now searchable based on substructure units. Once these materials are correctly catalogued and depicted, retrosynthetic construction becomes a more straightforward problem to address. This development aims to make the information on COFs more accessible and systematically organised.

Dr Kondinski is working together with **Dr Pavlo RUTKEVYCH (Research Fellow, CARES)** who is engaged in the development of an ontology tailored for zeolites. Zeolites are naturally occurring inorganic crystalline materials that can also be industrially synthesised. A significant part of their composition mirrors materials and minerals that are abundant in the Earth's crust. Owing to their impressive thermal stability and hollow structure, zeolites have become attractive heterogeneous materials in the realm of carbon capture and conversion.

In this reporting period, Dr Rutkevych has been working on an ontology meticulously designed to capture the chemico-physical properties of zeolites. This includes aspects such as structure, rational design, chemical composition, porosity, and synthesis methods. Given the crystalline nature of zeolites, significant effort has also been channelled into developing an ontological representation for crystalline materials at large. This broader representation encompasses details on unit cells, lattice parameters, atomic arrangements, and spatial categorisation. Such categorisation enables crystalline materials to be machine -actionable, thereby expanding the chemically accessible space within the knowledge graph.

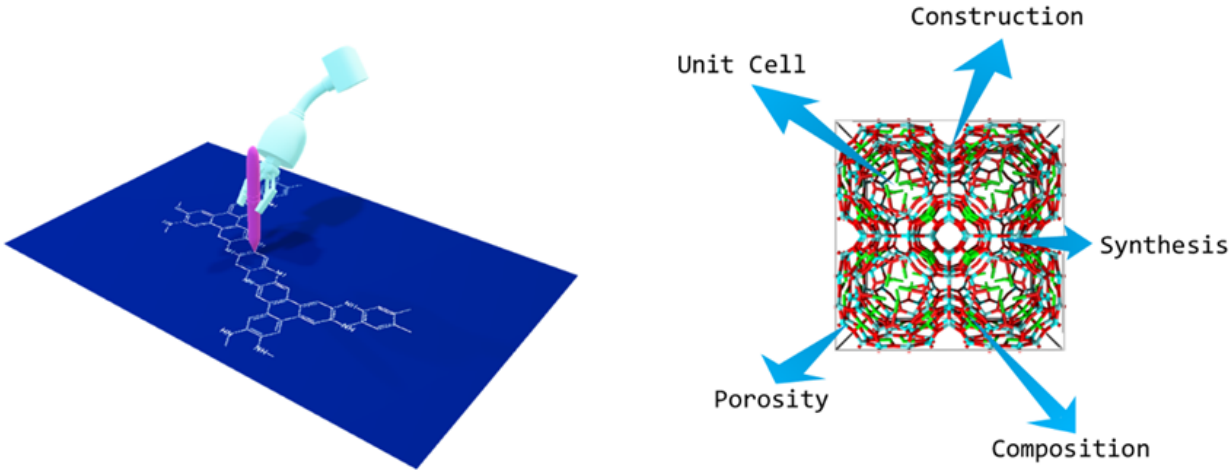


Figure 3.3: (Left image) Agent that automatically draws units of complex polymeric materials for carbon capture. (Right image) Ontology for the representation of crystalline and zeolitic materials relevant in carbon capture.

Dr Aleksandar KONDINSKI

Scientific output

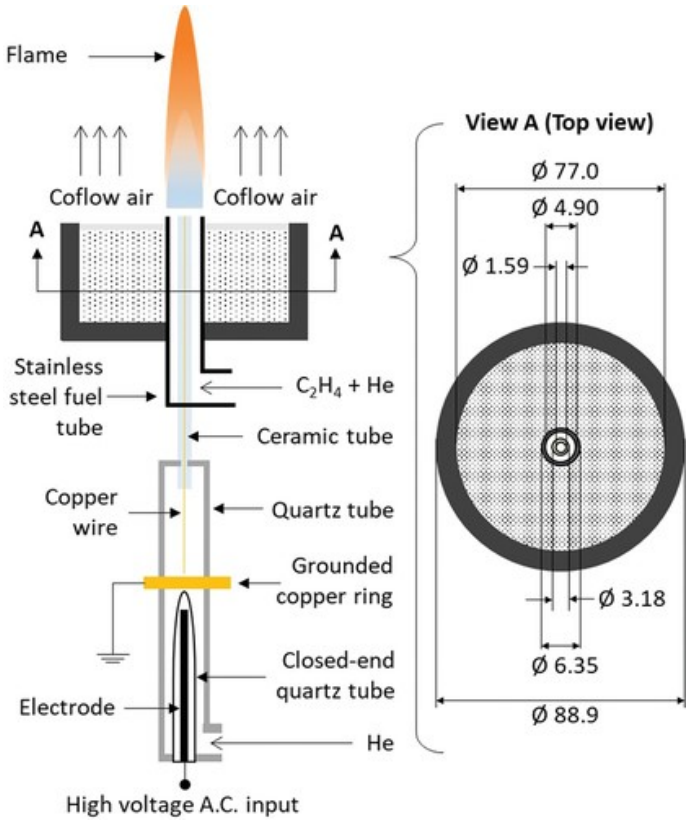
The following are the CREATE-acknowledged publications generated by IRP 3 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Investigation on the Effect of Charge Injection from Non-Thermal Plasma on Soot Formation in Laminar Coflow Diffusion Flame

Yong Ren Tan, Yichen Zong, Maurin Salamanca, Jacob W. Martin, Jochen A. H. Dreyer, Jethro Akroyd, Wenming Yang, and Markus Kraft, *Combustion Science and Technology*

DOI: 10.1080/00102202.2023.2206521

Abstract: A novel, modified coflow burner was developed to study the effect of charge injection from a non-thermal plasma into three helium-diluted laminar coflow diffusion ethylene flames. The frequency of the high voltage (HV) signal was varied to control the ion concentration (charge) injected into the flames. Optical emission spectroscopy was used to characterize the non-thermal plasma while a bias plate methodology was used to gauge the relative amount of charge generated. For different HV signal frequencies, the laser-induced fluorescence of OH, chemiluminescence of CH*, and laser-induced incandescence of soot in flames were measured. The OH and CH* measurements showed that the flames retained the classic flame shape with charge injection. Significant soot reduction was observed at low HV signal frequencies, corresponding to an increase in charge injection. Notably, at low HV signal frequency, soot reduction in highly concentrated (60%) ethylene flame is three times lower than the less concentrated (32%) ethylene flame. This can be attributed to the decrease in the injected charge to soot precursor concentration ratio when the concentration of ethylene in the flame is increased. These results demonstrate that the current system is a promising candidate for studying the charge effect from non-thermal plasma on soot formation in laminar coflow diffusion flames.

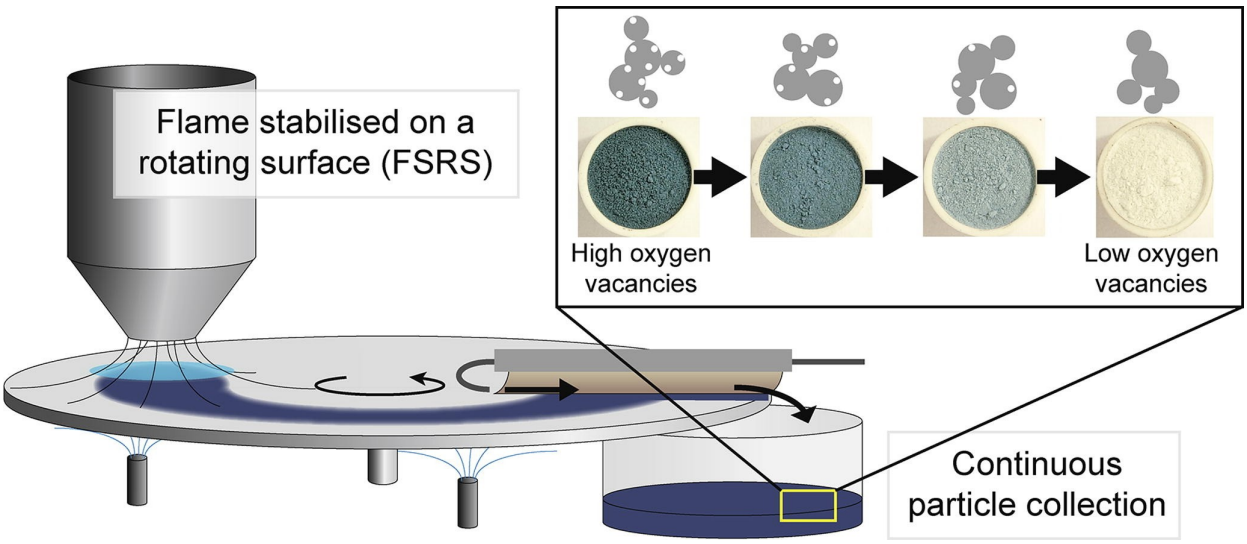


Effects of particle collection in a premixed stagnation flame synthesis of sub-stoichiometric TiO_{2-x} nanoparticles

Manoel Yohanes Manuputty, Rong Xu, and Markus Kraft, *Chemical Engineering Science*

DOI: 10.1016/j.ces.2022.118155

Abstract: Flame synthesis is a simple method to prepare sub-stoichiometric titanium dioxide (TiO_{2-x}) nanoparticles. A rotating stagnation plate is often used as a substrate and to provide a cooling mechanism. The collection of particles from the rotating plate could be done in two ways: the conventional interval particle collection (IPC) method and a continuous particle collection (CPC). The effects of the deposition time and the rotation speed on the properties of titanium dioxide (TiO_2) particles are investigated experimentally. For IPC, it was found that the properties of the collected samples are dependent on the deposition time. This creates an undesirable correlation between properties and synthesis yield. On the other hand, CPC approach allows for a continuous synthesis in which the particle properties are invariant with respect to the synthesis yield. The tunability of the particle properties is still achievable by controlling the rotation speed in the CPC.



Other activities and achievements

Mr Simon RIHM (PhD student, CARES) delivered presentations at these events below:

- Poster presentation on "Developing comprehensive digital twins of research laboratories: Introducing a systems engineering approach" at the DECHEMA Annual Meeting on Reaction Engineering in Frankfurt, Germany on 15 May 2023.
- An invited talk on the topic "Production of C^{2+} chemicals by electrochemical reduction of CO_2: mechanistic advances and technical issues" at the ACS Annual Green Chemistry & Engineering Conference 2023 in Long Beach, California on 13 June 2023.
- Poster presentation on "Connected Digital Twins of research laboratories" at CREATE Symposium 2023 in Singapore on 10 July 2023.

Dr Laura PASCAZIO's (Research Fellow, CARES) paper "Exploring the internal structure of soot particles using nanoindentation: A reactive molecular dynamics study" received the Institute of Physics Combustion Physics Group Ricardo Award for a paper published in 2019 or 2020 contributing to the significant technological advancement of combustion.

Dr Yichen ZONG (Senior Research Fellow, NUS) founded a spin-off from the C4T programme in September 2023. 3Y Energy will aim to establish Singapore's leadership in maritime decarbonisation by bringing pioneering decarbonisation solutions to vessels and heavy-duty vehicles. The founding team also includes Dr Xinyi ZHOU (non-CARES Research Fellow, NUS) and **Mr Jieyao LYU (CARES Visitor, NUS)**.

After being selected as a finalist at Pier71 Smart Port Challenge out of over 150 startups worldwide, 3Y Energy is now entering an incubator program under the Maritime & Port Authority of Singapore and NUS Enterprise. This will provide training and direct connections with industrial partners to commercialise their technology offering modular designs and retrofits to enable legacy engines to adopt alternative, carbon-neutral fuels without compromising performance. 3Y Energy will leverage CARES' expertise in combustion and fuel research to use advanced chemical simulations and full engine modelling to unlock the decarbonisation potential of fuels such as biodiesel, methanol, ammonia, and hydrogen .

Dr Zong has also been continuing to engage in connections with industrial partners such as City Energy for hydrogen utilisation in Singapore and PS Energy for the commercialisation of fuel additives.

Dr Zong gave a poster presentation on "Clean energy: Hydrogen transition" at CREATE Symposium 2023 in Singapore on 10 July 2023.

IRP 4

BETTER, CLEANER HEAT USAGE

Better, Cleaner Heat Usage is a new IRP 4 for Phase 2, replacing the former energy/electricity focus in Phase 1. This work is focused on high-performance thermal management and waste heat recovery research for improved, i.e., cleaner and more efficient heat usage in energy conversion technologies. IRP 4 addresses two key challenges in power generation systems: a) the efficient management of heat and b) the emission of harmful pollutants, which is particularly problematic in fuel-based technologies such as diesel engine power plants or marine engines. Regulations are increasingly stringent for these systems and a full understanding of the underlying phenomena is necessary to tackle this problem.

IRP 4 Principal Investigators:

Professor Epaminondas MASTORAKOS
University of Cambridge

Professor Alessandro ROMAGNOLI
Nanyang Technological University

Professor LEE Poh Seng
National University of Singapore

OVERVIEW

The work on maritime energy systems, pollution, and decarbonisation scenarios has continued during the reporting period. Liquid hydrogen energy systems are described in WP 4.3, while air pollution due to accidental leaks and measurements using drones fitted with sensors are described in WP 4.4. Significant interactions with the Maritime & Port Authority of Singapore took place, culminating in CARES' participation in a methanol bunkering test – a world's first on 27 July 2023. The dispersion simulations follow various levels of complexity, from Gaussian plume models to complex CFD around two ships mimicking bunkering operations.

Professor Epaminondas Mastorakos, PI
University of Cambridge

Update on work package 4.1

Engine combustion — best fuel, best operating condition

This Task has not made progress in the reporting period due to recruitment difficulties. A new researcher will start in October 2023 to finish this Task.

Update on work package 4.2

Closed power cycles—selection and analysis

There are no updates for work package 4.2 in this report due to recruitment difficulties in the last few months.

Update on work package 4.3

High-efficiency heat exchanger

Dr Mohamed Fadhel AYACHI's (Senior Research Fellow, NTU) current research activities are mainly focused on the development and assessment of LNG and LH_2 cold utilisation strategies for Singapore. To date, converting liquid hydrogen back to its gaseous state at ambient temperature calls for using the LNG terminal technologies, which are about vaporisers relying on either ambient air or seawater. The idea then is to come up with integrated solutions for Singapore to meet energy savings strategies that seek to exploit the LNG/LH_2 high-grade cold energy content and environmentally friendly objectives that support carbon capture and storage.

In this context, the current work consists of developing a baseline model associated with LNG cold utilisation. It refers to the current LNG terminal capacity in Singapore and provides some initial strategies (Figure 4.1). This model will serve as a baseline for the development of a larger scheme with optimal cold energy distribution, by considering 1) multiple utilisation opportunities

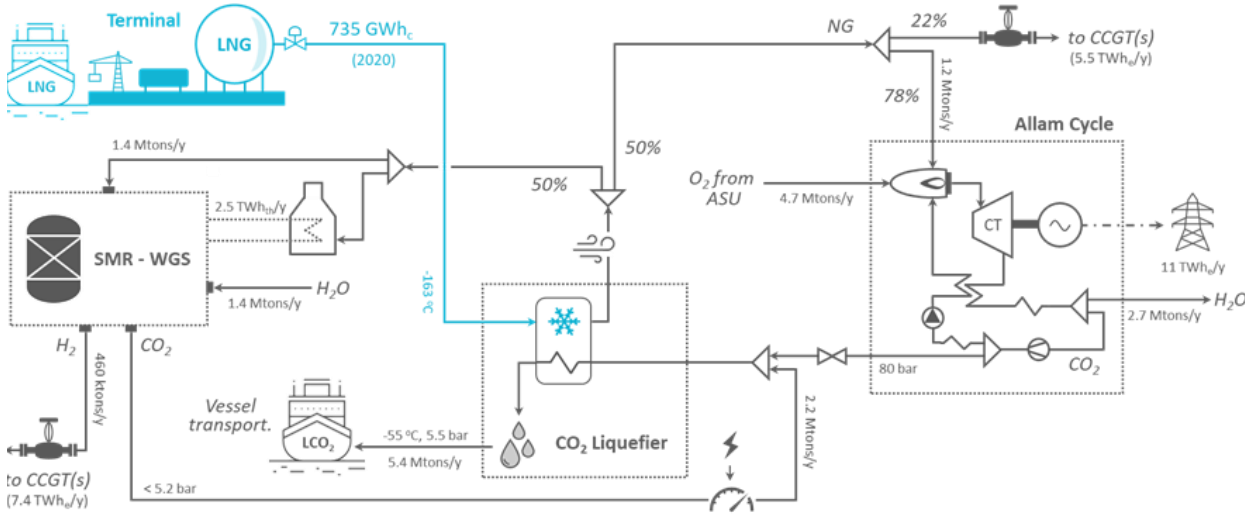


Figure 4.1: LNG cold utilisation associated to carbon capture and H_2 production.

Dr Mohamed Fadhel AYCHI

(including cryogenic cogeneration) and 2) synergy with a potential LH_2 import scenario.

On the other hand, part of the focus during this period consists of conducting mapping of the different hydrogen carriers suitable for Singapore and in having an understanding of the challenges that are mainly associated with the LH_2 carrier. It also explores how R&D associated to this carrier can contribute to an economically feasible pathway for the hydrogen supply chain (e.g., H_2 liquefaction processes, LH_2-to-H_2 reconversion processes). This will help in the development of an integrated process design that would enable an efficient recovery of the liquefaction energy consumed prior to shipment.

Update on work package 4.4

Process system model for the J-Park Simulator

Dr Yangyang LIU (Research Fellow, CARES) conducted numerical simulations using the computational fluid dynamics (CFD) technique to study the accidental ammonia leakage process during ammonia bunkering and provide safety assessments. After reviewing the current literature related to the simulation of ammonia release by CFD, Dr Liu consolidated the scheme for ammonia leakage simulation, including the leakage scenario, computational geometry and numerical method. The computational geometry was generated by SOLIDWORKS and then imported into CONVERGE CFD. For simulation, the Reynolds-Averaged Navier-Stokes approach with the k-ω SST turbulence model was applied. Fixed embedding and adaptive mesh refinement techniques were utilised for locally refining grids. Both vertical and horizontal ammonia leakage cases were carried out.

Figure 4.2 and Figure 4.3 show the ammonia distribution for horizontal and vertical leakage sce-

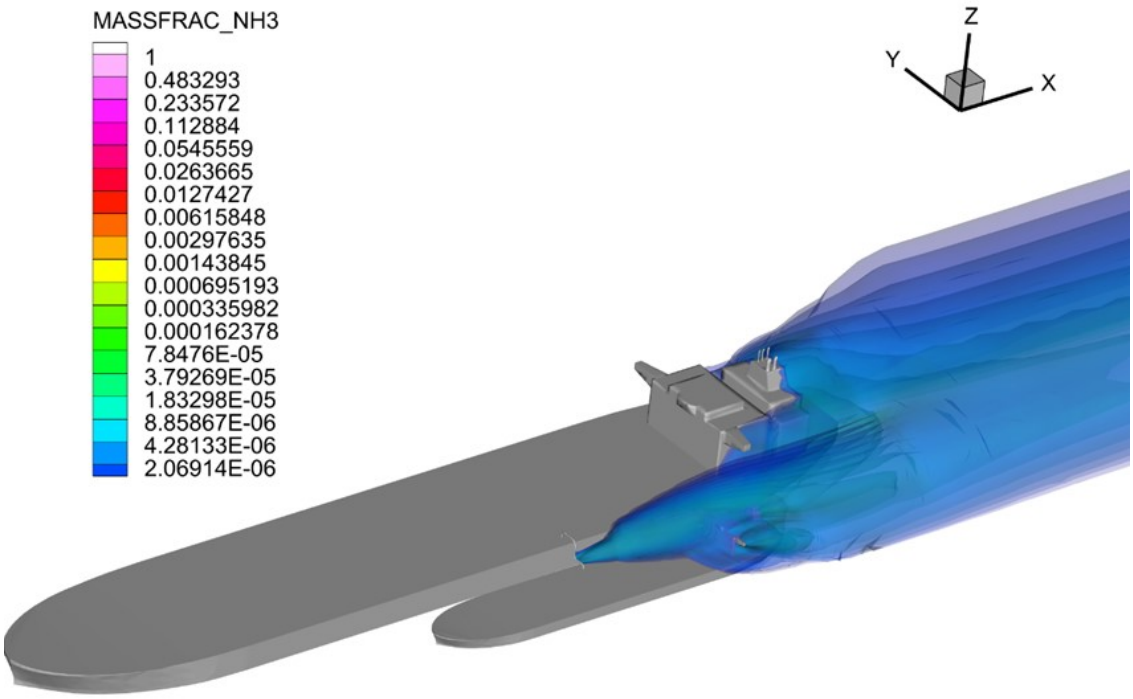


Figure 4.2: Ammonia distribution for horizontal leakage scenario.

Dr Yangyang LIU

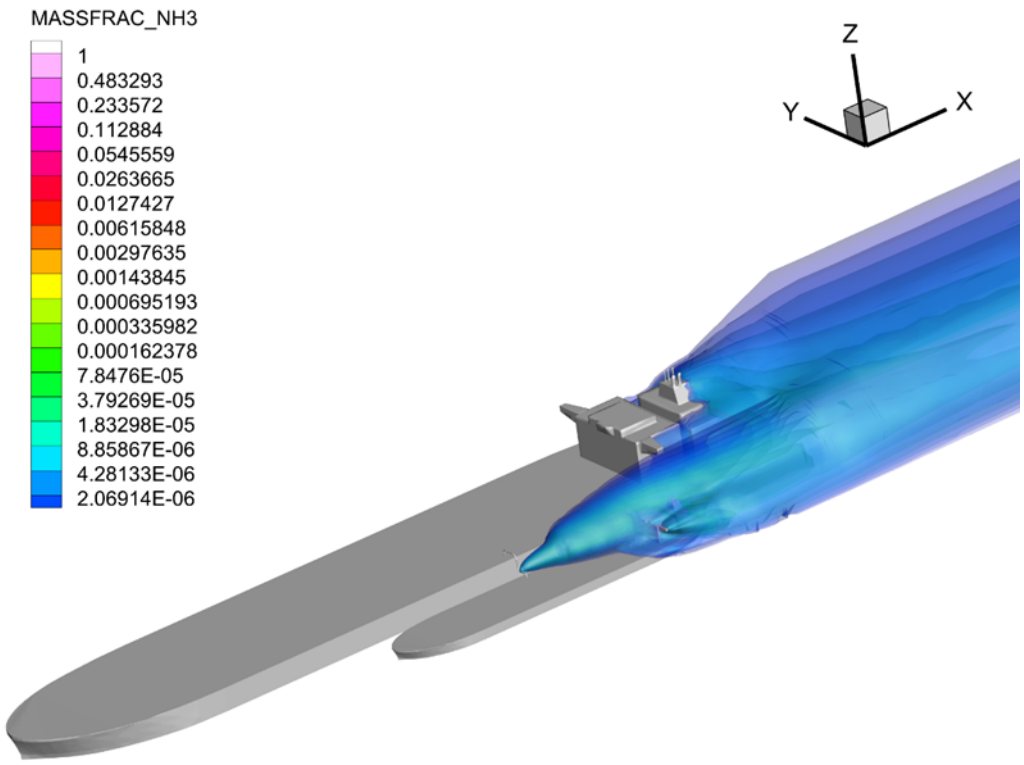


Figure 4.3: Ammonia distribution for vertical leakage scenario.

Dr Yangyang LIU

narios, respectively. Clearly, the superstructure parts on two ships affect the dispersion of ammonia in the near field. Compared to the horizontal leakage case, the vertical leakage has a more serious consequence with higher and further dispersion of ammonia. This means that, due to the toxic effect of ammonia, people on board may be exposed to a larger dangerous area where the concentration of ammonia exceeds the exposure limit. This study considered the effects of the existing tall and massive structures on board vessels on the dispersion of released ammonia in the near field. The dependence of the ammonia dispersion on the leakage position, atmospheric conditions, etc., will also be demonstrated. The findings of this study will contribute to the risk assessment and designing effective operational and mitigation control measures for ammonia bunkering operations.

Ms Li Chin LAW (Research Engineer, CARES) is exploring ship-based carbon capture and storage (CCS) technology as an alternative approach to reduce carbon emissions in shipping. Carbon capture is an energy-intensive technology; however, it can be optimised by integrating with heat recovery from high-temperature streams and LNG cold energy conservation. In this project, the potential energy savings with waste heat recovery and LNG cold energy conservation were quantified. Post-combustion CCS is the conventional CCS technology for flue gas treatment, alternatively, pre-combustion CCS which could promote waste heat utilisation was introduced. This concept combines the operation of two energy-intensive systems, namely hydrogen production and carbon capture. Energy assessment and comparison between three hydrogen production technologies and four carbon capture technologies have quantitatively shown that the combination of steam methane reforming (SMR) and pressure swing adsorber (PSA) is the most efficient technology for CO_2 reduction. Integrating SMR increases the CO_2 concentration in the syngas and reduces the flow rate of CCS feed. At the same time, the size and space needed for carbon capture are reduced, which implies a smaller cargo

loss. Ship-based SMR-PSA can be the stepping stone for ship propulsion using hydrogen fuel. With an on board SMR-PSA system, blue hydrogen can be produced on board of ship when required. This has resolved some of the challenges faced in bunkering and storage of liquefied hydrogen (LH_2). In addition, the issues of large LH_2 boil-offs and hazards associated with LH_2 handling are reduced with the shortened pipelines which can minimise LH_2 vaporisation. The model has suggested up to 70% of carbon reduction with a relatively low energy penalty. The proposed system offers flexible decarbonisation that can be gradually scaled over time. The results suggest that producing hydrogen on board the ship and capturing CO_2 at the reforming stage is an appealing marine decarbonisation strategy.

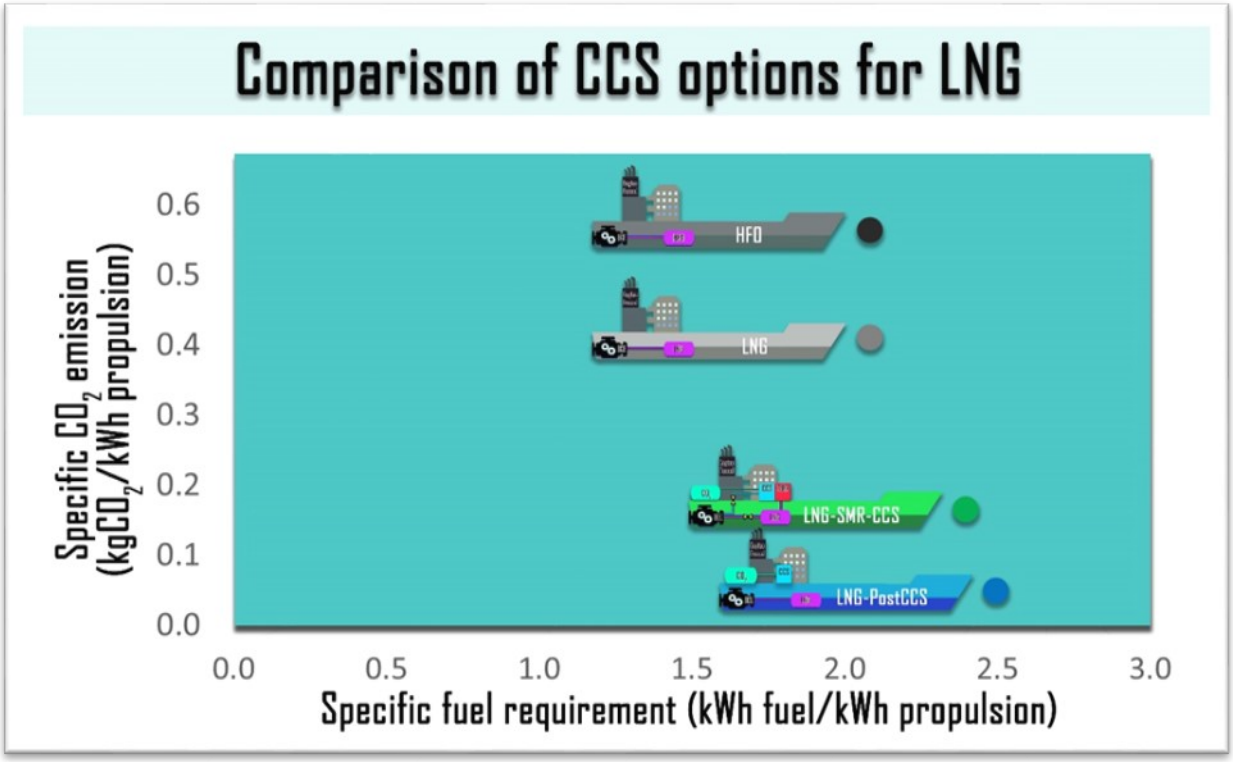


Figure 4.4: Specific CO_2 emission versus the specific fuel requirement of the proposed pre-combustion carbon removal and capture system (LNG-SMR-CCS) compared with conventional ships and ships with post-combustion carbon capture unit (LNG-PostCCS).

Ms Li Chin LAW

Dr Ramesh KOLLURU (Research Fellow, CARES) carried out Computational Fluid Dynamics (CFD) combined with Incompletely Stirred Reactor Network (ISRN) simulations to explore the evolution of chemically reacting species in the Marine Boundary Layer (MBL) and in the near field of a large ship. Various cases with the wind direction varying were studied. The Chemical Bond Mechanism (CBM IV) is used for modelling atmospheric chemistry reactions, while the Conditional Moment Closure model, integrated over space to give an ISRN approach, was used to model turbulence-chemistry interactions. The chemical reactions are solved in mixture fraction space and then exported to the CFD resolution. The initial concentrations used to estimate the evolution of chemical species are presented in Table 4.1, where h=0 refers to the background air and h =1 to the species concentrations at the ship's exhaust, assuming a typical large diesel engine. The baseline concentrations were acquired from Mastorakos [2], while the exhaust concentrations were sourced from the study by Kim et al. [1]. Figure 4.5 visually portray the evo-

Sno	Species	Concentration in ppb at the Exhaust	Concentration ppb at the Background
1)	Nitric Oxide (NO)	1111.148	0.182
2)	Nitrogen Dioxide (NO_2)	0.0	0.018
3)	Sulphur Dioxide (SO_2)	43.974	0.0
4)	Carbon Monoxide (CO)	58.016	0.0
5)	Ozone	0.0	20.3
6)	Methane (CH_4)	68.353	0.0
7)	Xylene (XYL)	0.220	0.35
8)	Toulene (TOL)	0.538	0.35
9)	Ethene (ETH)	1.871	0.35
10)	PAN	0.135	0.0
11)	PAR	4.2	4.9

Table 4.1: Concentration of chemical species at the background and at the exhaust.

lution of the conditional probability distribution function and scalar dissipation rates in mixture fraction space. Meanwhile, Figure 4.6 shows the absolute NO values along the length of the domain. The corresponding NO fluctuations in the mixture fraction space are depicted in Figure 4.7. In Figure 4.8, contour and line plots depict the evolution of the time-averaged NO within the wake region at CFD resolution. The simulations show the quick mixing achieved in the wake of the ship, due to the combined action of a downwash flow, a horizontal inward flow associated with a recirculation as shown in the streamline Figures 4.9, and the extra turbulence produced by the local shear. The plume does not behave as a point source, but rather as an emission from a source of finite size. In addition, strong asymmetry of the concentration is evident in the horizontal and vertical directions. These observations impact how ship emissions are to be included in regional-scale Air Quality Modelling and demonstrate the local effects that can appear.

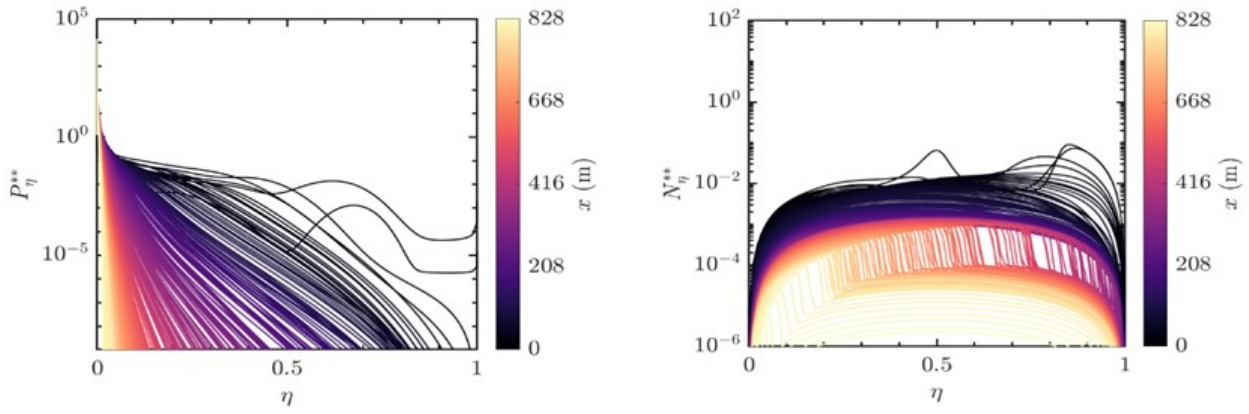


Figure 4.5: (left) Variation of probability distribution function in mixture fraction space; (right) Scalar dissipation rate in mixture fraction space

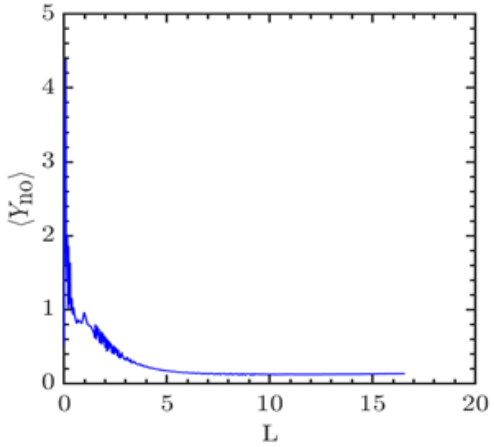


Figure 4.6: Variation of NO in physical space at ISRN resolution

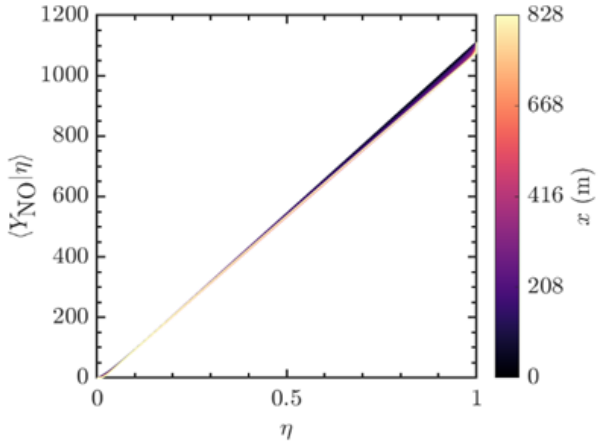


Figure 4.7: Variation of NO in mixture fraction space

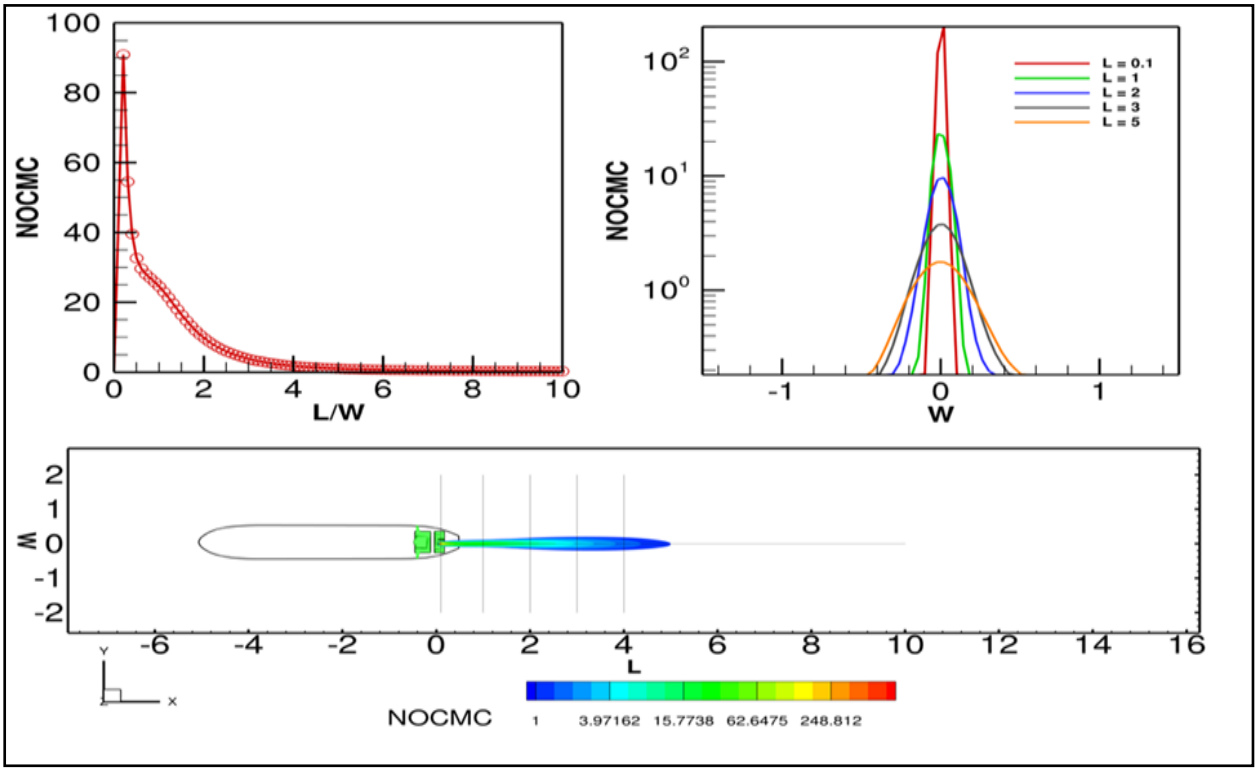


Figure 4.8: Unconditional plots of NO in physical space. The plot in the upper left corner presents a line plot illustrating the variations in NO along the length at W = 0 and H = 1. Conversely, the upper right figure illustrates the NO fluctuations across the xy plane, positioned at various L positions. The contour representation of NO is displayed at the bottom.

Dr Ramesh KOLLURU

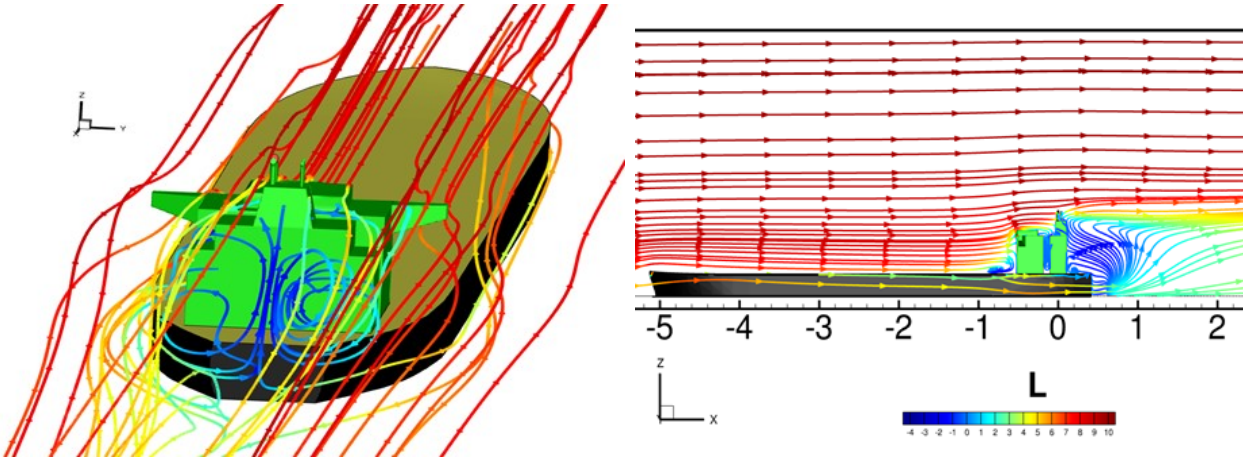


Figure 4.9: (Left) 3D Streamlines on the ship and (right) at section y = 0 plane. The model is generated in a 3D plane (X, Y, and Z). The spatial coordinates are in metres.

Dr Ramesh KOLLURU

Dr Molly HAUGEN (CARES Visiting Scientist, CAM) led a demonstration in April 2023 to showcase the ongoing work of sampling emission plumes with an unmanned aerial vehicle and tailored payload for specific monitoring purposes. Figure 4.10 shows a payload with a particle sensor and Figure 4.11 shows the sampling structure in more detail. The setup shown considers important variables for monitoring mobile emissions sources and gives a method for monitoring maritime emissions for research applications, as well as regulation enforcement efforts.

As shown in Figure 4.11, the UAV is capable of carrying multiple different sensors and can sample from outside the UAV downwash due to the 90 cm sampling probe. The April demonstration served as a showcase for the subsequent bunkering trial in July. Trial preparations for the July testing period began soon after the April demonstration, with high interest gained from government and industrial attendees. A rapid collaboration with NUS and CREATE allowed for risk assessments, trial testing plans, and backup plans to be created.

The goal of the bunkering trial was to demonstrate that this UAV setup could be adapted for use during at-sea monitoring of new fuel bunkering within Singapore's port. The team worked directly with the Maritime & Port Authority of Singapore to create a plan to monitor any fugitive emissions during the planned trial in July. The cooperative project is a foundation for future research and collaborations within Singapore across multiple sectors and University groups.

Figure 4.10: Drone demonstration outside of CREATE Tower showing the influence of the unmanned aerial vehicle (UAV) on the plume it is sampling. Here, the payload is fitted for particle detection.

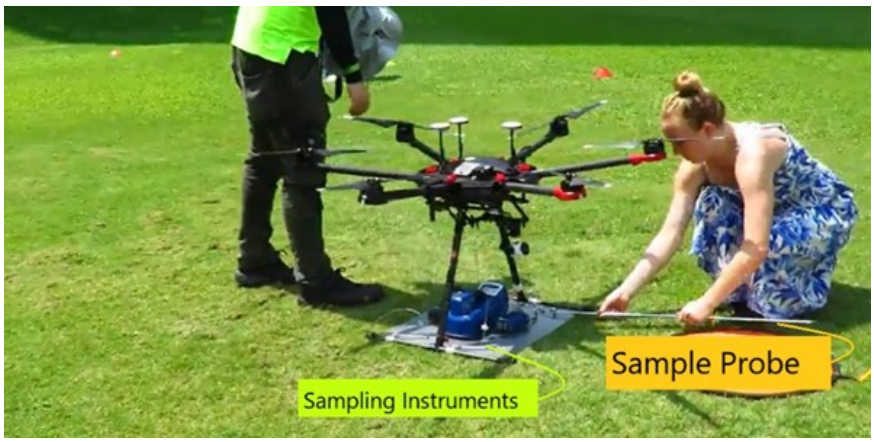


Figure 4.11: The Sample Probe protrudes 90 cm from the UAV's center, enabling sampling from outside the UAV's downwash. The sampling instruments are also shown. Here, the UAV is equipped with particle instruments.

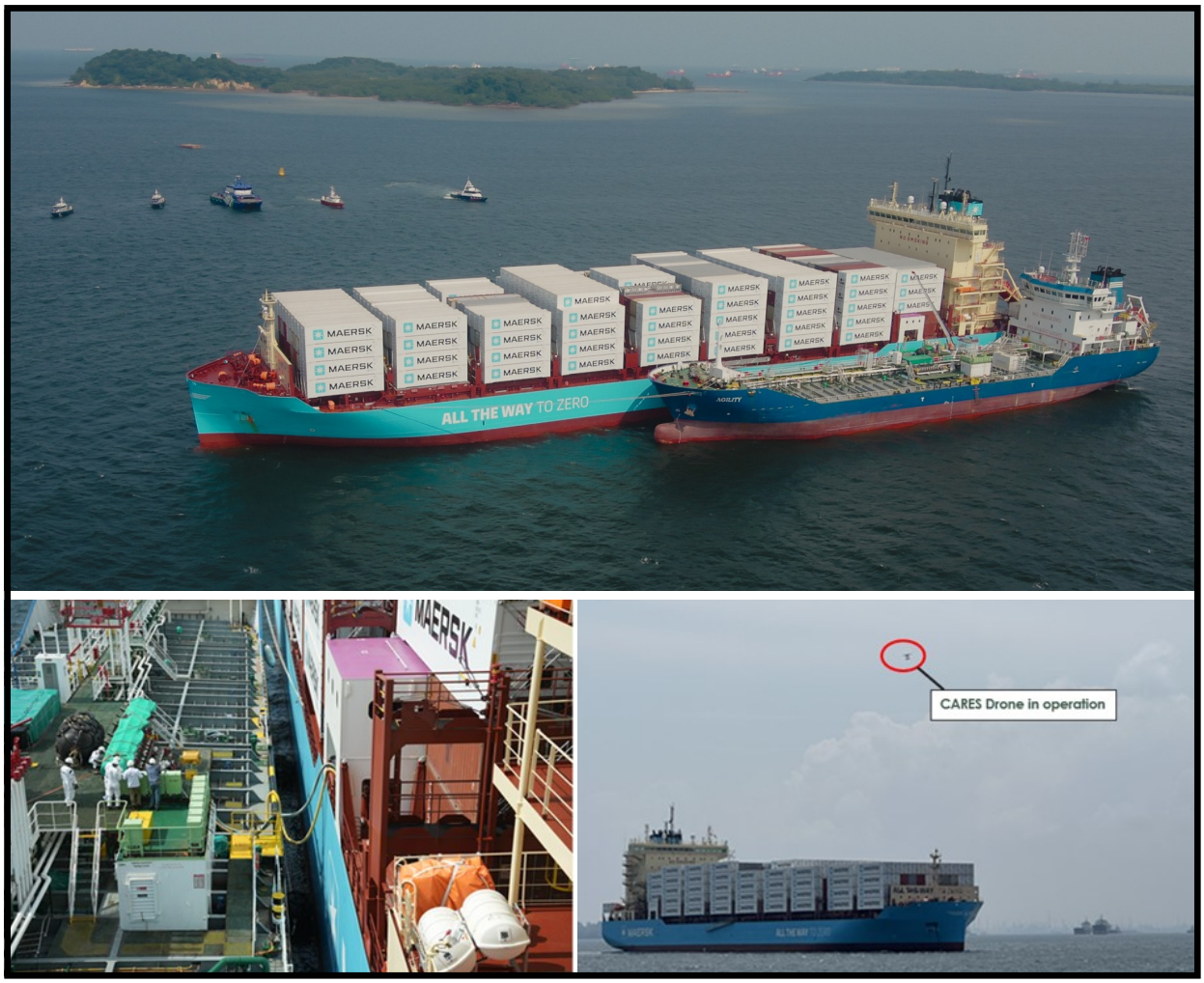


Figure 4.12: Pictures of the methanol bunkering operation on 27 July 2023. Top and bottom-left photo supplied by Maritime & Port Authority of Singapore. Bottom-right photo taken by CARES.

In addition to taking point sampling with the UAV, the team can integrate plume dispersion and mixing estimates to give a more robust understanding of the plume characteristics. An example of this is shown in Figure 4.13 where Dr Savvas GKANTONAS (Research Associate, CAM) has created methanol vapour heat maps, shown for a worst-case scenario (according to MPA) of a 25,000 kg spill and a wind of 5 m/s that was present on the test day. Based on the flammability limits of methanol vapour and the capabilities of the methanol sensor, we have set 500 ppm (mass fraction) as a maximum safe level for the drone operation and hence identified no-fly and safe flight zones (Figure 4.13).

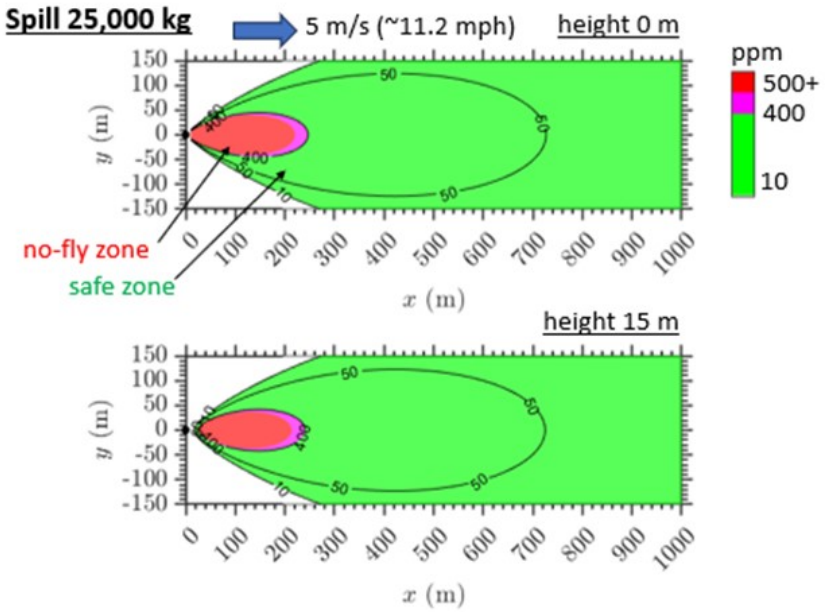


Figure 4.13: Methanol vapour heat maps with no-fly and safe zones indicated. Here it is assumed that a 25,000 kg spill incident occurs and the wind speed is 5 m/s (from left to right). The source is assumed to be at point x=0, y=0 and height=0 m and x stands for the distance downwind.

Dr Savvas GKANTONAS

Using dispersion modelling, more scenarios can be analysed. Before the tests, we have conducted a thorough assessment using estimates for the methanol leakage rates, the consequent evaporation occurring from a circular liquid spill and finally, the vapour dispersion under different atmospheric conditions. Examples of leakage rate and the resulting spill (pool) radius are given in Figure 4.14. Based on the circular spill, the evaporation rate was approximated using the empirical formulas of Sutton and Pasquill [3-4] and Deutsch [5]. As shown in Figure 4.15, the Sutton and Pasquill model gives consistently lower estimates of the evaporation rate and hence the amount of vapour that is to be dispersed. In an interest to have a more conservative estimate with regards to detection limits, we chose the Sutton and Pasquill model for evaporation estimates and further coupled it with a standard Gaussian dispersion model to produce methanol dispersion estimates as in Figure 4.16 and the heat maps of Figure 4.13. Together with the UAV data, the dispersion estimates can be used to help the maritime community learn how leaks could influence urban pollution in Singapore, as well as environmental/ atmospheric repercussions, specifically for future fuels that get adopted as maritime fuel decarbonises.

References:

[1] Kim, H. S., C. H. Song, R. S. Park, G. Huey, and J. Y. Ryu. "Investigation of Ship-Plume Chemistry Using a Newly-Developed Photochemical/Dynamic Ship-Plume Model." Atmospheric Chemistry and Physics 9, no. 19 (October 9, 2009): 7531–50. https://doi.org/10.5194/acp-9-7531-2009.

[2] The conditional moment closure approach for atmospheric pollution problems E. Mastorakos, Engineering Depariment, Cambridge University, UK , Transactions on Ecology and the Environment vol 66, © 2003 WIT Press, www.witpress.com, ISSN 1743-3541

[3] Sutton OG. Wind structure and evaporation in a turbulent atmosphere.Proc Royal Soc London, Series. 1934;A146:701-722.

[4] Pasquill F. Evaporation from a plane, free liquid surface into a turbulent air stream.Proc Royal Soc London, Series. 1943;A182:75-95.

[5] Deutsch S. Verdunstung aus Flüssigkeitslachen unter atmosphärischen Bedingungen, Universität Dortmund; 1995.

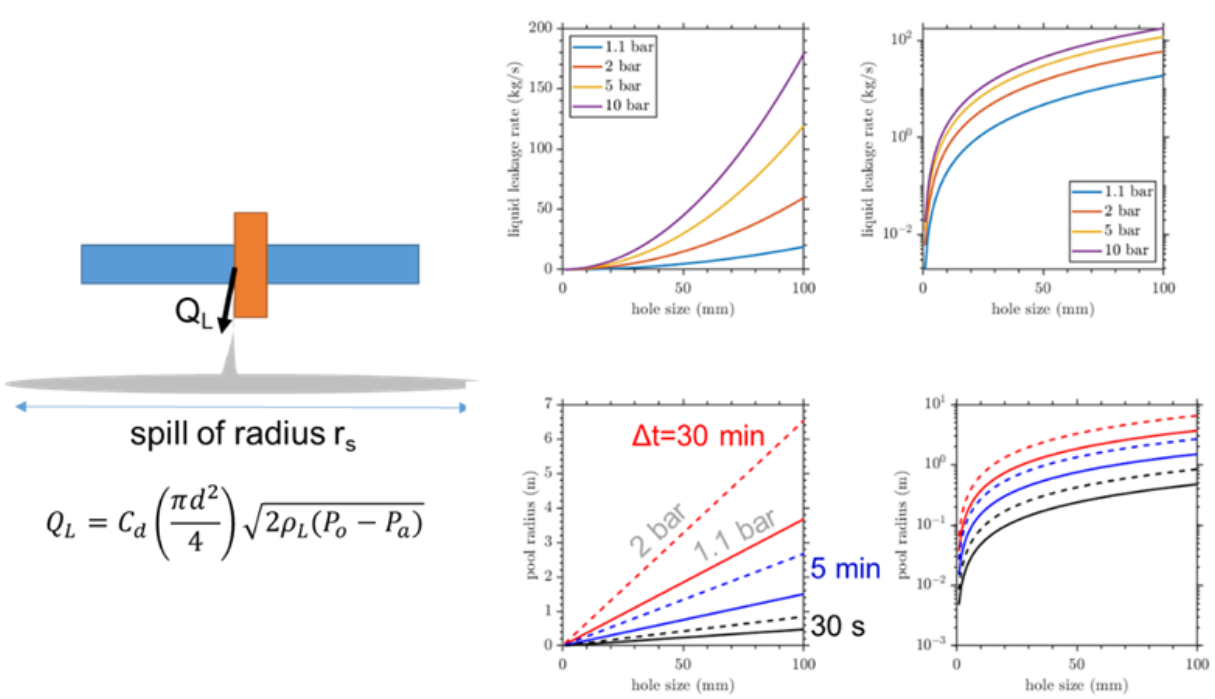


Figure 4.14: Estimates of methanol leakage rate and accumulation in a circular pool. The leakage rate is based on a characteristic hole size d, the relative pressure and a discharge coefficient (here C_d=0.6). If the event lasts Δt and results in a circular spill with a constant thickness of 1 mm above the sea surface (assuming no mixing), then the pool radius can be estimated.

Dr Savvas GKANTONAS

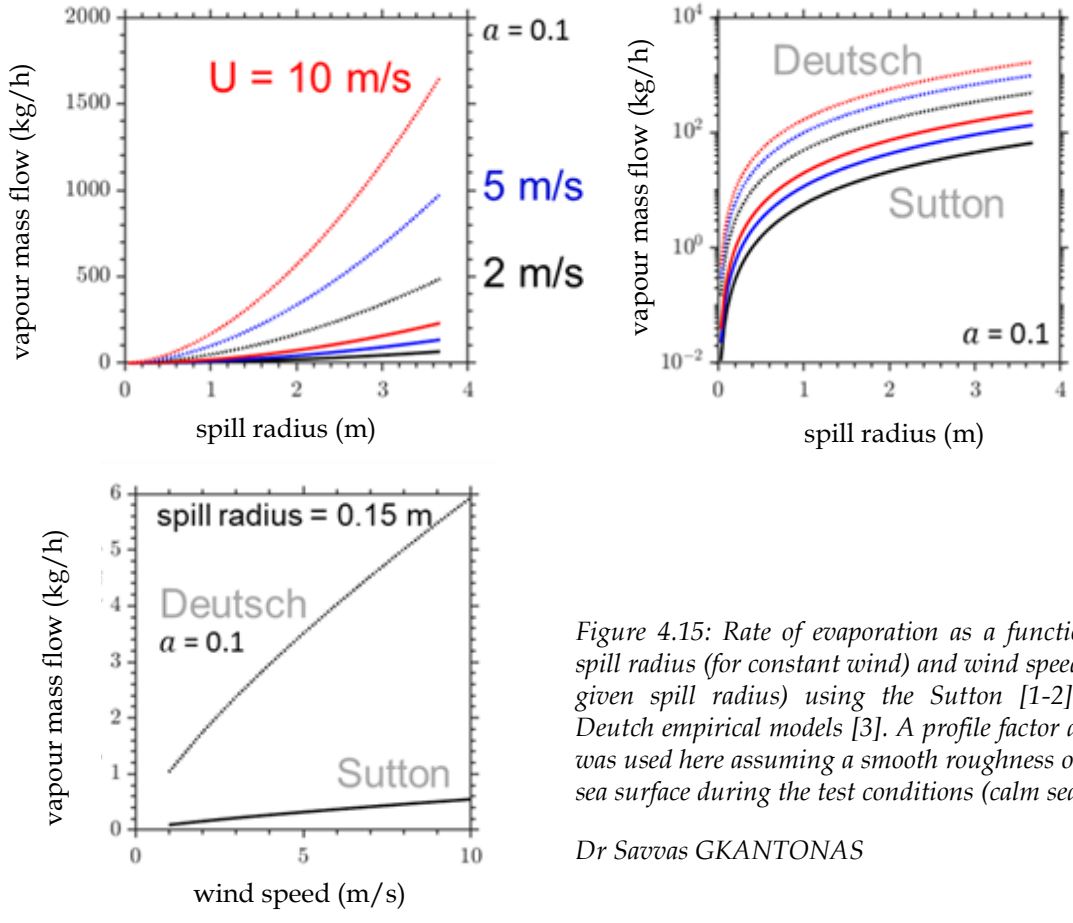


Figure 4.15: Rate of evaporation as a function of spill radius (for constant wind) and wind speed (for given spill radius) using the Sutton [1-2] and Deutch empirical models [3]. A profile factor a=0.1 was used here assuming a smooth roughness on the sea surface during the test conditions (calm sea).

Dr Savvas GKANTONAS

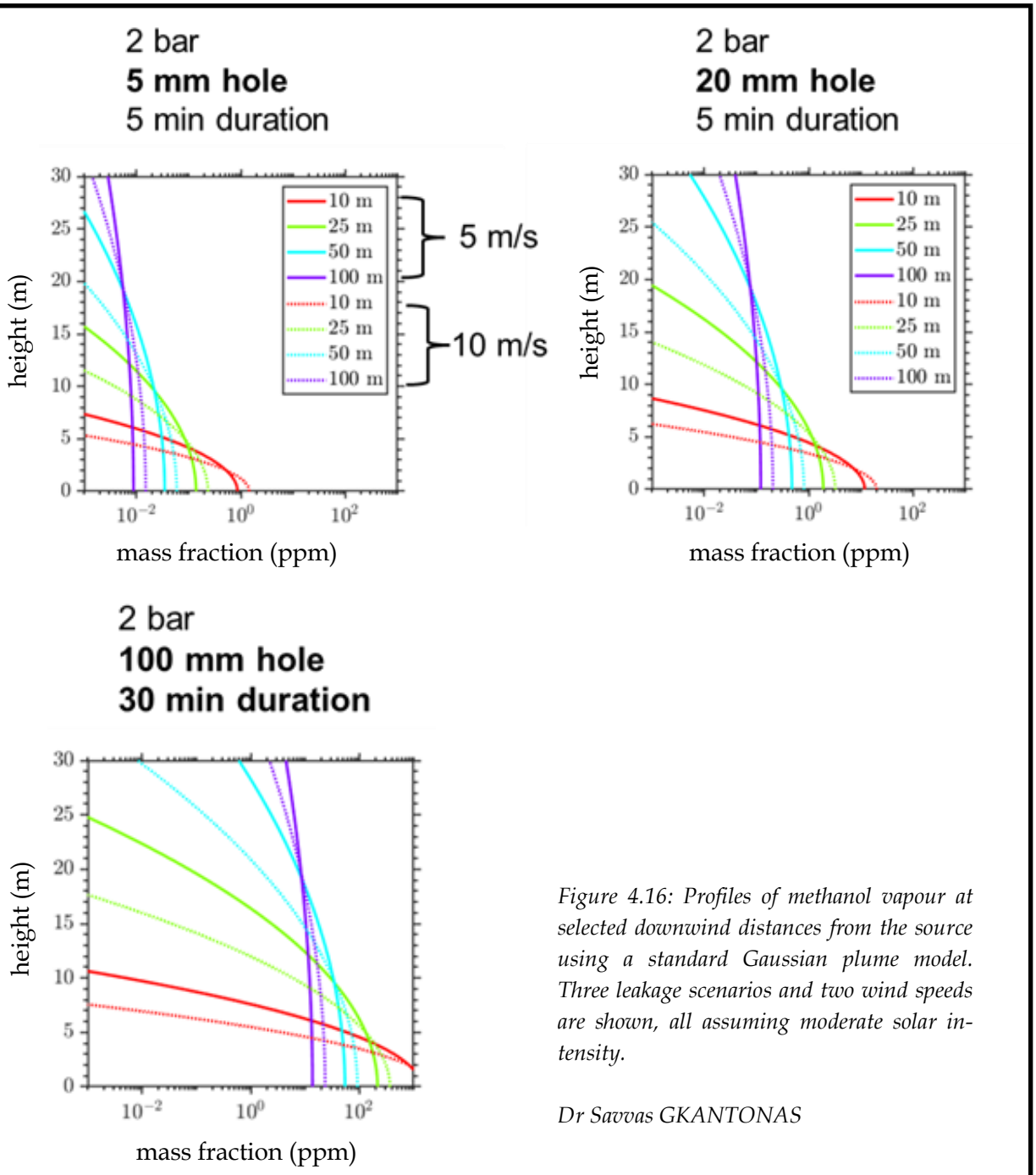


Figure 4.16: Profiles of methanol vapour at selected downwind distances from the source using a standard Gaussian plume model. Three leakage scenarios and two wind speeds are shown, all assuming moderate solar intensity.

Dr Savvas GKANTONAS

Other activities and achievements

Dr Molly HAUGEN (CARES Visiting Scientist, CAM) led a 2-part drone event consisting of a seminar and demonstrator at CREATE Tower and UTown Green at NUS on 20 April 2023. This demonstration brought in researchers, industry leaders, and government officials in Singapore.

Dr Haugen worked directly with the Maritime & Port Authority for the world's first ship-to-containership methanol bunkering operation on 27 July 2023 at the Raffles Reserved Anchorage in Singapore. This included adapting the UAV's launch location, assessing the safety zone around the bunking ship, and creating best practices for this type of emission monitoring, assisted by **Mr Chun Siong SIM (CARES Lab Manager, CARES)**.

Ms Li Chin LAW (Research Engineer, CARES) engaged in various activities:

- Won the Best Presentation Award for the online presentation titled "Estimation of Energy Efficiency of Blue Hydrogen Production Onboard of Ships" at the International Conference on Maritime Energy Management and Research (ICMEMR) from 11 – 12 May 2023 in Paris (virtual conference).
- Presented a poster titled "Low-carbon Maritime Transport" at CREATE Symposium 2023 in Singapore on 10 July 2023.
- Participated in the Masterclass on Maritime Decarbonisation organised by the Singapore Institute of Technology on 20 and 21 July 2023.
- Working to publish a new paper with King Abdullah University of Science and Technology (KAUST) on a project related to cryogenic CO_2 capture.

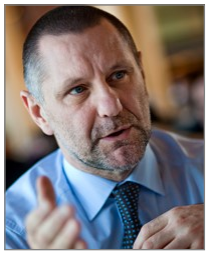
Ms Law and Dr Haugen's research were highlighted by Singapore's national news outlet, *The Straits Times* in the write-up of CREATE Symposium 2023

IRP BB

BETTER BUSINESS: PATHWAYS TO INDUSTRIAL DECARBONISATION

The Better Business IRP acts as an incubator for ideas from all other IRPs and will support the acceleration and scaling of the technology outputs from the programme. It will examine different possible business models and compare the situation in Singapore with other important chemical clusters worldwide, engaging with stakeholders to identify the potential benefits and co-benefits of each technology arising from the programme.

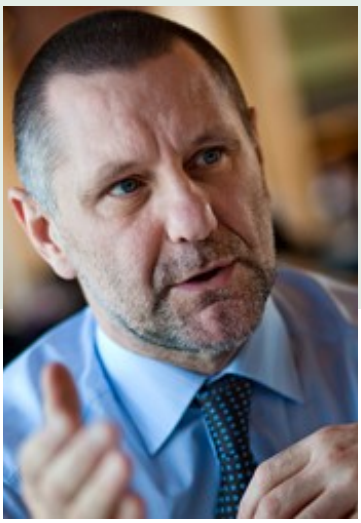
IRP BB Principal Investigators:



Professor Steve EVANS
University of Cambridge

Professor S. VISWANATHAN
Nanyang Technological University

Professor Kenneth HUANG Guang-Lih
National University of Singapore



OVERVIEW

Over the last few months, we have focused on detailed planning to complete these following tasks on time and on cost. These plans are in place and being delivered. Research on business model innovations related to solar energy adoption continues with the manuscripts undergoing revision based on initial feedback. A study on the use of green hydrogen-based synthetic fuel production as a carbon utilisation method has completed and this has been accepted for publication in the journal *Energies*. Another paper related to optimisation for circular economy entitled "An Efficient Approximation to the Pull Policy for Hybrid Manufacturing and Remanufacturing Systems with Setup Costs" has been published in *Institute of Industrial and System Engineering (IISE) Transactions*. The project on how strengthening institutions for VC investment influences the pollution behaviour of firms in China's chemical and energy-intensive sectors has been and will be presented at more international conferences. This work has also been submitted to a top journal – *Strategic Management Journal*. Based on the first study, we continue to conduct empirical analyses on the different roles of VC types (government VCs and private VCs) in influencing the green innovations of focal firms and their underlying mechanisms. A new project on the role of the chief sustainability officer on the company's sustainability performance in terms of emissions, and energy use has generated some interesting results and we are currently working on the manuscript. In addition, a new project on ecosystem-view transformation enabled and empowered by advanced digital technologies is in the process of further data collection from industry and is now in stage 2 of data collection, which focuses on refining of the design and strategy. For the Emerging Opportunities Fund (EOF) project, we have a manuscript ready titled "Decarbonization in the Oil and Gas Sector" and will be submitting it to a journal soon.

Professor Steve Evans, PI
University of Cambridge

Update on work package BB.1

Business model innovation potentials

Dr Lemy MARTIN (Research Fellow, NTU) continues to work with **Prof S. VISWANATHAN (PI, NTU)** on business model innovations related to solar energy adoption, with the first manuscript being expanded to include a numerical study and full market pricing scenarios based on initial feedback. This work has been accepted for presentation at INFORMS Annual Meeting in October 2023 in USA. This additional work also ties in with the second manuscript regarding hybrid pricing mechanisms for solar third-party ownership models.

Research has also been done on the possibility of using green hydrogen-based synthetic fuel as a carbon utilisation option for Singapore. Given the commitment to net zero emissions by 2050, Singapore needs to consider multiple decarbonisation pathways. Carbon utilisation methods such as synthetic fuel production can function as a fast interim solution as the country transitions towards net zero. This study considers three scenarios: a baseline scenario where crude-oil based fuel continues to be produced and consumed as-is, a local production scenario where imported green hydrogen and locally captured carbon function as feedstock for local synfuel production, and an overseas production scenario where locally captured carbon is exported to produce synfuel abroad and then imported back to Singapore for consumption. Using data acquired from the current literature, we compute a carbon utilisation price (CUP), which is the estimated price of utilising captured carbon to produce synfuel, alongside an adjusted CUP called the consequential carbon utilisation price (CCUP) that also considers the avoided emissions from crude oil-based fuel production. We find that overseas production is more economically viable than local production due to the expensive hydrogen feedstock cost, which is very costly to transport under current technology. We also conduct sensitivity analysis by looking into several cost parameters such as carbon feedstock costs, fuel shipping costs, economies of scale, and shipping emission taxes to see their impact on the CCUP. The manuscript has been accepted for publication by *Energies*.

Prof Viswanathan together with his collaborators at Nanyang Business School has completed a paper related to optimisation of production and inventories for remanufacturing in a circular economy. Their paper entitled "An Efficient Approximation to the Pull Policy for Hybrid Manufacturing and Remanufacturing Systems with Setup Costs" has been published in *Institute of Industrial and System Engineering (IISE) Transactions*.

Update on work package BB.2

Role of the CSO's in Firms' Sustainability Disclosure and Sustainability Performance

Dr Yan WANG (Research Fellow, NTU) and **Prof S. VISWANATHAN (PI, NTU**) delved into their analysis of the impact of the chief sustainability officer (CSOs) on a firms' sustainability disclosure and sustainability performance. They sought to investigate whether the CSOs gender and educational background would impact the firm's ESG disclosure score and carbon emissions, but unfortunately, no evidence was found. In addition to carbon emissions, they analysed whether the CSO has an impact on other business aspects. They found CSOs' positively impacted on company decisions to implement initiatives to make use of energy more efficiently and to outline the company's attention to helping reduce global emissions of greenhouse gases. However, it was not evident that CSOs had an impact on a company's coal use, electricity use, natural gas use, or crude oil use. From these results, they proposed that the role of CSO in the past might have mainly focused on the company's sustainable rating and sustainable policy set, and as it takes time for these policies to be implemented, the positive role of CSO in reducing emissions might be seen in the near future. They are currently working on the manuscript.

Update on work package BB.3

Venture capital policy and firm pollution in the chemical and energy-intensive industries

Dr Michelle Xiaomin FAN (Research Fellow, NUS) continues to work with **Prof Kenneth HUANG (PI, NUS)** on the study investigating how strengthening institutions for VC investment influences the pollution behaviour of firms in China's chemical and energy-intensive sectors. This study has been and will be presented at a number of prominent international conferences (see more in "Other activities and achievements" section). After several rounds of revisions based on the comments from these international conferences, this manuscript will undergo review at a top-tier journal, *Strategic Management Journal*.

Building upon the first project, they continue to investigate the various roles of different VC firms (government-supported VC, GSVC firms and Private VC, PVC firms) in influencing the focal firm's green innovation in a new project. Based on the sample of representative firms in the energy-intensive industries from 2004 and 2016, they adopted an exogenous shock that has differential impacts on the treatment group and control group to explore the differences between them after the policy shock regarding green innovations. They found preliminary results that firms funded by GSVC firms produce less green innovations than firms funded by PVC firms. Taking the perspective of the resource-based view, the potential mechanism for this pattern may lie in the different sources of competitiveness gained by GSVC firms and PVC firms. Specifically, GSVC firms obtain their main competitive advantage through their non-market strategy such as political connections while PVC firms obtain theirs by employing market-based strategy including developing strong green technological innovations. This work sheds light on the underlying mechanisms of different VC firms by testing and incorporating key moderators and through further data analyses.

Update on work package BB.4

Industrial sustainability and ecosystem trends

Guided by **Prof Steve EVANS** (**PI, CAM**), **Ms Can CUI** (**PhD student, CARES**) is in the midst of collecting the latest data on emerging technologies from all IRPs, and on analysing these for sustainable business opportunities. These will become documented in Deliverable 9, "Tentative business plan for each emerging technology", which is a set of statements describing the potentiality and the possible business model and scaling pathway, for the most promising technologies from each IRP.

They are also in the midst of data collection and analysis for Deliverable 10, "Roadmap for industrial decarbonisation" which will offer a roadmap for decarbonisation of the Singapore chemical sector. They are collecting data from other nations documents and policies, industry reports, and local interviews (e.g., Singapore Business Federation, Maritime & Port Authority).

Ms Cui has furthered data collection from industry and is now in stage 2 of data collection by refining the design and strategy. The focus is on how technology companies can innovatively interact with novel partners beyond the traditional value chain to create sustainable value, i.e., how can companies think outside of their own industry to formulate unconventional collaborations, etc. Preliminary data reveals different attitudes and considerations in terms of their understanding towards sustainability and collaboration, partnership strategy with companies from different areas and how to drive sustainable value, and challenges in the formulation of collaboration mechanisms.

Scientific output

The following are the CREATE-acknowledged publications generated by IRP BB during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

C4T IRP BB: An Efficient Approximation to the Pull Policy for Hybrid Manufacturing and Remanufacturing Systems with Setup Costs

Geoffrey A. Chua, Yan Feng, Juan Ramon L. Senga, and S. Viswanathan, *IISE Transactions*

DOI: 10.1080/24725854.2023.2253294

Abstract: We consider a continuous-review inventory control problem for a hybrid manufacturing and remanufacturing system with product recovery and setup costs. Van Der Laan et al. (1999b) proposed a *pull policy* but finding optimal parameters requires an exhaustive search and a single cost function evaluation is itself complex. We propose a tractable approach to finding these parameters using an interim policy called double (r, Q) with parameters (r_m, Q_m, r_r, Q_r). When the inventory position of the serviceable item reaches r_r, a remanufacturing lot size Q_r is setup if recoverable inventory is sufficient. Otherwise, we allow the inventory position to decrease further. As it drops to r_m, a manufacturing lot size Q_m is placed. Unlike the pull policy, this interim policy suspends the remanufacturing option when inventory position is less than r_r. This facilitates an efficient approximation of the recoverable inventory which decouples the double (r, Q) problem into two standard (r, Q) problems. It can then be efficiently solved using a modification of existing (r, Q) algorithms for two instances. Numerical studies show that our approach performs well relative to the optimal pull policy with parameters estimated from an extensive Simulation-Optimization method and other heuristics found in literature. The approach is also extended to correlated demand and arrivals.

Other activities and achievements

Prof Kenneth HUANG (PI, NUS) presented "Attaining Sustainability? The (Unintended) Consequences of Venture Capital Investments on Firms' Environmental Performance" at the INSEAD Doriot Entrepreneurship Conference from 15—16 June 2023 in Singapore; DRUID Annual Conference from 10—12 July 2023 in Lisbon, Portugal; and the International Association for Chinese Management Research (IACMR) Conference from 14—18 June 2023 in Hong Kong.

Prof Huang also presented "An Examination of Venture Capital Investments and Firms' Environmental Performance" at the Academy of Management (AOM) Annual Meeting from 4—8 August 2023 in Boston, USA. Prof Huang's listed presentations here is a joint work with **Dr Michelle Xiaomin FAN (Research Fellow, NUS)** and Prof Jiaxing YOU (Non-C4T PI, Xiamen University)

Prof Huang has been awarded the Management and Organization Review (MOR) Best Senior Editor Award. MOR is published by Cambridge University Press and is the premier journal for ground-breaking insights about management and organisations in China and global comparative contexts.

Prof Steve EVANS (PI, CAM) has been elected as Honorary Treasurer of the Academia Europaea. Prof Evans has also won a joint bid with Harvard and Tsinghua Universities for an "International Sustainability Research Platform" for BMW Germany.

Dr Lemy MARTIN (Research Fellow, NTU) gave a poster presentation on "Internal Carbon Pricing on Multi-Unit Firms" at CREATE Symposium 2023 in Singapore on 10 July 2023.

IRP JPS

THE J-PARK SIMULATOR

IRP JPS is an overarching research activity, with the ultimate purpose to show how research coming from each IRP affects the CO_2 output in Singapore and in particular the operations on Jurong Island. The research uses the latest ideas from Semantic Web technologies and Industry 4.0 to integrate real-time data, knowledge, models and tools to fulfil objectives such as simulation and optimisation in cross-domain and multi-level scenarios. One of the focuses is to create superstructures of models contained within the developed ontologies for industrial parks to provide an accurate and fast-to-evaluate approximation of computationally expensive mathematical models for process industry plants in high dimensions.

IRP JPS Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Raymond LAU Wai Man
Nanyang Technological University

Professor Iftekhar KARIMI
National University of Singapore

OVERVIEW

Over the past six months, we have improved the architecture and underlying technologies of the J-Park Simulator (JPS) to increase its autonomy and connectivity to the physical world. We have integrated domain-specific application ontologies to achieve interoperability within the knowledge graph. We have developed the Derived Information Framework (DIF) to semantically annotate dynamic and automated information flow through the knowledge graph. The DIF aims to lower the entry barrier for researchers to model any real-world cascading events. We have also developed a Forecasting agent to predict time series based on the DIF.

Furthermore, as part of an attempt to automate and digitalise laboratory operations, we have developed multiple mobile applications to view and control laboratory equipment and to access and register asset information. These mobile applications improve the decision-making on the energy -savings and efficiency of laboratory operations. We have also extended the visualisation of data from the CARES laboratory with an analytical dashboard for laboratory and facility managers to monitor and analyse various building performance metrics in real-time.

Using knowledge graph technologies, we have improved the digital twin for smart cities by consolidating data from various domains to assess how flooding scenarios impact a city's population, buildings, and property values. We are also developing a multi-domain and multi-scale energy model for smart cities with district heating optimisation, forecasting and emission dispersion modelling capabilities.

We are also working on an updated version of the Marie Knowledge Graph Question Answering (KGQA) system, which aims to use pre-trained Large Language Models (LLMs) to translate natural language questions into SPARQL queries to retrieve information from the knowledge graph.

Professor Markus Kraft, PI
University of Cambridge

Update on work package JPS.1

Big data — sensors and data modelling

Dr Yong Ren TAN (Software Developer, CARES), **Mr Wilson ANG (Software Developer, CARES)**, **Ms Xinhong DENG (Software Developer, CARES)**, **Mr Hou Yee QUEK (Research Associate, CARES)**, and **Mr Michael LAKSANA (Software Developer, CARES)** have implemented laboratory automation solutions as part of the creation of a digital twin of the CARES laboratory. They used a dynamic representation of data from various domains, such as chemistry, assets, and buildings, to demonstrate how automation can enhance the laboratory's performance, safety, and sustainability to aid Facility and Laboratory Managers.

Mr Ang, Mr Quek, and **Ms Li Ting PHUA (Project Officer Intern, CARES)** have extended the ontology for Building Management System devices (OntoBMS) and the BMS Instantiation agent to include devices such as Valves, Variable Air Volume systems (VAVs), and Make-up Air Units (MAUs). These devices, their corresponding sensors, and time series can be viewed via the existing BMSQueryApp, allowing users to track the status and make informed decisions regarding the energy-saving capabilities of various devices.

Mr Laksana developed a system to standardise and accelerate the instantiation and deployment of sensors and microcontrollers for laboratory automation. He created two agents to support this workflow: the Post Processing agent, which retrieves the raw data collected by the sensor, down samples and processes the data into useful values, and instantiates the time series, and the Device Instantiation agent, which creates the triples relevant to the sensor, sensor readings and the microcontroller. He tested this framework with the development of an automated fume hood monitoring and alert system.

In the process of creating a digital twin of the CARES laboratory, a common issue being observed in the laboratory is fume hood sashes left open when the devices are not in use. This results in a constant high airflow supplied to the fume hood and high energy consumption. The developed system prevents this issue by notifying users and the laboratory manager to close the fume

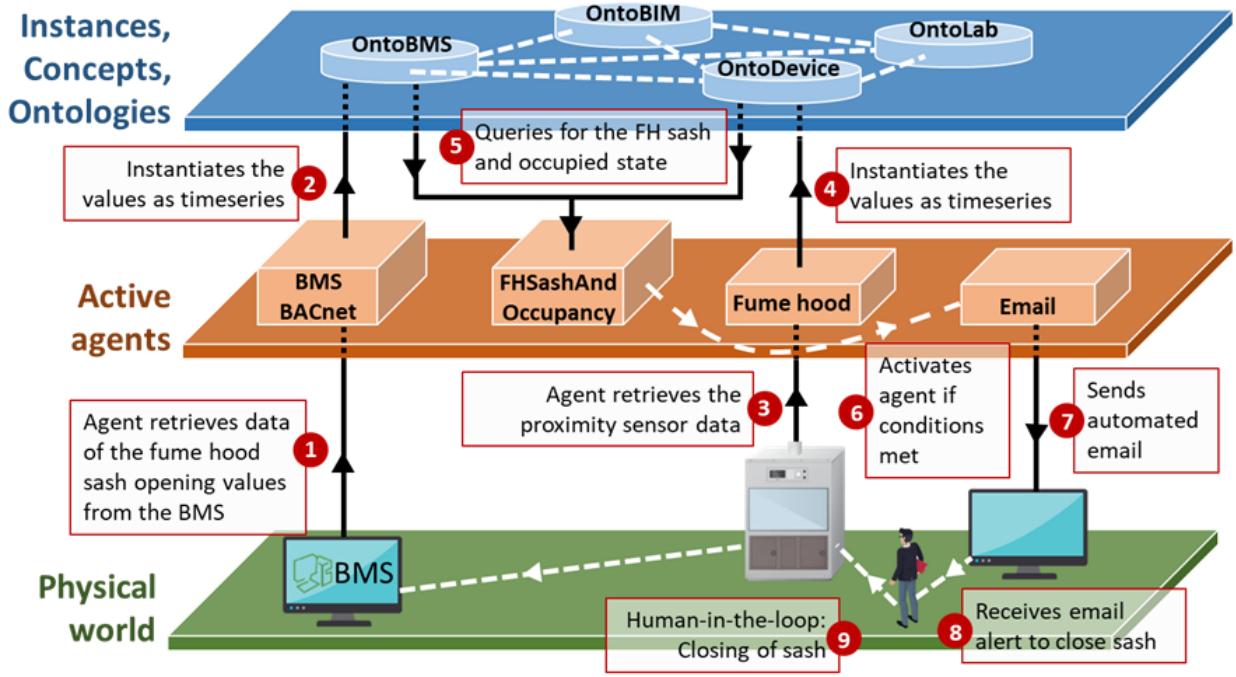


Figure 5.1: A sample workflow of the automated fume hood monitoring and alert system, allowing the monitoring of the status of a fume hood and produce alerts when the sash is not closed properly.

The following devices (FH-04) are unoccupied and have a sash opening above the threshold of 20.0%. Please close the sash for these fumehoods and walkin-fumehoods if they are unoccupied and not in use. Listed below are the fumehoods, walkin-fumehoods, their occupied state and sash opening values:

Devices	Occupied State	Sash Opening
FH-01	This device does not have an occupied state.	17.66 % since the following timestamp: 2023-07-06 17:14:35 PM SGT
FH-02	This device does not have an occupied state.	11.68 % since the following timestamp: 2023-07-06 17:14:35 PM SGT
FH-03	Not occupied since the following timestamp: 2023-07-03 13:57:22 PM SGT	10.48 % since the following timestamp: 2023-07-06 17:14:35 PM SGT
FH-04	Not occupied since the following timestamp: 2023-07-06 17:15:01 PM SGT	50.50 % since the following timestamp: 2023-07-06 17:14:35 PM SGT
FH-05	This device does not have an occupied state.	12.84 % since the following timestamp: 2023-07-06 17:14:35 PM SGT
FH-06	This device does not have an occupied state.	18.54 % since the following timestamp: 2023-07-06 17:14:35 PM SGT

Figure 5.2: Example alert email sent to laboratory personnel to notify them of currently unused fume hoods with open sashes.

hood sash when not in use, improving laboratory safety and efficiency.

The system uses a proximity sensor to monitor fume hoods and determine whether they are occupied. Based on the data collected by the proximity sensor, the occupancy of the fume hood is derived and updated into the knowledge graph. Mr Ang developed a Fume Hood Sash and Occupancy agent to retrieve the occupancy status and the fume hood sash position from the Building Management System BACnet (Building Automation and Control Network) at regular intervals. If the fume hood is unoccupied and the sash position exceeds a threshold, this agent prompts the Email agent to send out an alert email to the appropriate laboratory personnel, reminding them to close the sash. Figure 5.1 summarises the workflow of the system, and Figure 5.2 illustrates an example alert email that is sent to the laboratory personnel.

Ms Deng worked on multiple Android mobile applications as part of the overall CARES laboratory automation solutions. She improved the BMSQueryApp by allowing users to control the selected laboratory device state by writing to the knowledge graph. To enhance data security, Ms Deng also integrated an open-source authentication and authorisation tool, Keycloak, into the mobile application, allowing users to be assigned different roles, such as 'manager' and 'regular user'. Upon logging in to the app, different user groups are granted different levels of access to the resources within the application, and a pop-up window notifies users of trying to access unauthorised resources.

Dr Tan and Ms Deng have also designed the Asset Management mobile application to streamline laboratory management in CARES. This mobile application allows users to scan QR codes to access asset information instantly, register new assets, book equipment digitally, and notify users regarding maintenance schedules, thereby enhancing the productivity and quality of the laboratory operation. With the development of further features, such as energy usage monitoring of assets, users could also monitor their experiment's energy consumption.

To support this work, Mr Ang and Mr Laksana have developed an ontology called OntoAsset-Management, which represents asset information such as the assignee, location, identifiers such as serial number, manuals, related purchase documents and their details. Figure 5.4 shows how a workstation can be semantically represented using a part of this ontology. Mr Laksana is also developing an Asset Manager agent to retrieve, update and delete asset instances in the knowledge graph, which works in conjunction with the Asset Management mobile application.

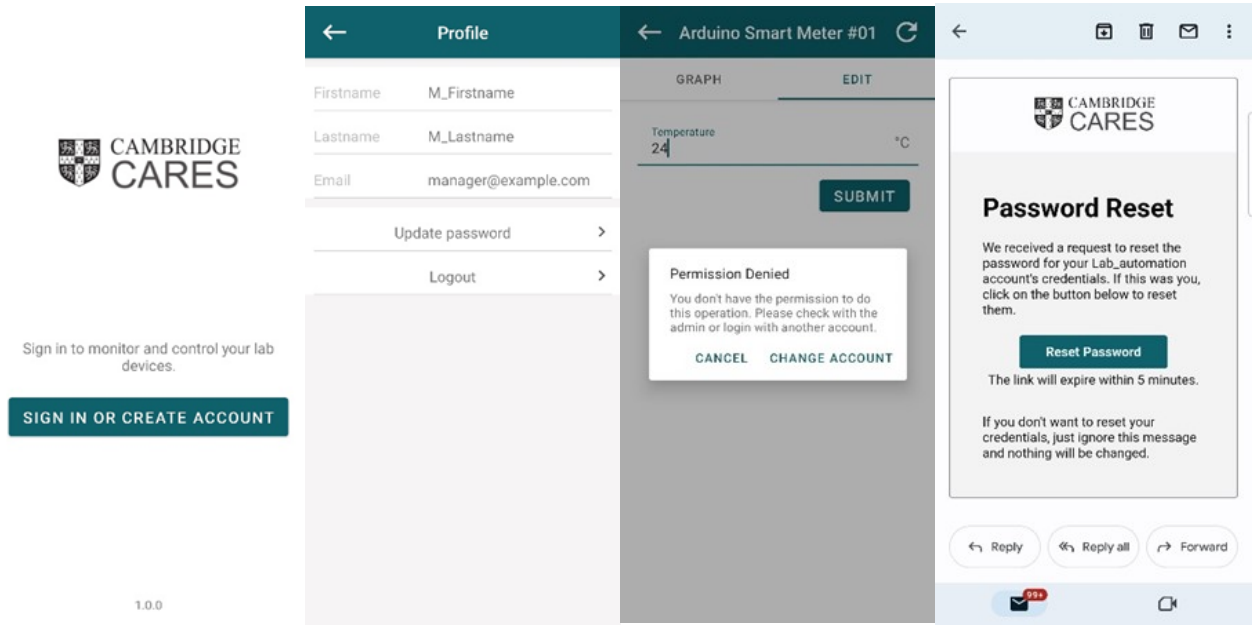


Figure 5.3: Integration of open-source authentication and authorisation tool, Keycloak, with the mobile application.

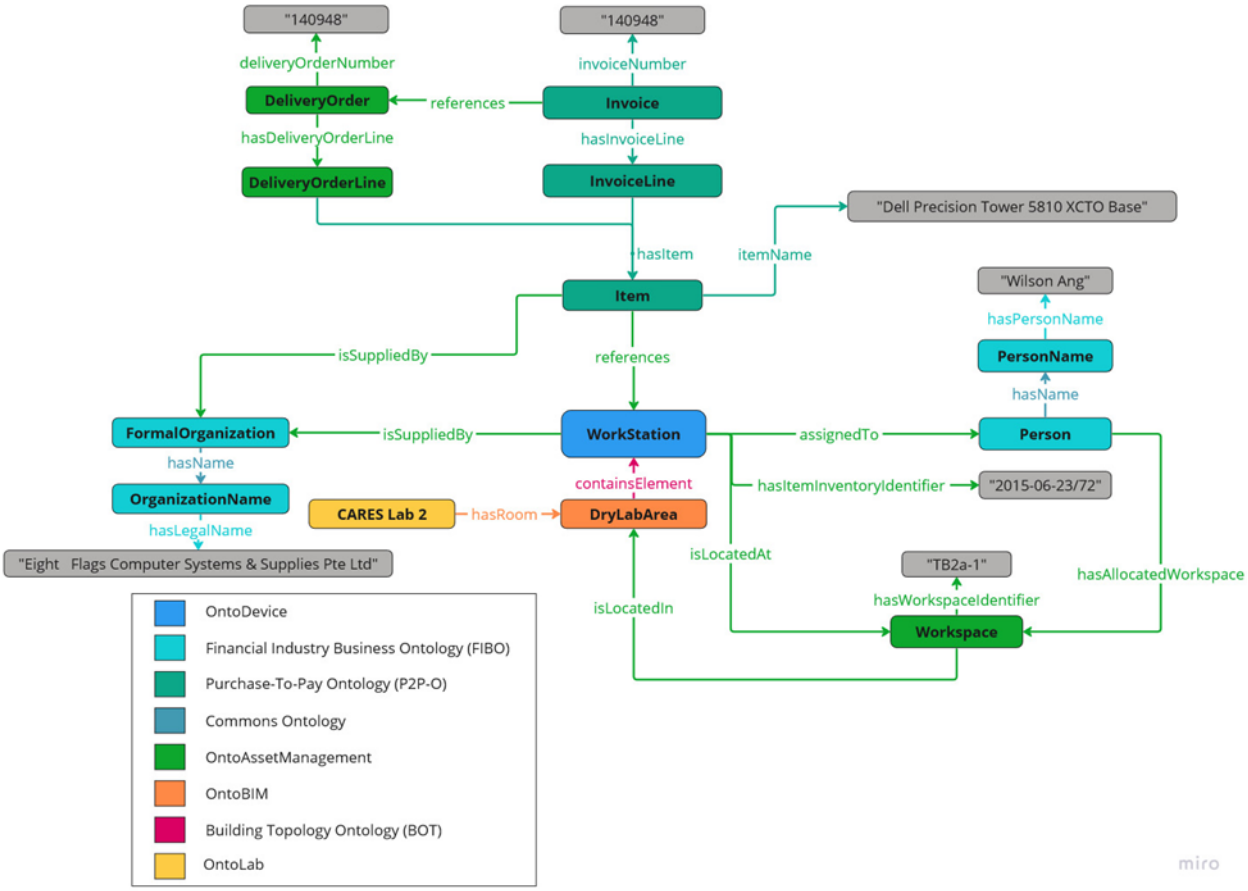
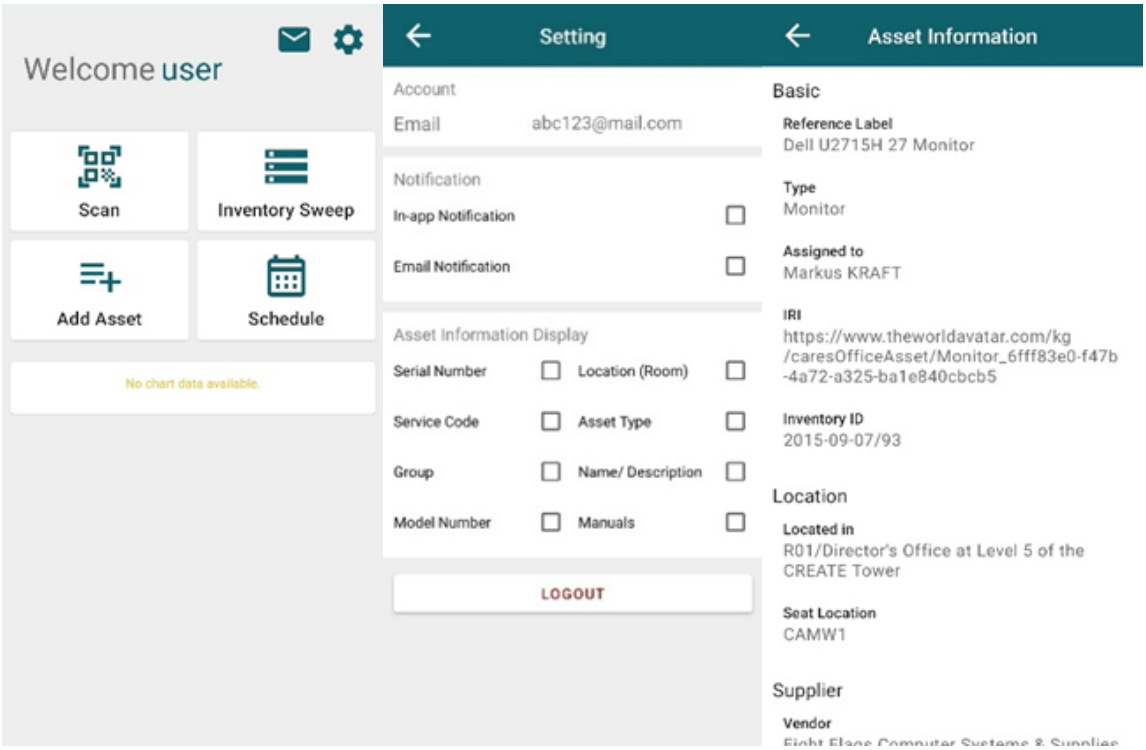


Figure 5.4: Semantic representation of a workstation using a part of the OntoAssetManagement ontology.



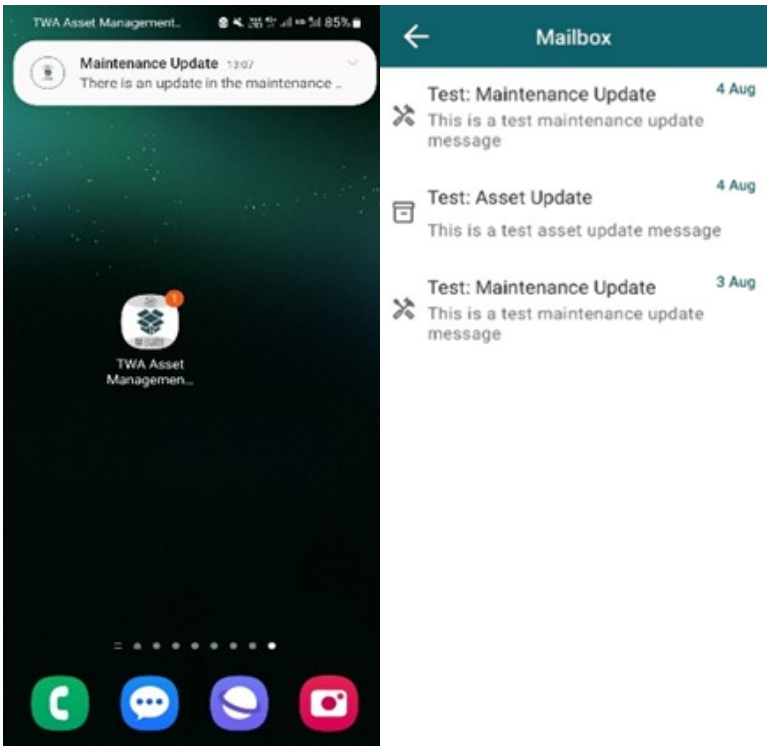


Figure 5.5: Features of the Asset Management mobile application: scanning QR codes to access asset information, displaying specific information regarding assets and user notifications regarding maintenance schedules and asset updates.

Update on work package JPS.2

Surrogate models, superstructure and architecture development

Mr Jiaru BAI (PhD Student, CAM), **Dr Kok Foong LEE (Software Developer, CARES)**, **Mr Markus HOFMEISTER (PhD Student, CAM)**, **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)** and **Dr Jethro AKROYD (Senior Research Fellow, CARES)** developed the Derived Information Framework (DIF) to semantically annotate how information can be derived from others in a dynamic knowledge graph (Figure 5.6). The DIF uses a lightweight ontology to markup provenance, an agent template to standardise agent operations, and a framework to propagate information changes using agents' actions. The DIF aims to lower the entry barrier for researchers to model any real-world cascading events, thereby helping in transitioning various real-world scenarios to be represented in a dynamic knowledge graph. The DIF can track and document the calculations and re-execute the computations when accessing outdated information, enabling automated integration of new information and ensuring constant access to up-to-date insights in the domain of interest.

Mr Hou Yee QUEK (Research Associate, CARES) developed the Data Bridge agent to improve data interaction and migration within the knowledge graph as well as from external data sources such as relational databases endpoints, in anticipation of the integration of more data across domains and scales. As part of standardising sensor data instantiation, this agent also supports receiving and instantiating time series from other sensor-based agents.

Mr Mingchuan TIAN (Software Developer, CARES) developed the GeoSegment agent, which utilises deep neural networks and the K-means clustering algorithm to partition geospatial raster data into meaningful segments, extract useful information from the raster data and instantiate it based on OntoSemanticSegmentation, an ontology developed to represent polygon segments. This agent enables an efficient instantiation of large geospatial datasets. Using the GeoSegment agent, Mr Tian instantiated various types of raster data, including satellite imagery, land-use patterns, and terrain models, to evaluate

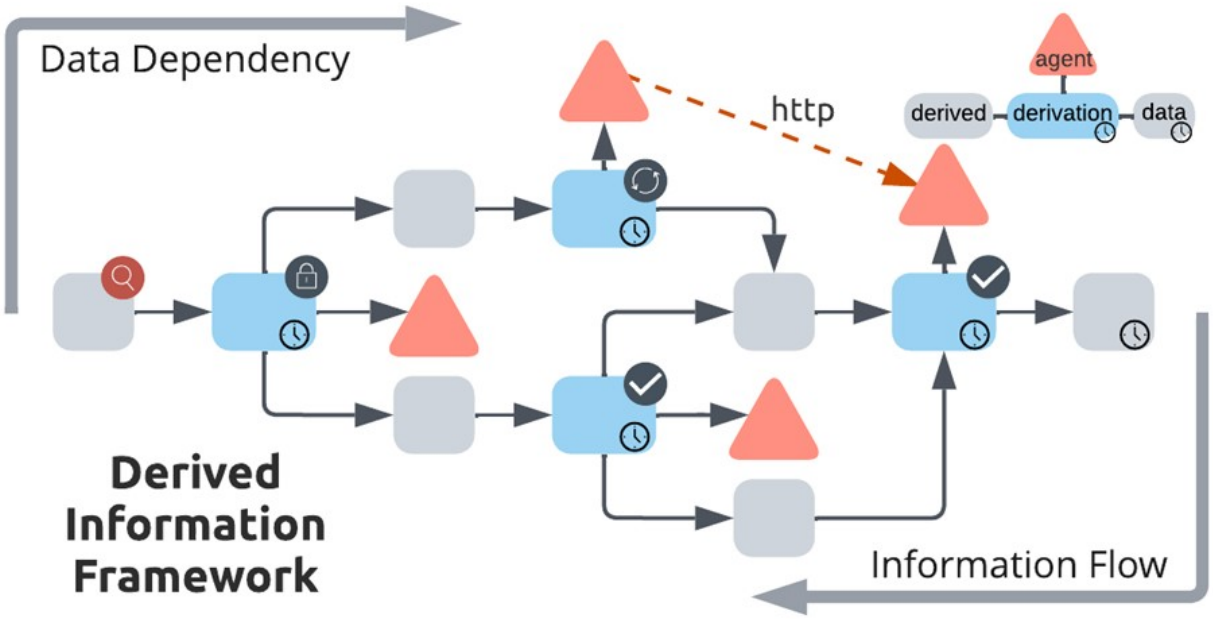


Figure 5.6: Schematic of the dual capability of the Derived Information Framework (DIF) in tracking data dependency (provenance) and updating the subsequent information flow.

its efficacy and versatility. The instantiated terrain data can also be used in the C4T EOF3 project (Impact of Singapore's Shipping Activities on Urban Air Quality), where the dispersion model estimates pollutant dispersion using data from various domains, one of which is terrain information.

Dr Mosbach, Dr Akroyd and **Dr Feroz FARAZI (Research Fellow, CAM)** have designed a fully automated workflow to verify FAIR (Findability, Accessibility, Interoperability, Reusability) principles compliance of data and metadata used in research experiments and applications. Two layers for this workflow development have been defined: the abstraction and implementation layers, as illustrated in Figure 5.7.

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES) is involved in training, supporting, and providing guidance, especially to new team members, concerning documentation, questions on software design, agent development, and non-functional requirements such as performance and scalability.

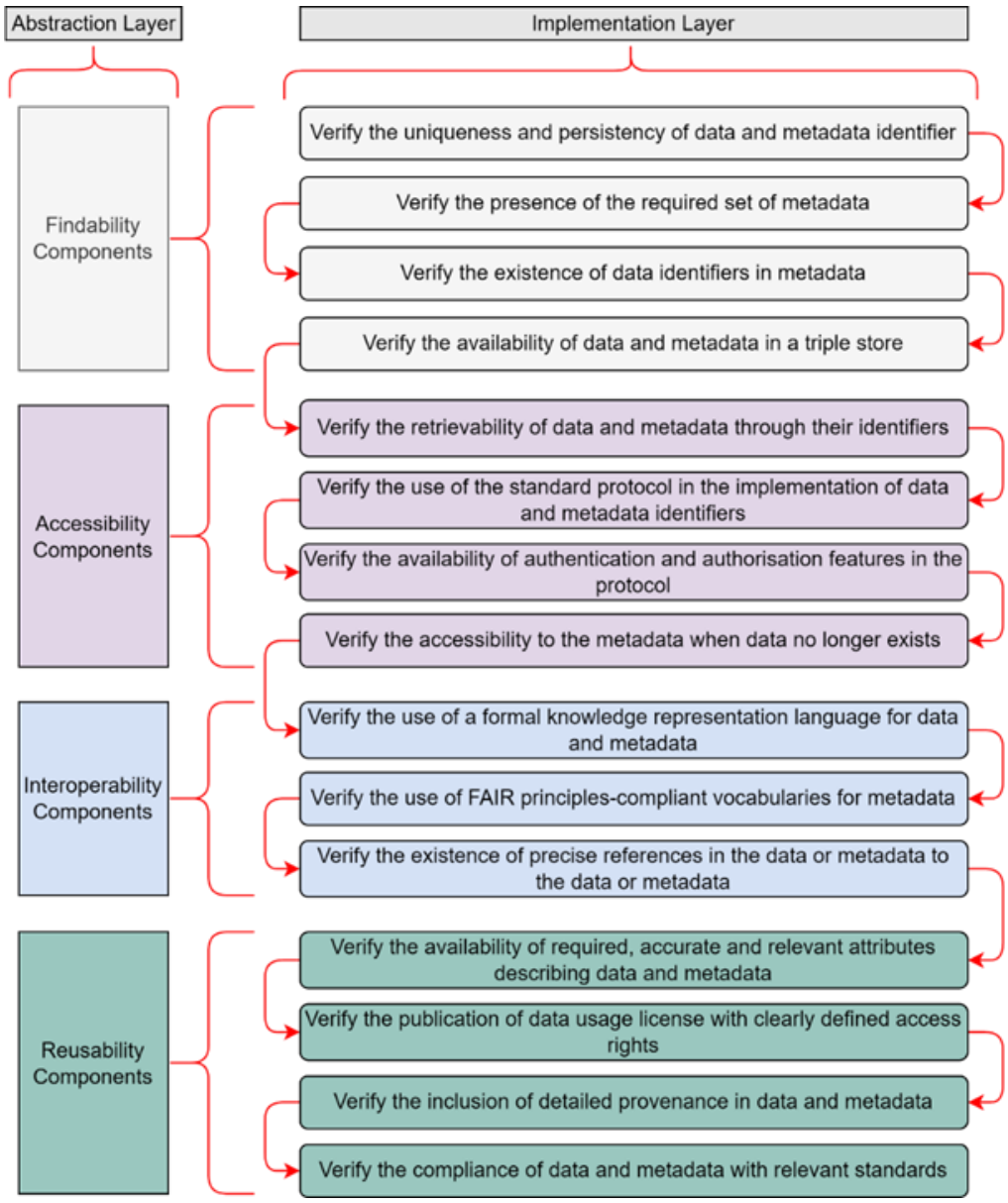


Figure 5.7: The proposed workflow for verifying FAIR compliance of data and metadata used in research experiments and applications via the World Avatar dynamic knowledge graph.

Update on work package JPS.3

Implementation

Dr Aleksandar KONDINSKI (Research Fellow, CARES), **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, **Dr Jethro AKROYD (Senior Research Fellow, CARES)**, **Dr Yong Ren TAN (Software Developer, CARES)**, **Mr Simon RIHM (PhD Student, CAM)**, and **Mr Jiaru BAI (PhD Student, CAM)** have assessed the technical feasibility of the 'CreatorSpace', aiming to enhance connectivity between researchers and decarbonisation specialists. The feasibility study, titled "Hacking decarbonisation with a community-operated CreatorSpace", focused on the intersection of human creativity and artificial intelligence (AI) in decarbonisation. The CreatorSpace is envisaged as a virtual, semantic platform, mirroring the essence of hackerspaces and makerspaces, designed to foster collaboration among chemists, engineers, and material scientists, integrating chemical knowledge across various scales and technologies. The study employed a 'backcasting' approach which highlighted areas such as sustainable aviation fuels and carbon capture as prospective pathways.

Mr John ATHERTON (PhD Student, CAM) completed his work on energy markets, curtailment and battery placements in Britain and conducted comparative curtailment analysis. He also modelled and observed battery dispatch behaviour for a sample day to evaluate its performance.

Ms Wanni XIE (PhD Student, CAM) developed a system for decarbonising the UK power system based on a knowledge graph approach. She assessed the carbon tax impact of adopting Small Modular Reactors (SMRs) in the UK power system and analysed the effects of SMR placements on the population and power transmission efficiency. The study considers diverse renewable power scenarios and determines cost-effective SMR numbers while optimising power flow to balance transmission loss and population risk. The UK has been chosen for this proof of concept because data are readily and publicly available.

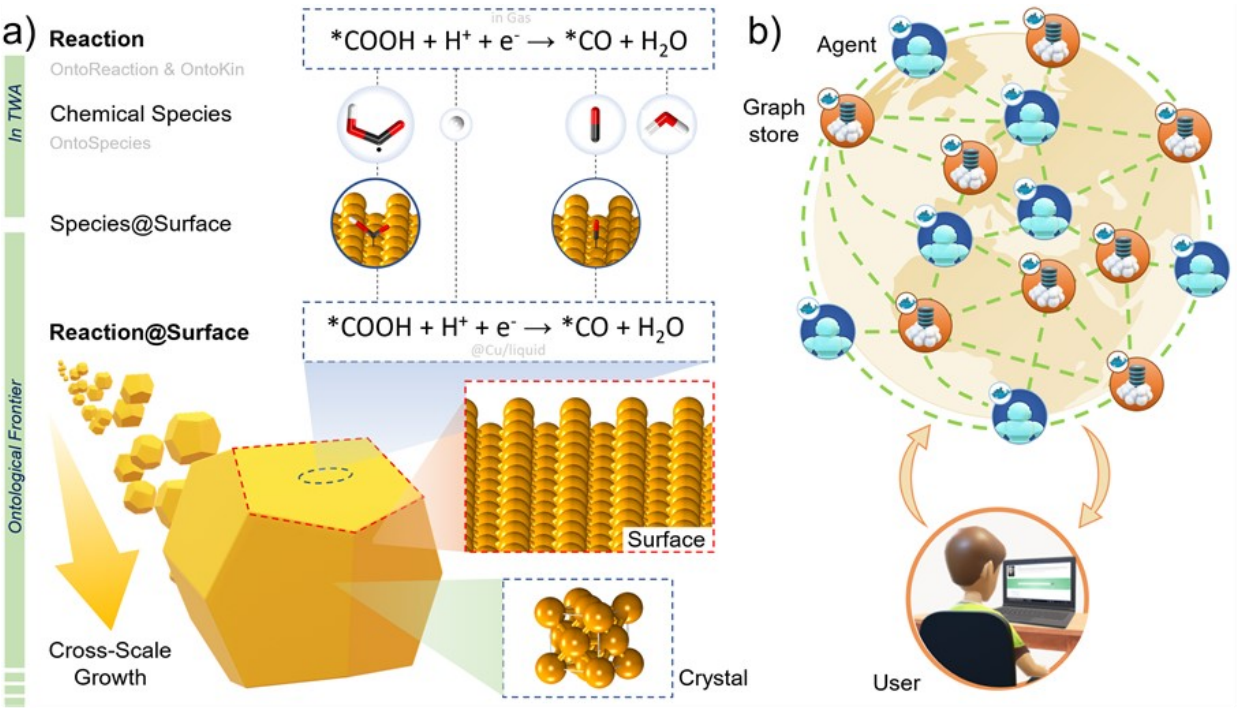


Figure 5.8: The existing and the new ontological frontier illustrated in terms of chemical and materials models (left); The CreatorSpace using distributed, containerised software to integrate chemical data with autonomous computational agents in a dynamic knowledge graph (right).

This work can easily be extended and applied to other regions where data is available, including Singapore.

Mr Markus HOFMEISTER (PhD Student, CAM) developed digital twins for smart cities using semantic and knowledge graph technologies. He successfully completed his project assessing flood scenarios' impact on people, buildings, and property values. Two research papers stemming from this work have been submitted and are currently under review, one detailing the benefits of our approach to the practitioner community itself and the other describing the technical details. **Mr Shin Zert PHUA (Software Developer, CARES)** has developed a context-aware Routing agent to supplement the current insights on flooding with a more holistic perspective. This includes minimum rescue times under flooded road conditions, strategic planning of emergency service coverage and critical path analyses to foster flood resilience and post-disaster recovery.

Leveraging the Derived Information Framework described in Work Package JPS.2, Mr Hofmeister has implemented a Forecasting agent for predicting time series within the World Avatar. He is currently linking a district heating optimisation system with integrated forecasting and emission dispersion modelling for the city of Pirmasens in Germany, where data are readily and publicly available. This work showcases capabilities to support multi-domain and multi-scale energy modelling for smart cities.

Mr Jieyang XU (Masters Student, CAM), **Dr Feroz FARAZI (Research Fellow, CAM)**, Dr Akroyd, and Dr Mosbach investigated the impact of changes in fuel price on regional inequality within the context of scenarios where air source heat pumps replace domestic gas heating in the UK, where data are readily and publicly available. Mr Xu formulated an inequality index to facilitate comparisons of regional inequality between scenarios and developed an ontology called OntoRegionalAnalysis to describe the UK regional data. By understanding the impacts of changing the electricity-to-gas price ratio and contrasting them with projected fuel prices, the study enables forecasting of future inequality trends, providing policymakers with valuable insights for informed energy decisions. This work can easily be extend and applied to other regions where data is available, including Singapore.

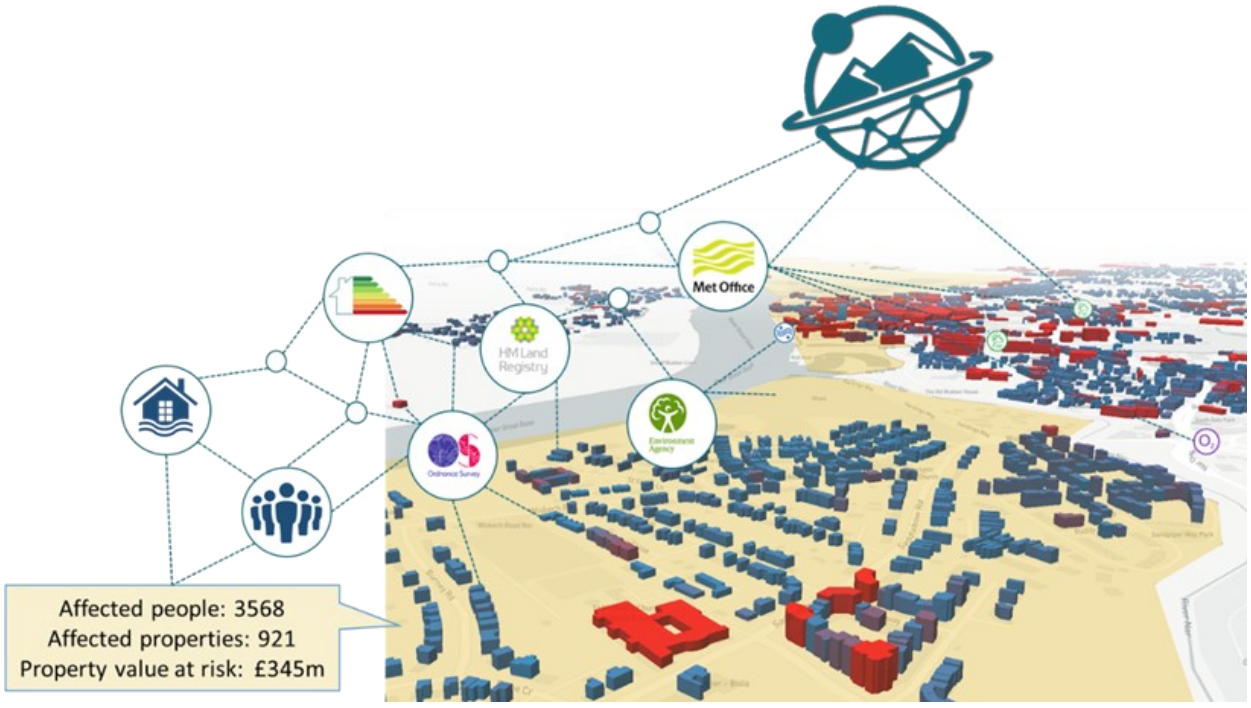


Figure 5.9: Schematic depiction of how the World Avatar dynamic knowledge graph combines cross-domain data to automatically assess the potential impact of anticipated flooding events.

Mr Jiying CHEN (PhD Student, CAM), Dr Farazi, Dr Akroyd, and Dr Mosbach integrated data regarding the energy performance of the built environment with its geospatial data. Given the heterogeneous nature of geospatial and energy sector data, we need an integrated system to manage and evaluate energy performance data. The World Avatar knowledge graph, together with its autonomous computational agents, provides a dynamic, interconnected representation of data to understand urban energy performance. The workflow consists of extracting CityGML building features from geodatabases, retrieving building and energy parameters using Ontology-Based Data Access (OBDA) mapping and instantiating and visualising the building data, as illustrated in Figure 5.10.

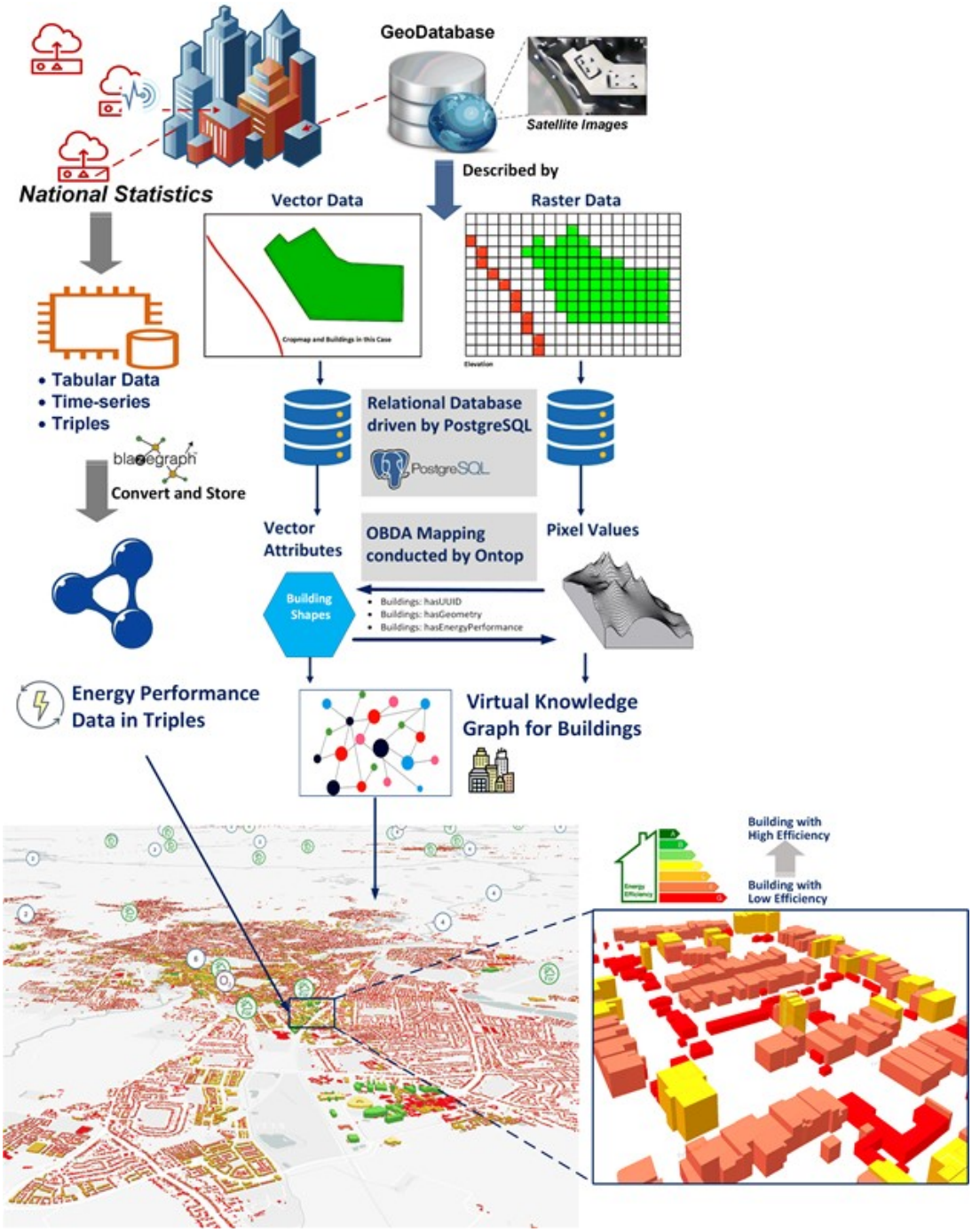


Figure 5.10: Workflow for integrating geospatial descriptions of buildings and their energy performance using the World Avatar dynamic knowledge graph.

Update on work package JPS.4

Model analysis and visualisation

Mr Hou Yee QUEK (Research Associate, CARES) is extending the real-time visualisation of the CARES laboratory with an analytical dashboard based on the open-source Grafana platform (Figure 5.11). This dashboard displays various time series of assets in the laboratory and their building management system. This dashboard supports the laboratory and facility managers through real-time monitoring and analysis of building performance metrics such as energy consumption, laboratory conditions, equipment usage, and fault detection.

Figure 5.11: An analytical dashboard displaying the ambient temperature for various rooms in the CARES laboratory.

Ms Shaocong ZHANG (Software Developer, CARES) has developed a web interface that will be used to visualise the results of a model of the Singapore energy system that allows the exploration of pathways to decarbonisation. The model will include scenarios such as varying transport consumption, building consumption and CO_2 removal. Ms Zhang has developed a front-end visualisation that takes input configurations as HTTP requests and renders the results as charts.

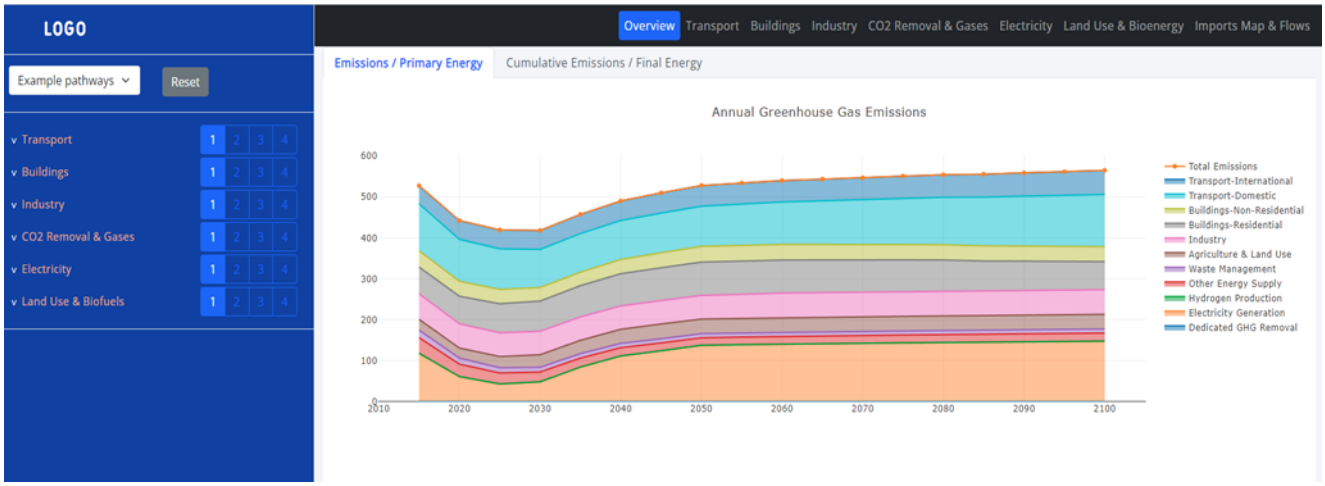


Figure 5.12: Prototype of the web interface displaying the results of the Singapore energy system model.

Mr Xiaochi ZHOU (PhD Student, CAM), **Ms Mehal AGARWAL (Software Developer, CARES)**, and Ms Zhang completed the third iteration of the Marie Knowledge Graph Question Answering (KGQA) system, which uses joint entity recognition and entity linking models. They conducted systematic tests to evaluate the performance of the system. The Marie KGQA system offers data regarding chemical reactions and characteristics associated with energy storage and conversion including batteries, fuel cells, and catalysts. This system has the potential to facilitate the advancement of cleaner energy systems and contribute to the shift towards low-carbon alternatives.

Dr Laura PASCAZIO (Research Fellow, CARES) and **Mr Dan TRAN (Software Developer, CARES)** are working on the fourth iteration of the Marie KGQA system using pre-trained Large Language Models (LLMs) to translate questions in natural language into SPARQL queries that can be executed against knowledge graphs. Mr Tran has developed a data-parallel fine-tuning pipeline for T5 and Llama models. He is currently porting the fine-tuned models to C++ for high-performance inference.

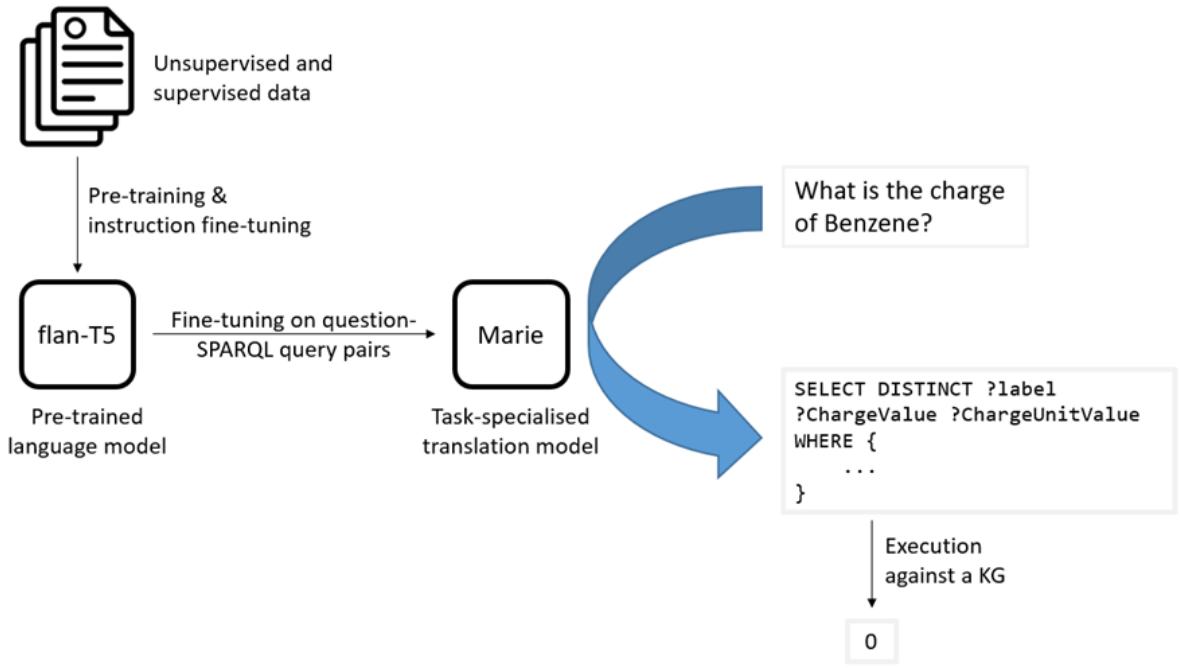


Figure 5.13: Workflow for the fourth iteration of Marie Knowledge Graph Question Answering (KGQA) that can convert natural language questions into SPARQL queries for execution against knowledge graphs.

Scientific output

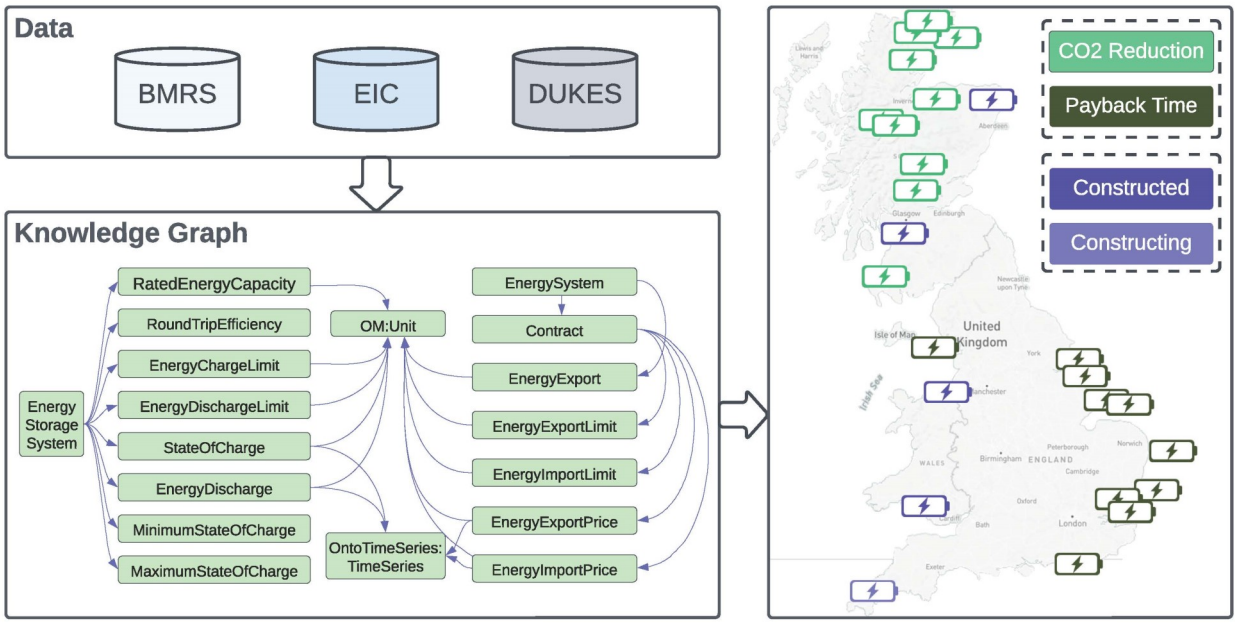
The following are the CREATE-acknowledged publications generated by IRP JPS during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

British wind farm ESS attachments: curtailment reduction *vs.* price arbitrage

John Atherton, Jethro Akroyd, Feroz Farazi, Sebastian Mosbach, Mei Qi Lim, and Markus Kraft, *Energy & Environmental Science*

DOI: 10.1039/D3EE01355C

Abstract: Energy storage systems (ESSs) are a potential solution to the rising issues of electricity price volatility and curtailment of British wind energy. This study performs an extensive and knowledge graph supported investigation into 47 potential wind farm ESS co-location sites. While all ESSs achieved payback due primarily to price arbitrage, results indicate English/Welsh sites (typically with offshore wind) had quicker payback times owing to higher capacity factors presenting more opportunistic charging times. Conversely, while batteries co-located with Scottish wind farms attained slower payback times, they accomplished greater curtailment reductions, which could be used to displace marginal selling from generally fossil fuelled sources.



Other activities and achievements

Mr Jiaru BAI (PhD Student, CAM) presented the Derived Information Framework at the 2nd Annual Symposium of The Turing Interest Group on Knowledge Graphs held in the University of London on 16 June 2023.

Mr Shin Zert PHUA (Software Developer, CARES) and **Mr Markus HOFMEISTER (PhD Student, CAM)** presented their work on weather resilience in smart cities at the 9th Applied Energy Symposium in Japan from 2 - 7 September 2023 and at the Science of Cities Symposium in Singapore on 5 October 2023. **Mr Hou Yee QUEK (Research Associate, CARES)** will also present the value of interoperable building and energy simulations using a dynamic knowledge graph for decarbonising cities at the Science of Cities Symposium in Singapore.

Prof Markus KRAFT (PI, CAM) presented results from the World Avatar (TWA) at several events including:

- An executive summary of the World Avatar project outcomes and use cases to Singapore's Ministry of National Development (MND) on 12 April 2023.
- A talk entitled "Flood risk assessment with the World Avatar project" at the Asia Climate Forum in Singapore on 20 April 2023.
- A presentation to AstraZeneca called "The World Avatar Project – a universal digital twin: Future of lab automation" on 27 April 2023.
- A keynote at the Isaac Newton Institute in partnership with the Alan Turing Institute called "The World Avatar project – a universal all-encompassing digital twin" in Cambridge on 7 June 2023.
- As part of the nationwide "Digitaltag" initiative in Germany, Prof Kraft showed results from the World Avatar in his hometown of Pirmasens on 16 June 2023.
- A keynote talk on "Big Data and Climate Change: How Cities Can Become More Resilient and Efficient" at the RISUD Annual International Symposium (RAIS) in Hong Kong on 6 July 2023.
- A presentation titled "Low-carbon hydrogen innovations at Cambridge CARES" at a TUMCREATE and SGInnovate panel discussion on 26 July 2023.
- An executive summary of the World Avatar project outcomes and use cases to the Qatar Environment & Energy Research Institute (QEERI) on 4 August 2023.

CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

CLIC is a flagship programme in the Science of Learning initiative to harness advancements in neuroscience to develop training programmes for lifelong flexible learning. The research team has made significant headway since the commencement of the program. Investigators in the four different workgroups have worked continuously and collaboratively to ensure an optimal and cohesive task battery, data collection, organisation and analysis.

Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

OVERVIEW

The Centre for Lifelong Learning and Individualised Cognition (CLIC) is a programme in the Science of Learning initiative that leverages progress in neuroscience to develop lifelong flexible learning training programs. CLIC aims to improve lifelong learning and cognitive agility through innovative cross-disciplinary research and intends to translate its findings into an integrated model of learning that can be applied in day-to-day life. The CLIC team has experienced numerous achievements in the last six months. Since the last update, our researchers have successfully concluded participant recruitment, marking a significant milestone for the team. Subsequently, our research team has been diligently focused on data analysis and drafting manuscripts tailored for journal submissions.

In May 2023, a week-long writing bootcamp was hosted at the University of Cambridge, jointly organised by Professors Victoria Leong, Henriette Hendriks, and Michelle Ellefson, and led by Professor Trevor Robbins. The workshop was attended by researchers from the School, Social and Cognition Workgroups where they were mentored on consolidating their analyses and findings and worked on drafting the research manuscript on the CLIC adult data.

The Neuroimaging Workgroup successfully concluded their data collection phase in June 2023 and has since been dedicated to analysing both the behavioural and neuroimaging data from the final group of participants. Simultaneously, they have embarked on the development of a new training program set to be implemented in Phase 2 of the study. This novel training program, known as the Structure Learning-based Cognitive Flexibility Suite (SLiCX), introduces an innovative element by incorporating colour as an additional dimension to the symbols utilised in the Structure Learning intervention previously employed in WP0.2's Main Study. Pilot studies are in the pipeline to assess the potential impact of colour and determine the most suitable experimental conditions for both adults and adolescents.

The School Workgroup has been consistently collaborating with the Singapore Examination & Assessment Board (SEAB) to create inventive and adaptive thinking measures for educational institutions. This ongoing partnership encompasses the co-creation of innovative assessments and their integration into schools. Professor Michelle Ellefson and Dr Teo Chew Lee are at the helm of this collaborative endeavour, with active involvement from both the Cognition and Social teams, with the primary aim to explore the interplay between neuroscience research, practical applications, and policy.

As CLIC draws nearer to the end of Phase 1, a series of outreach and engagement events were organised and held between August to September to discuss areas of lifelong learning and brain health. Our researchers engaged with agencies and policy makers involved in education and research through tailored workshops which offered insights into integrating our findings into policies and practice.

Separately, the team also organised The Brainiverse Experience: Jetting to Better Brain Health &

Learning which was targeted towards engaging the public to explore flexible thinking and learning, brain health and overall mental well-being. This gave CLIC the opportunity to connect the public with CLIC's research on cognitive abilities. The event was held over two days at the ArtScience Museum, which included talks by Professor Robbins, and guest speakers Professor David Rowitch and Professor Sarah-Jayne Blakemore from the University of Cambridge. The event also included interactive booths from the different workgroups, an earthquake challenge for secondary school students, and an art competition for students with special needs. The Brainiverse Experience was also graced by the British High Commissioner, Her Excellency Kara Owen, which elevated the event and made it more meaningful.

The team has been actively involved in the educational outreach, conducting workshops, manuscript preparation as well as conference presentations. The School Workgroup has organised three workshops, including one run by Professor Ellefson, Dr Teo, Dr Peter Seow and Dr Nastassja Lopes Fischer on "Making Sense of the Brain and the Science of Learning" held at the National Institute of Education (NIE). Additionally, PhD student Emma Sam, and Dr Liu Chia-Lun from the Social and Neuroimaging Workgroup attended conferences where they presented their posters to an international audience. Finally, the team has also published two protocol papers which stands as crucial reference point for future manuscripts. We expect several research papers to be drafted in the upcoming months.

As we approach the conclusion of Phase 1 in our study, our researchers are meticulously preparing for a smooth transition and commencement into Phase 2 along with the fresh challenges and insights it will bring to our research endeavours.

Professor Annabel Chen Shen-Hsing
Director of CLIC, NTU

Professor Zoe Kourtzi
Director of CLIC, CAMBRIDGE

Update on Cognition Workgroup

Assessing Cognitive Flexibility, Other Executive Functions and Learning in Healthy Young Adults

In April, the Cognition team successfully completed the data collection phase of the CLIC adult characterisation study, marking a significant achievement for the CLIC project. Subsequently, they hosted a workshop in Cambridge in May, where **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM), Prof Zoe KOURTZI (Co-Director, CAM), Prof Barbara SAHAKIAN (Senior Scientific Advisor, CAM), Prof Annabel CHEN (Co-Director, NTU)** and **Assoc Prof Victoria LEONG (Co-Deputy Director, NTU)** provided guidance to CLIC research fellows in consolidating their analyses and findings for manuscript development.

The Cognition workgroup meticulously assessed the results and drafted the manuscript for the CLIC adult study. The research protocol for the CLIC adult study (Tong et al., 2023) was published in July, marking the first of several papers planned for publication from the Cognition workgroup. Additionally, the group will be facilitating a workshop for early career researchers from NTU and Cambridge, fostering connections and collaboration opportunities for joint manuscripts and collaborative projects.

In August, CLIC held a series of impact events, which included an Engagement with Policymakers on 25 August which brought together key stakeholders and researchers to delve into crucial topics related to lifelong learning and brain health. The Brainiverse Experience and The Brainiverse Interactive were organised on 26 August and 8 September respectively as a unique science festival. The aim was to engage the public and convey the processes and findings of CLIC's research in a less academic setting. See the "Other activities and achievements" section for more details.

Dr Ke TONG (Research Fellow, NTU) and **Dr Xinchen FU (Research Fellow, NTU)** contributed significantly to data analysis and manuscript preparation for the CLIC studies, including research protocols and reviews**.** Dr Tong led and contributed to the preparation of several CLIC manuscripts, including the CLIC adult study research protocol, CLIC adult main study manuscript, and a review on cognitive flexibility across lifespan. Dr Fu also contributed to the manuscript on cognitive flexibility across the lifespan and to the data analysis and drafting of the infant exploratory studies paper. She is also responsible for the testing sessions and analysis for the infant creativity testing.

Ms Natalie Philyra HOO (Research Assistant, NTU) made valuable contributions to both adult and infant testing projects in CLIC. In the adult testing domain, she managed Part 2 testing sessions, handled IRB ethics amendments, and prepared the Brainiverse booth for the Creative Dance AI segment. Additionally, she played a crucial role as a scribe during the Engagement with Policymakers event, prepared the Program booklet, and effectively managed administrative matters with A*STAR. In infant testing, Natalie demonstrated strong leadership as a project lead, overseeing recruitment, scheduling, testing sessions, data transfer, coding, and analysis, all of which significantly contributed to the research.

Mr Kean Mun LEE (Research Assistant, NTU) spearheaded the renewal of CLIC's Data Management Plan, ensuring compliance with NTU's standards. He processed, cleaned, and organised cognitive data from the WP0.1 Adult study, and supported the School Workgroup's collaboration with the Singapore Examinations and Assessment Board in developing assessment questions. Mr Lee also played a crucial role in organising the Adult Brain Health, Learning, and Wellbeing Workshop during the Engagement with Policymakers event. Additionally, he led the design efforts for the Cognition Team's booth called Neuronauts at The Brainiverse Interactive.

Mr Shamsul Azrin JAMALUDDIN (Research Associate, NTU) played a pivotal role in organising the CLIC Impact Events, managing communications, logistics, and venue procurement. Nota-

bly, Mr Jamaluddin served as the primary point of contact for The Brainiverse Experience, effectively managing communication and coordination with both internal and external stakeholders. His responsibilities encompassed organising site visits at the ArtScience Museum venue and collaborating closely with the events management company to determine event requirements. Moreover, he assumed a crucial role in the preparation of essential documents for procuring the venue and securing the services of the event management company. Finally, Mr Jamaluddin efficiently managed the logistical aspects for The Brainiverse Experience keynote speakers and Cambridge Principal Investigators during their stay in Singapore. His contributions have been instrumental in the successful execution of the CLIC Impact Events.

Figure 6.1: Pictures from the Brainiverse Experience on 26 August. Bottom photo shows Prof Sarah-Jayne BLAKEMORE (non-CLIC PI, CAM) delivering her closing keynote, "Sensitive periods of brain, cognitive and social development in human adolescence".

The following study has been pre-registered by the Cognition Workgroup on the Open Science Framework Registries

Workgroup	Title	Submission Links
WP0.1 Cognition	Assessing Cognitive Flexibility, Other Executive Functions and Learning in Healthy Young Adults	Pre-registration link: https://osf.io/6rc9h

Update on Schools Workgroup

Translation to Education: Assessing Cognitive Flexibility, Other Executive Functions and Learning in Healthy Adolescents

The School Workgroup continues to work with the Cognition and Social Workgroup to analyse the data collected during the WP0.1 Study. **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** worked closely with the Adults and Neuroimaging Working Groups members (**Dr Ke TONG (Research Fellow, NTU)** and **Ms Marisha Barth UBRANI (Research Assistant, NTU)**) to ensure that data analysis, and coding procedures are properly aligned across all workgroups. Dr Lopes Fischer is leading the school team to conduct data analysis and modelling of the adolescent data in collaboration with the Cognition and Social Workgroups. She presented key findings and project milestones during the Cambridge Data Analysis Bootcamp in May 2023.

Ms Phillis FU (Research Associate, NTU) has been working on preprocessing the psychometric social variables from the Adolescents' dataset and for the coding of the Alternate Uses Task data. **Ms Shilpi TRIPATHI (Research Associate, NTU)** has been working with **Dr Chew Lee TEO (co-PI, NTU)** on the analysis of the psychometric social variables from the Adolescents' dataset and on the validation of the Contextual Linguistic Profile Questionnaire (CLiP-Q) for the Adolescents' dataset and within Singapore's context.

The School Workgroup is working closely with **Prof Henriëtte HENDRIKS (co-Deputy Director, CAM)** and the Social Workgroup to generate publication from these data. **Ms Jen Hui LIM (Research Associate, NTU)** and **Ms Gabrielle ONG (Research Assistant, NTU)** are also working on the literature review together with Dr Teo for a manuscript on the interdisciplinarity middle depicting a collaborative framework between cognitive neuroscience and educational research.

Since April 2023, members of the School Workgroup have been preparing for The Brainiverse Experience and activities specially designed for adolescents called "Brainiverse Challenge". Ms Fu was the main coordinator representing the School Workgroup, managing the logistics, publicity and external dissemination efforts through CLIC's social media accounts. The school team led the design and enactment of the following events within Brainiverse:

- *Brainiverse Challenge" was a contest within The Brainiverse Experience where teams of students were tasked to build construction models on a tremor machine. Dr Peter Seow invited colleagues from the Science Centre Tinkering Lab to host the event which was attended by 30 students and 10 parents and received overall good reviews. The earthquake installation was set up for the public to try during the follow-up event The Brainiverse Interactive.
- Brain science in art and science performance: The team invited local Krump dancer (Ms Michelle ANG) and her team 'OXYMORONS' to showcase a powerful performance which intricately blended power and subtlety through dance. The performance was a testament to the fusion of art and cognitive flexibility. Following the performance, the panel consisting of the dancer, a musician Prof Eddy WONG (non-CLIC PI, NIE), and Dr Lopes Fischer delved into a thought-provoking discussion on the enthralling interplay between artistic expression and cognitive flexibility. The video will be uploaded to the team's YouTube channel.

The School Workgroup conducted a series of workshops and lectures for educators at the National Institute of Education (NIE), see the "Other activities and achievements" section for more details.

Prof David HUNG (PI, NTU), Prof Ellefson, Dr Teo, and Dr Nastassja Lopes Fischer conducted a session at the Engagement with Policymakers event on 25 August during "Workshop 2: Adolescent Brain Health, Learning and Wellbeing". Ms Tripathi and Ms Lim supported the session as

scribes. On top of members from the CLIC project, this session involved representatives from agencies such as the National Research Foundation (NRF), the Agency for Science, Technology and Research (A*STAR), and the Ministry of Education (MOE).

The School Workgroup has been working with the Assessment Research (Assessment for Learning) Department in the Singapore Examination & Assessment Board (SEAB) to develop school-based tasks to measure inventive and adaptive thinking. This collaborative work involves the co-design of new assessment items and implementing these items in schools in Singapore. This collaboration is significant in its contribution to understanding the nexus between neuroscience research, practice and policies. Dr Lopes Fischer and Ms. Fu are the leading researchers in this work. This sub-workgroup of work is composed of representatives from the Cognition and Social Workgroups, and Mr Timothy LEE (Project Manager at the Office of Education Research, NIE). Prof Ellefson is co-leading this sub-workgroup together with Dr Teo.

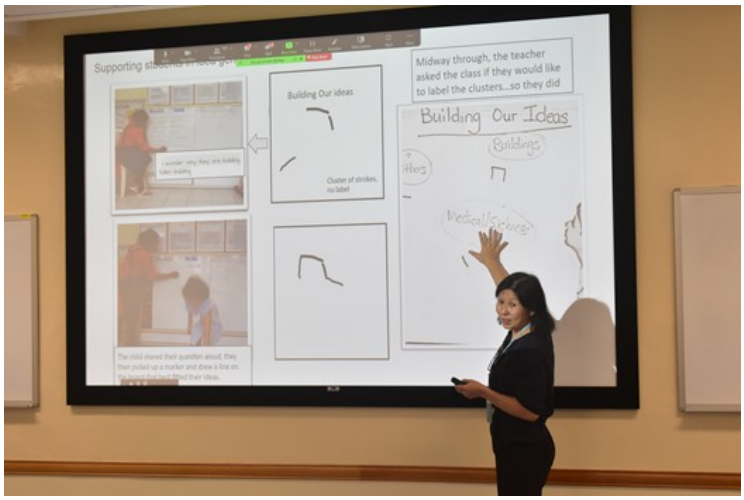


Figure 6.2: CLIC's Workshop at NIE titled "Making Sense of the Brain and the Science of Learning" on 22 August showcasing the latest findings of educational neuroscience and learning sciences to educators in an interactive session.

Figure 6.3: School Workgroup members interacting with the general audience during The Brainiverse Experience event at the Art Science Museum on 8 September 2023.

The following study has been pre-registered by the Schools Workgroup on the Open Science Framework Registries

Workgroup	Title	Submission Links
WP0.1 Translation to Education	Assessing Cognitive Flexibility, Other Executive Functions and Learning in Healthy Adolescents	Pre-registration link: https://osf.io/md4tv/

Update on Social Workgroup

Cognitive Flexibility and Its Association with Linguistic Preferences, Decision-Making, Tolerance of Uncertainty and Perceived Social Support

The Social Workgroup has continuously been collecting data from online questionnaires and lab-based cognition data for WP0.1. As of April 2023, data collection for WP0.1 has been completed and N=400 adult participants have fully completed the full WP0.1 study (both the online and face-to-face portions). The Social Workgroup Research Fellows and PhD student have been diligently assessing the incoming data's quality. This includes scrutinising participants' attentiveness during online survey completion and identifying any missing data. Additionally, they have been closely monitoring any potential issues with the online Qualtrics survey platform. Furthermore, the Social Workgroup has prepared and submitted pre-registrations for hypotheses related to socio-cognitive variables in the adult study.

Researchers from the Social Workgroup have also been conducting data analyses of the social data; the Research Fellows presented some of the results from the data analyses at the Writing Bootcamp in May 2023. Furthermore, the Social Workgroup were actively involved in the CLIC Impact Events where they created exhibits on linguistics, decision-making, and conducted a gameshow. Finally, **Prof Georgios CHRISTOPOULOS (PI, NTU**) and **Prof Henriëtte HENDRIKS (Deputy Director, CAM)** co-led a workshop discussing how social factors and future technologies can impact lifelong learning during CLIC's Engagement with Policymakers in August.

Prof Hendriks made a residency visit to Singapore in May 2023. During her visit she had meetings with several key people at CARES and met Prof Subodh MHAISALKAR (CREATE) to discuss the progress of the project, and potential office space options in CREATE. She made use of this time to have in person discussions with Prof Christopoulos and the Social Workgroup to discuss the data analyses and write initial outlines for papers related to multilingualism. She is currently taking the writing forward mainly with **Dr Nadhilla Velda MELIA (Research Fellow, NTU)**. She gave a talk in the Science of Learning in Education Centre (SoLEC) at NIE on the linguistic parts of the CLIC project, which was well attended. In her role as co-Deputy Director of CLIC, Prof Hendriks has also been involved in the organisation of the Writing Bootcamp together with **Prof Michelle ELLEFSON (PI, CAM)** which took place from 12-17 May. The Writing Bootcamp allowed the team in Singapore and Cambridge to look at the results in detail (focussing on the cognition data) and led to an initial draft of a first paper based on this dataset. Prof Hendriks was also closely engaged with **Assoc Prof Victoria LEONG (co-Deputy Director, NTU)** in the organisation of the CLIC Impact Events on 25 and 26 August and 8 September. Prof Hendriks took responsibility for the interactive elements of the events and returned a second time to Singapore in August to attend and help with the final preparations of the event.

Dr Shengchuang FENG (Research Fellow, NTU) has been analysing social decision-making data in adults and examining language entropy's connection to cooperativeness. He presented preliminary results at the Cambridge Writing Bootcamp. He is also exploring the relationship between social decision-making and neural resting state data. Dr Feng is currently preparing the manuscripts for these analyses.

Dr Melia oversees data quality checks, preprocessing, and analysis of sociocognitive questionnaires. Her focus is on social variables like tolerance of uncertainty, perceived social support, and multilingualism. She conducts a range of analyses, including descriptive statistics, reliability assessments, correlations, exploratory and confirmatory factor analyses, and investigates how these variables moderate the relationship between cognitive flexibility and structure learning. She presented some of her findings, particularly

related to multilingualism, at the Cambridge Writing Bootcamp. Currently, she is collaborating with Prof Hendriks on papers for publication based on these results. Additionally, Dr Melia was also part of the organising committee for The Brainiverse events.

Ms Emma Sam Yoke LOO (PhD Student, NTU) was involved in the CLIC Impact Events where she contributed to the development of a career-related game. Additionally, her poster on the association between cognitive flexibility, career adaptability, career exploration, and perceived employability was accepted for presentation at the Organizational Neuroscience Conference in Rotterdam, Netherlands from 15 – 17 June 2023.

Mr Akshay ABRAHAM (Research Associate, NTU), **Ms Hui Shan YAP (Research Assistant, NTU)** and **Ms Yuan Ni CHAN (Research Assistant, NTU)** have been involved in the CLIC Impact Events to develop and prepare the decision-making and career related games. Mr Abraham was also involved in recruiting and training Student Assistants to run and explain the tasks to guests.

The following study has been pre-registered by the Social Workgroup on the Open Science Framework Registries

Workgroup	Title	Submission Links
WP0.1 Social	Cognitive Flexibility and Its Association with Linguistic Preferences, Decision-Making, Tolerance of Uncertainty and Perceived Social Support	Pre-registration link: https://osf.io/ay9gr

Update on Neuroimaging Workgroup

Neuroimaging: Structure Learning Training and Cognitive Flexibility

Since the previous report submission in April 2023, the Neuroimaging Workgroup has completed data collection and has been working on analysis of the behavioural and neuroimaging data of the final participant pool. Data collection was completed by end June 2023 with a total of 108 participants (Training = 54, Control = 54) recruited.

In addition, two new Research Fellows, **Dr Deepika SHUKLA (Research Fellow, NTU)** and **Dr Eleanor Wei Shi KOO (Research Fellow, NTU)** joined the team. Both Dr Shukla and Dr Koo received training to familiarise themselves with the protocol of WP0.2's main study, which includes the cognitive-behavioural task batteries and the three MRI scan sequences (multi-parameter mapping (MPM), magnetic resonance spectroscopy (MRS) and resting-state fMRI administered at the pre- and post-MRI data collection timepoints).

Prior to **Dr Chia-Lun LIU's (Research Fellow, NTU)** departure, he conducted separate handover sessions with Dr Shukla and Dr Koo. Dr Shukla has been tasked with MRS data acquisition and analysis, while Dr Koo will be taking over MPM, resting-state fMRI and the behavioural data.

Since joining the Neuroimaging Workgroup, Dr Shukla has worked on rectifying errors such as issues arising from data oversampling and spectral shift. She has also implemented BIDS data formatting for the MRS portion of the neuroimaging data. Dr Shukla is currently working on MRS data analysis to ensure the quality and accuracy of the data. In addition, preliminary MRS data has shown inconsistency in voxel placements in the DLPFC region in pre- and post-MR sessions, which poses a potential limitation in using quantified GABA levels in assessing possible training effects. Based on these results, Dr Shukla is currently conducting quantified assessments for MRS voxel placements on standard brain templates, specifically the DLPFC region.

Dr Koo is currently optimising the pre-processing steps and further analyses of resting-state fMRI data, focusing on using the data for connectome-based predictive modelling. She plans to perform predictive analysis to correlate the functional connectivity matrix and the behavioural data. With the help of **Ms Min HONG (Research Associate, NTU)** and **Ms Winlynn CHOO (Research Associate, NTU)**, Dr Koo is also working on implementing standardised formatting for neuroimaging data according to BIDS and documentation of processing procedures and pipelines.

The behavioural data analysis was collaboratively conducted by **Mr Wei Ler KOO (Research Assistant, NTU)**, **Ms Janet TAN (Research Assistant, NTU)**, **Ms Marisha Barth UBRANI (Research Assistant, NTU)** and Ms Choo in line with the analysis pipelines previously discussed. To streamline the process of data analysis, the cognitive tasks measuring the construct of cognitive flexibility were delegated to the team members. Mr Koo oversaw the analysis of Task Set Switching Where (TSS Where), Task Set Switching What (TSS What) and Wisconsin Card Sort Task (WCST), Ms Ubrani was in charge of analysis of Colour Shape Task (CST) and Trails Making Test (TMT), and Ms Tan focused on the analysis of Intra-Extra Dimensional Task (IED) and Probabilistic Reversal Learning (PRL). Concurrently, they were also involved in the analysis of the cognitive tasks such as working memory and inhibition tasks, language and numeracy tests, and the creativity tasks. Separately, Ms Tan was responsible for the analysis of intelligence tasks and structure learning (SL) data. She also cleaned and preprocessed data for questionnaires administered at pre- and post-intervention timepoint to extract demographic information of participants and their scores on social constructs. Finally, Ms Choo has also helped to fix scripts that the others were working on for their analysis.

Ms Ubrani, with the assistance of 2 student assistants, reviewed the responses of the language and numeracy tests – Woodcock-Johnson IV (WJIV) test of achievements and Wechsler Abbreviated Scale of Intelligence (WASI-II). The manual scoring of the creativity tasks Alternate Uses Task

(AUT) and Remote Associates Task (RAT) were performed in line with the scoring criteria of WP0.1 and an inter-rater reliability score was computed to ensure a high level of agreement between the raters.

Research assistants from the team pre-processed and cleaned the behavioural data. The data was then inspected for outliers and tested for assumptions of normality and equal variances. Appropriate statistical tests were applied to address the non-normality distribution of the datasets. The means-testing of the Control versus Training group showed no significant differences in task performance between the two groups due to limited power. As a result, further analyses were conducted using permutation tests or models. The behavioural data was also aggregated according to domains to compute factor scores for cognitive flexibility, working memory, inhibition, and creativity. However, when these factor scores were used for means analysis, no significant differences between the Training and Control groups were detected.

Among the 54 Training participants, two participants' data were excluded due to errors during administration of SL training stages. The remaining SL data was pre-processed by Ms Tan and classified into learning and strategy types according to the same criteria employed by WP0.1. As shown in Figure 6.4, this produced a final number of 45 Learners, 4 Slow-learners and 3 Non-learners. The number of participants who employed Maximising strategy (N=29) was the highest, followed by Mixed strategy (N=19) and lastly Matching strategy (N=4). These findings have implications for further analysis and the modifications to the SL design in Phase 2 of the study.

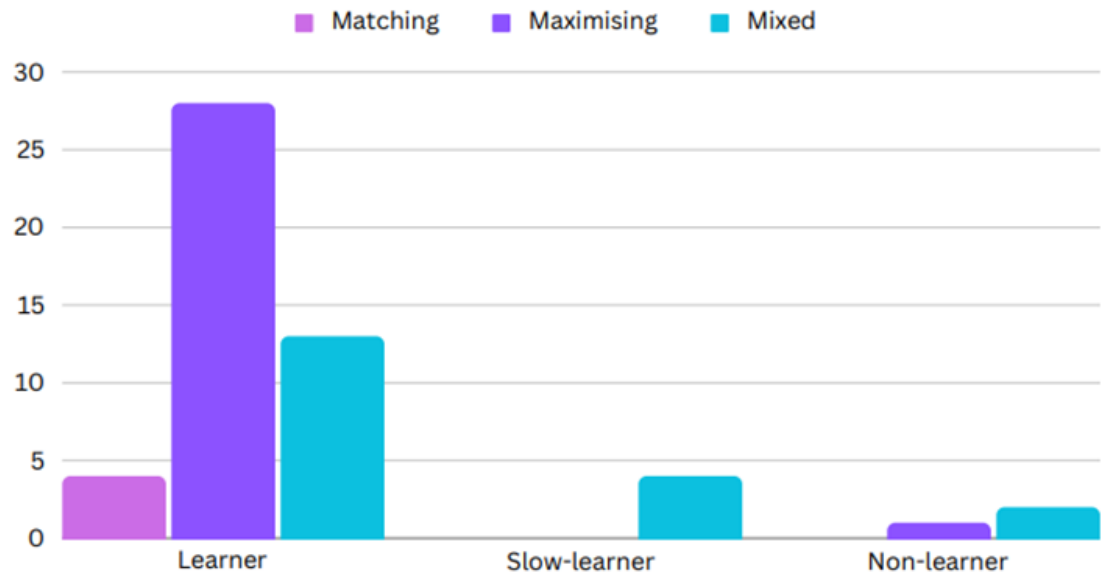


Figure 6.4: Number of participants classified by learning and strategy type

Dr Liu and Ms Ubrani employed ex-Gaussian modelling on the CST data to extract tau value, which measures how quickly participants decide to switch to a colour-based or shape-based response. As an incomplete dataset was used previously, this model will now be used on the full dataset. Semantic Network Analysis has been explored by Mr Koo and Ms Choo, and preliminary results have been obtained, but further exploration is still ongoing. Ms Tan is currently working on applying the reinforcement learning model to IED and PRL to obtain the inverse temperature value, which is an indicator of participants' exploitation tendencies.

Other analysis methods will also be tested to better understand the links between the behavioural data collected at different timepoints of study. Ms Tan will perform linear regressions to understand

how SL and cognitive tasks may predict one another. At the same time, she will examine the performance during the testing stages of SL (Generalisation and Reversal) using a linear mixed model. Ms Ubrani will attempt to conduct a median split performance on RAT and correlate it to Verbal Fluency to see how convergent thinking relates to divergent thinking. She will also run a Semantic Distance Analysis for AUT by employing a natural language processing dictionary to understand how far in meaning the participants' responses are from the task's prompts. Lastly, Ms Ubrani will employ a linear mixed model on the CST reaction time data to explore the response-congruency effects on reaction time.

Neuroimaging Data Quality Check and Analysis: Since the last meeting with **Prof Annabel CHEN (co-Director, NTU)** and **Prof John SUCKLING (PI, CAM)** in March, Dr Liu has attempted follow-up resting-state fMRI analyses suggested in the meeting. For example, extrinsic and intrinsic functional connectivity were further explored by defining specific brain regions anatomically using an alternative set of atlases. Voxel-Based Quantification (VBQ) analysis was assisted by Ms Hong to confirm that the mentioned "central point artifact" derived from the MPM results was independent of the analysis method. While the focus of resting-state fMRI analysis remained on functional connectivity within the cognitive flexibility network and between networks, further data- and hypothesis-driven approaches have been attempted by Dr Liu. Preliminary results identified functional connectivity between cognitive flexibility and frontal-parietal and visual cortico-striatal circuits in resting-state fMRI. These results were presented by Dr Liu at the 29th Annual Meeting of the Organisation for Human Brain Mapping in Montréal, Canada from 22 -26 July 2023.

Dr Shukla and Dr Liu discussed the most updated neuroimaging protocol with Dr Diana ROTARU (non-CLIC Research Fellow, CAM), ensuring that data acquisition and analysis are aligned with the Cambridge team. Artefacts and imaging protocol changes for MRS and MPM had been discussed and tested for their feasibility in current protocol optimisation. Phantom and human test scans were performed to ensure pre- and post-MRI data reproducibility and longitudinal assessments in terms of consistent placements of voxel on the dorsal-lateral prefrontal cortex. Data processing and GABA quantitation with tissue correction pipelines have been developed, and data processing and quantification for WP0.2 data have been completed. The results from phantom and test scans were presented to Prof Chen and Prof Suckling, identifying the issue of in-scanner T1 MRI downshift in reference to the immediate scout scan. Dr Shukla is currently rectifying the issue to prevent voxel misalignment. The corrected brain tissue fractions will be used to get quantified GABA levels from left and right DLPFC regions, which will be correlated with the cognitive test scores obtained pre- and post-training sessions. For additional analysis of MRI structural data, Dr Shukla, with the support of Ms Hong, will be exploring the use of Voxel-Based Morphometry (VBM) analysis on detecting changes in grey and white matter as well as subcortical volumes between pre- and post-MRI sessions.

Development of SLiCX programme for Phase 2

Concurrently, while performing the data analyses, the Neuroimaging Workgroup is developing a new SL training program to be administered in Phase 2 of the study called the Structure Learning-based Cognitive Flexibility Suite (SLiCX). SLiCX will introduce colour as an additional dimension to the symbols used in the SL intervention from WP0.2's Main Study. Pilot studies are currently being planned to test the potential colour effect and the experimental conditions suitable for adults and adolescents. This initiative is led by Dr Koo and supported by Mr Koo, Ms Tan and Ms Ubrani. It is also guided by Research Fellows from other workgroups - **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)**, **Dr Ke TONG (Research Fellow, NTU)**, and **Dr Shengchuang FENG (Research Fellow, NTU)**. Multiple rounds of discussions were held within the team to plan for the SLiCX pilot studies.

In anticipation of heavy computational needs for WP0.2 Main Study, Ms Choo has been tasked to maintain the REDCap servers (Figure 6.5) and the 2 servers that she helped to procure and set up

for CLIC (CLIN40002 and CLIN40003), ensuring that any updates and installation to the backend is successfully brought to production. CLIN40002 is a Windows Server that is used in WP0.1 modelling analysis. Meanwhile, CLIN40003 is an Ubuntu server used for WP0.2 modelling analysis. The CLIC REDCap servers are composed of UAT and production servers, in which UAT can only be accessed via the NTU network and acts as a testing platform for agendas related to REDCap. The production web server is accessible via the internet and is targeted to host the recruitment and survey for Phase 2 of CLIC. To help with a better rolling out of REDCap usage in Phase 2, **Ms Natalie Philyra HOO (Research Assistant, NTU)**, **Ms Shilpi TRIPALTHI (Research Associate, NTU)**, **Dr Deepika SHUKLA (Research Fellow, NTU)** and **Ms Yuan Ni CHAN (Research Assistant, NTU)** have been elected as the secondary administrators for REDCap. They will work alongside Ms Choo to set up questionnaires and decide on member's roles once the surveys for Phase 2 are confirmed. Ms Choo also works with Dr Liu and Ms Ubrani to ensure that the details of the DMP provided are accurate.

Dr Sheng Hung CHUNG (Research Engineer, NTU) is responsible for overseeing the CLIC IT infrastructure, especially the overall maintenance of CLIC data storage and server computing infrastructure. The Network Attached Storage (NAS) provided by NTU CITS (Centre for IT Services) is a clustered file storage that enables multiple researchers/workstations to retrieve data from a centralised disk via a dedicated secured shared drive. After comparing the specifications for CLIC's third and fourth servers, Dr Chung has obtained quotations for the two servers. Under CLIC's admin assistance, the third server (OS: Ubuntu, the only GPU-equipped server of CLIC) was successfully procured in February. Currently, Dr Chung is making his best efforts to strengthen the server's security before the server is made available to the CLIC members. The fourth CLIC server is currently under procurement by CLIC's admin. It is tentatively an Ubuntu server. Dr Chung also helps in maintaining the CLIC Google Workspace. Ms Choo is also helping to plan data storage usage and optimise the existing servers in preparation for the behavioural data modelling and heavy neuroimaging data analyses for WP0.2 data.

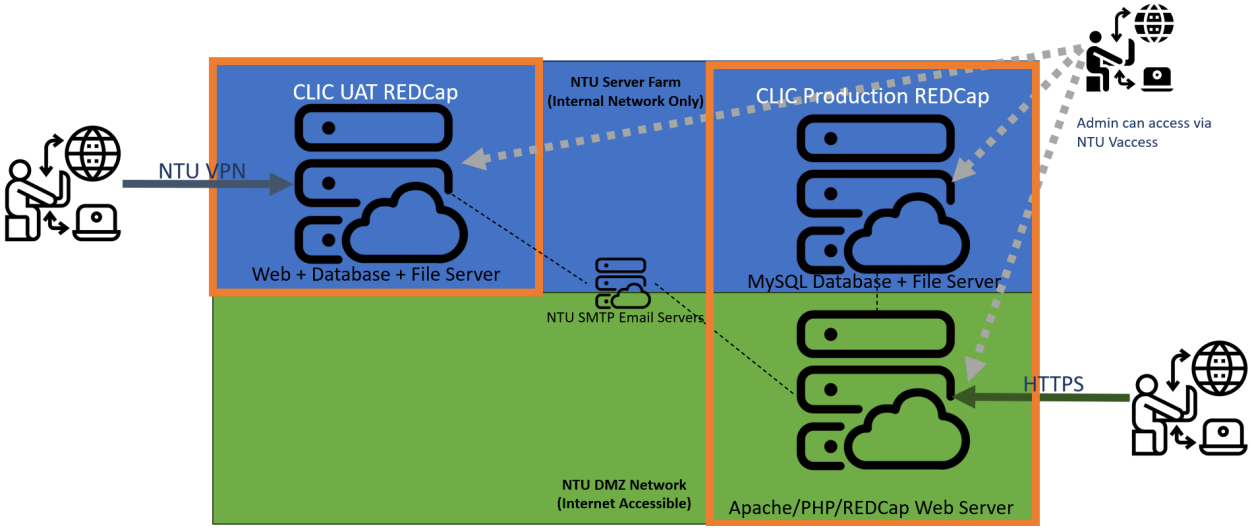


Figure 6.5: CLIC REDCap Infrastructure

The following study has been pre-registered by the Neuroimaging Workgroup on the Open Science Framework Registries

Workgroup	Title	Submission Links
WP0.2 Neuroimaging	Structure Learning Training and Cognitive Flexibility	Pre-registration link: *Pending Submission*

Scientific output

The following are the CREATE-acknowledged research protocol papers generated by CLIC during the reporting period.

Potential cognitive and neural benefits of a computerised cognitive training programme based on Structure Learning in healthy adults: study protocol for a randomised controlled trial
Chia-Lun Liu, Xiaoqin Cheng, Boon Linn Choo, Min Hong, Jia Li Teo and Wei Ler Koo, *Trials*
DOI: 10.1186/s13063-023-07551-2

Description: Cognitive flexibility refers to the capacity to shift between conceptual representations particularly in response to changes in instruction and feedback. It enables individuals to swiftly adapt to changes in their environment and has significant implications for learning. The present study focuses on investigating changes in cognitive flexibility following an intervention programme--Structure Learning training.

Study protocol: How does cognitive flexibility relate to other executive functions and learning in healthy young adults?
Ke Tong, Yuan Ni Chan, Xiaoqin Cheng, Bobby Cheon, Michelle Ellefson, Restria Fauziana, Shengchuang Feng, Nastassja Fischer, Balázs Gulyás, Natalie Hoo, et al., *PLOS ONE*
DOI: 10.1371/journal.pone.0286208

Description: Cognitive flexibility (CF) enables individuals to readily shift from one concept or mode of practice/thoughts to another in response to changes in the environment and feedback, making CF vital to optimise success in obtaining goals. However, how CF relates to other executive functions (e.g., working memory, response inhibition), mental abilities (e.g., creativity, literacy, numeracy, intelligence, structure learning), and social factors (e.g., multilingualism, tolerance of uncertainty, perceived social support, social decision-making) is less well understood. The current study aims to (1) establish the construct validity of CF in relation to other executive function skills and intelligence, and (2) elucidate specific relationships between CF, structure learning, creativity, career decision making and planning, and other life skills.

Other activities and achievements

CLIC Impact Events

CLIC held an Engagement with Policymakers on 25 August 2023, which was attended by officials and key stakeholders in the education and research sector in Singapore to delve into crucial topics related to lifelong learning and brain health. This event brought together individuals from the National Research Foundation, Ministry of Education, Ministry of Social and Family Development, SkillsFuture Singapore, Early Childhood Development Agency, Institute for Adult Learning and the Agency for Science, Technology and Research.

The event consisted of four comprehensive workshops:

1. Childhood Brain Health, Learning and Wellbeing led by **Prof Topun AUSTIN (co-PI, CAM)**, **Assoc Prof Victoria LEONG (co -Deputy Director, CAM)** and Prof David ROWITCH (non-CLIC PI, CAM)
2. Adolescent Brain Health, Learning and Wellbeing led by **Prof Michelle ELLEFSON (PI, CAM)**, **Prof David HUNG (PI, NTU)** and **Dr Chew Lee TEO (co-PI, NTU)**
3. Adult Brain Health, Learning and Wellbeing led by **Prof Annabel CHEN (co-Director, NTU)**, **Prof Barbara SAHAKIAN (Senior Scientific Advisor, CAM)** and **Prof John SUCKLING (PI, CAM)**
4. The Ideas Express: Designing the Future Learning led by **Prof Henriëtte HENDRIKS (co-Deputy Director CAM)** and **Prof Georgios CHRISTOPOULOS (PI, NTU)**

This engagement event breaks down current research as well as CLIC's findings, and identifies strategic opportunities, challenges, and recommendations tailored to the local landscape. These workshops offered valuable insights for educational and research policymakers to integrate cutting-edge research into policies and practices.

The CLIC team organised a 2-part science festival at the ArtScience Museum in Singapore to engage the public to explore the fascinating world of flexible minds, learning, and mental well-being. The first event, titled The Brainiverse Experience on 26 August consisted of plenary talks, an earthquake challenge competition for secondary school students, and an art competition for special needs students on the topic "Neurodiversity: No Brain is the Same". **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM)** was invited to give the opening keynote titled "Cognitive Flexibility as the Gateway to Successful Decision-making, Creative Thinking and Optimal Brain Function". In his talk, he emphasised the significance of research on cognitive flexibility and the underlying cognitive neuroscience.

In the follow-up Brainiverse Interactive event on 8 September, the Cognition team research staff presented CLIC's research and implications to a curious and diverse audience using interactive booths and games. The combined Brainiverse events significantly amplified the reach and impact of CLIC's research to more than 1500 attendees.

Talks, workshops, and presentations

At the inaugural Organizational Neuroscience Conference hosted by Erasmus University in Rotterdam, Netherlands, from 15 -17 June, **Prof Georgios CHRISTOPOULOS (PI, NTU)** chaired the first session titled "PDW: Neuroscience technologies and tools: making sense of it all". He also organised two workshops on fMRI and Heart Rate methods at the 83rd Annual Meeting of the Academy of Management in Boston, USA, from 4 – 8 August.

Prof Ellefson conducted a workshop for specialists in MOE on 21 August on the educational research the CLIC School Workgroup have been conducting.

Prof Ellefson, Dr Teo, **Dr Peter SEOW (co-PI, NTU)** and **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** delivered the workshop "Making Sense of the Brain and the Science of

Learning" at the National Institute of Education (NIE) on 22 August which consisted of an interactive session where speakers discussed the latest findings on Educational Neuroscience and Learning Sciences. The workshop included hands-on activities and an interactive discussion to help educators understand how they can support learners in developing their cognitive, social-emotional and academic abilities. This workshop saw a total of 126 attendees, who participated either in person or through the online streaming platform.

Dr Teo also hosted a talk for Prof Sarah-Jayne BLAKEMORE (non-CLIC PI, CAM) titled "Sensitive periods of social brain development in adolescence" which was organised in collaboration with the Science of Learning in Education Centre (SoLEC) at NIE.

Dr Lopes Fischer and Dr Katherine Guangji YUAN (non-CLIC Research Fellow, NIE) delivered a workshop at NIE titled "Introduction to R" in August 2023. Dr Lopes Fischer returned a second time to NIE as an invited lecturer for the NIE course titled "AGE06E Neurodiversity and The Learning Experience" led by **Asst Prof Azilawati JAMALUDIN (co-PI, NIE)** in September 2023.

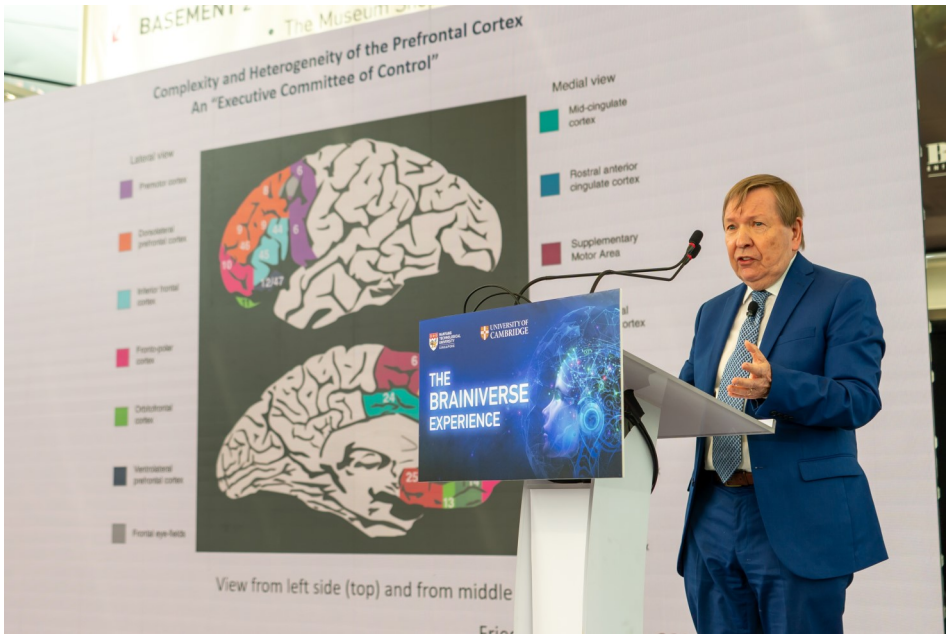
The CLIC team delivered two poster presentations, one was titled "Gonna change my way of thinking to stay employed: The relationship between cognitive flexibility and career adaptability" at the Organizational Neuroscience Conference hosted by Erasmus University in Rotterdam, Netherlands, from 15 -17 June. The second was titled "Resting-state fMRI functional connectivity predicts individual flexibility in structure learning" at the 29th Annual Meeting of the Organisation for Human Brain Mapping in Montréal, Canada from 22 -26 July 2023.

Other awards and activities

Prof Christopoulos received the "Early Career Investigator Award" at the 83rd Annual Meeting of the Academy of Management in Boston, USA.

As part of the CLIC's efforts in applying research findings to education, researchers from the different workgroups have been collaborating with external stakeholders (i.e., MOE's Singapore Examinations and Assessment Board – SEAB) in the co-design of new assessment tools based on CLIC's research about cognitive flexibility.

Prof Christopoulos and Prof Sahakian published an opinion paper titled "Cognitive flexibility: the science of how to be successful in business and at work" on 13 April 2023 in The Conversation, exploring the relationship between cognitive flexibility and business success. This popular science article has been republished by both the World Economic Forum and the Society of Human Resource Management on their websites.



Pictures from the CLIC Impact Events. Top photo shows Prof Trevor Robbins delivering his opening keynote on 26 August. The bottom two photos are the public engagement activities on 8 September.

CKG

CITIES KNOWLEDGE GRAPH

Cities Knowledge Graph (CKG) aims to transform city planning related data, information and knowledge into a semantic and extensible platform – a knowledge graph. The proposed CKG would be similar to a knowledge management system for urban planning, integrating information from various sources and domains, evaluating planning proposals against visions and targets set for future urban development, and supporting policymakers and planners by mapping interesting planning directions. It further ties together existing 3D geo-databases, as well as novel analysis, simulation and visualisation tools developed by CARES and SEC, contributing to the development of an unprecedented knowledge graph called the "The World Avatar (TWA)".

CKG Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Stephen CAIRNS
(April 2020 – June 2022, moved from SEC)
ETH Zürich

Professor Martin RAUBAL
(July 2022 – present)
ETH Zürich

OVERVIEW

Cities Knowledge Graph is an Intra-CREATE Thematic Grant project in the 'Cities' thematic area. The project brings together expertise from CARES, the host institution of the project, and SEC (the Singapore-ETH Centre, established by ETH Zürich - the Swiss Federal Institute of Technology Zürich) and its Future Cities Laboratory Global programme. The team is led by PIs Prof Dr Markus Kraft (University of Cambridge) and Prof Dr Martin Raubal (ETH Zürich). Dr Pieter Herthogs (Senior Researcher, SEC) is Co-Investigator and Project Leader. Dr Aurel Von Richthofen (Team Leader Cities, Arup Germany), Prof Dr Stephen Cairns (ETH Zürich and Monash University Indonesia) and Prof Dr Franziska Sielker (TU Vienna and University of Cambridge) are Co-Investigators of the project.

Over the past six months, we have made significant new additions to the knowledge graph. We finalised and deployed the OntoZoning, OntoBuildableSpace and OntoPlanningRegulations ontologies. We also integrated domain-specific application ontologies to achieve interoperability by linking building ontologies together to distinguish the geometry from other semantic properties. We developed an urban metabolism ontology and various scenarios to represent and compute the sum of technical and socioeconomic processes occurring in urban areas. We developed scenarios to estimate electricity and drinking water demands of given plots of land in Singapore over a year, according to the 'present' and the potential 'future' built environment.

We updated the existing City Energy Analyst (CEA) agent to retrieve weather data and terrain data from the knowledge graph to improve the accuracy of CEA simulations of building energy demands and solar energy generation. We developed a Traffic Routing agent which supports strategic and tactical planning for smart cities and disaster recovery efforts. We also developed two input agents, Open Meteo agent and Open Street Map agent, which are responsible for augmenting the knowledge graph with information such as weather data and building usage data to be used by other applications.

The team developed the Suitable Site Selector demonstrator, which allows users to compare multi-domain information and evaluations for up to five selected plots. Users can compare between 'present' and 'future' data and analyse deltas between the 'present' and 'future' using the graphical user interface. We also developed a user-friendly knowledge administration panel for the Cities Knowledge Graph, to manage ontologies and rules of inference within dynamic geospatial knowledge graphs.

The project closed in September 2023 with a successful Completion Event in which the outcomes were presented to a large in-person and online audience including representatives of governments, construction and engineering industries, and academia.

Professor Markus Kraft, PI
University of Cambridge

Professor Martin Raubal, PI
ETH Zürich

Update on work package 1

Developing master-planning ontologies

Following the ontology validation workshop organised for the Urban Redevelopment Authority (URA) in March 2023, the team shared all necessary materials for URA to internally review, test, and validate the three URA-specific ontologies developed by the project (OntoZoning, OntoPlanningRegulations, and OntoBuildableSpace) and the project's Programmatic Plot Finder application, a demonstrator of a regulatory search engine supporting site search tasks in city planning. The team also integrated the received feedback.

Ms Ayda GRIŠIŪTĖ (PhD Researcher, ETH Zürich) extended the script for calculating the allowed Gross Floor Area (GFA) to cover all plots across Singapore. The newly generated dataset increased allowable GFA value availability from 29% (33,641 plots) to more than 76% (85,988 plots). The dataset also increased the granularity of allowable GFA values per plot; almost 71,000 plots in Singapore have more than one allowable GFA value. The generated allowable GFA and urban planning regulation datasets enable new types of queries, e.g., case-based search, regulation change assessment or plot ranking.

Dr Chenyi CAI (Researcher, SEC) is augmenting the GFA calculation workflow to include the representation of 3D buildable space concepts (e.g., footprints, volumes) using the OntoCityGML ontology. She developed the first conceptual draft of the implementation and will continue to work on the semantic representation of regulations and geometric visualisation of buildable space. This work could serve as a basis for comparing existing buildings and allowable build space in a 3D format.

The team has finalised and deployed the OntoZoning, OntoBuildableSpace, and OntoPlanningRegulations ontologies on the World Avatar knowledge graph.

Dr Andrea BARTOLINI (Postdoctoral Researcher, SEC) and **Dr Pieter HERTHOGS (Senior Researcher, SEC)**, with support from Ms Grišiūtė have developed the first version of an ontology for urban metabolism called OntoUrbanMetabolism, to represent the sum of technical and socio-

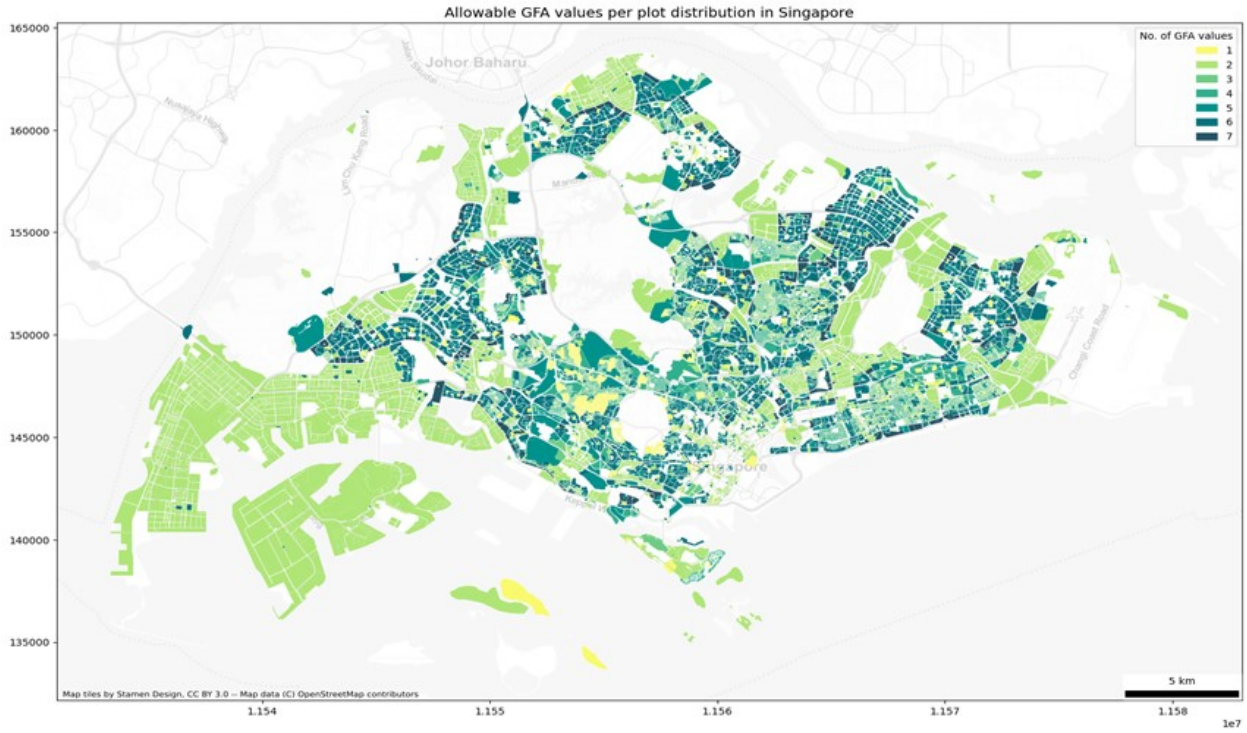


Figure 7.1: The number of allowable Gross Floor Area (GFA) values per plot across all plots in Singapore.

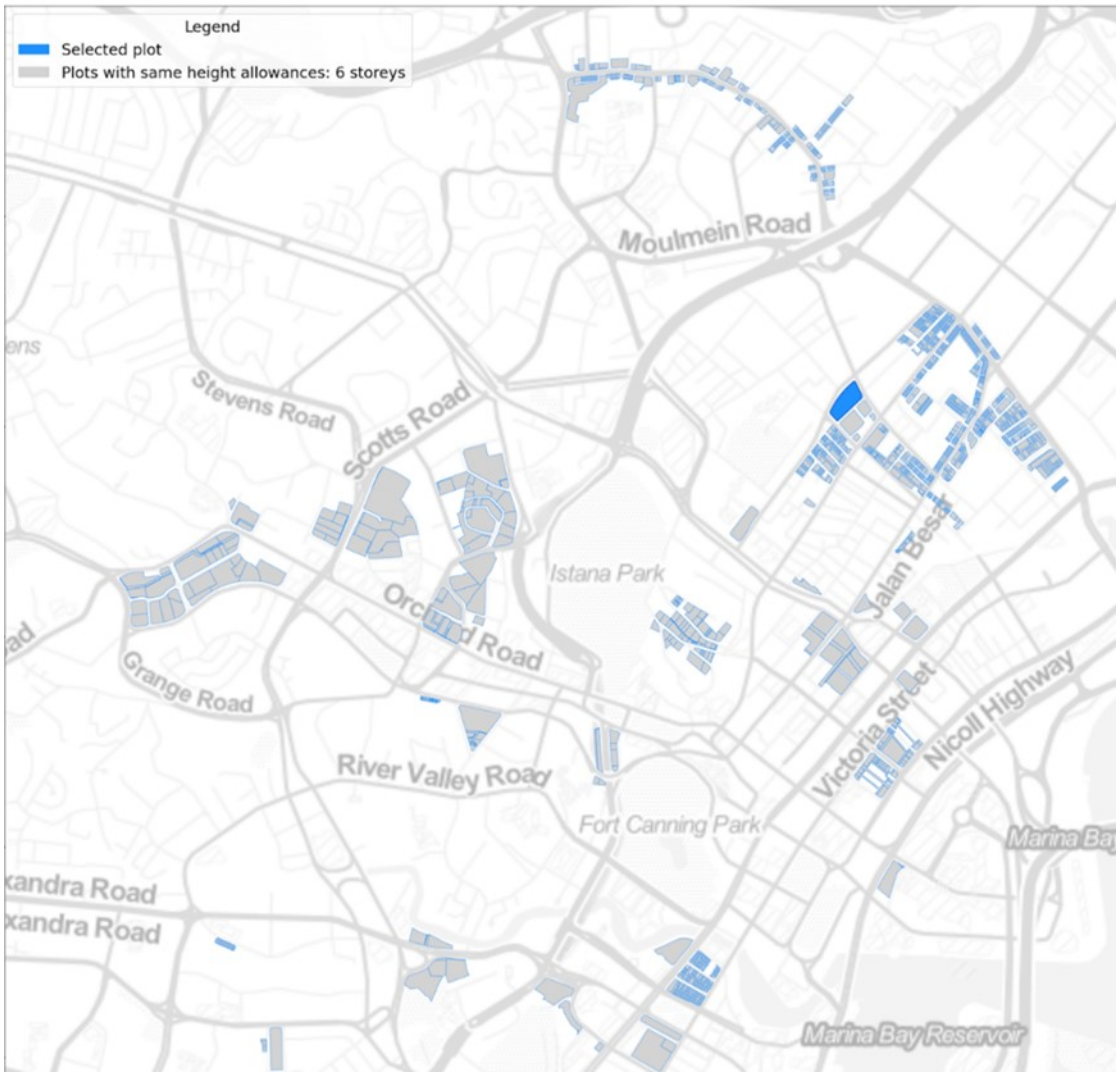


Figure 7.2: Results from a case-based search query, retrieving plots with the same allowed number of stories.

economic processes occurring in urban areas, generating different types of resource flows, and having other types as outputs of the process itself. Such an ontology defines a common language to describe the resource flows needed to sustain the functioning of urban areas.

This ontology also represents data from different technical domains on different spatial and temporal resolutions. Dr Bartolini developed a prototype application to compute the metabolism of selected plots in Singapore, leveraging available public datasets. The application estimates yearly electricity and drinking water metabolisms of these land plots based on the current built environment, and according to development scenarios computed using allowable GFAs as defined by the OntoBuildableSpace ontology.

Furthermore, Dr Bartolini will couple the semantically represented data as input to sample infrastructure simulation models, such as power systems simulations, and will also link a semantic description of the built environment within a plot to its urban metabolism.

Dr Sebastian MOSBACH (Senior Research Fellow, CARES), **Dr Jingya YAN (Research Fellow, CARES)** and **Mr Hou Yee QUEK (Research Associate, CARES)** worked on integrating domain-specific application ontologies to achieve interoperability within the dynamic knowledge graph. For city model visualisations, Dr Yan and Mr Quek established two properties to link a central building concept from the Building Topology Ontology (BOT) with their geometry features in Industry Foundation Classes (IFC) and CityGML,

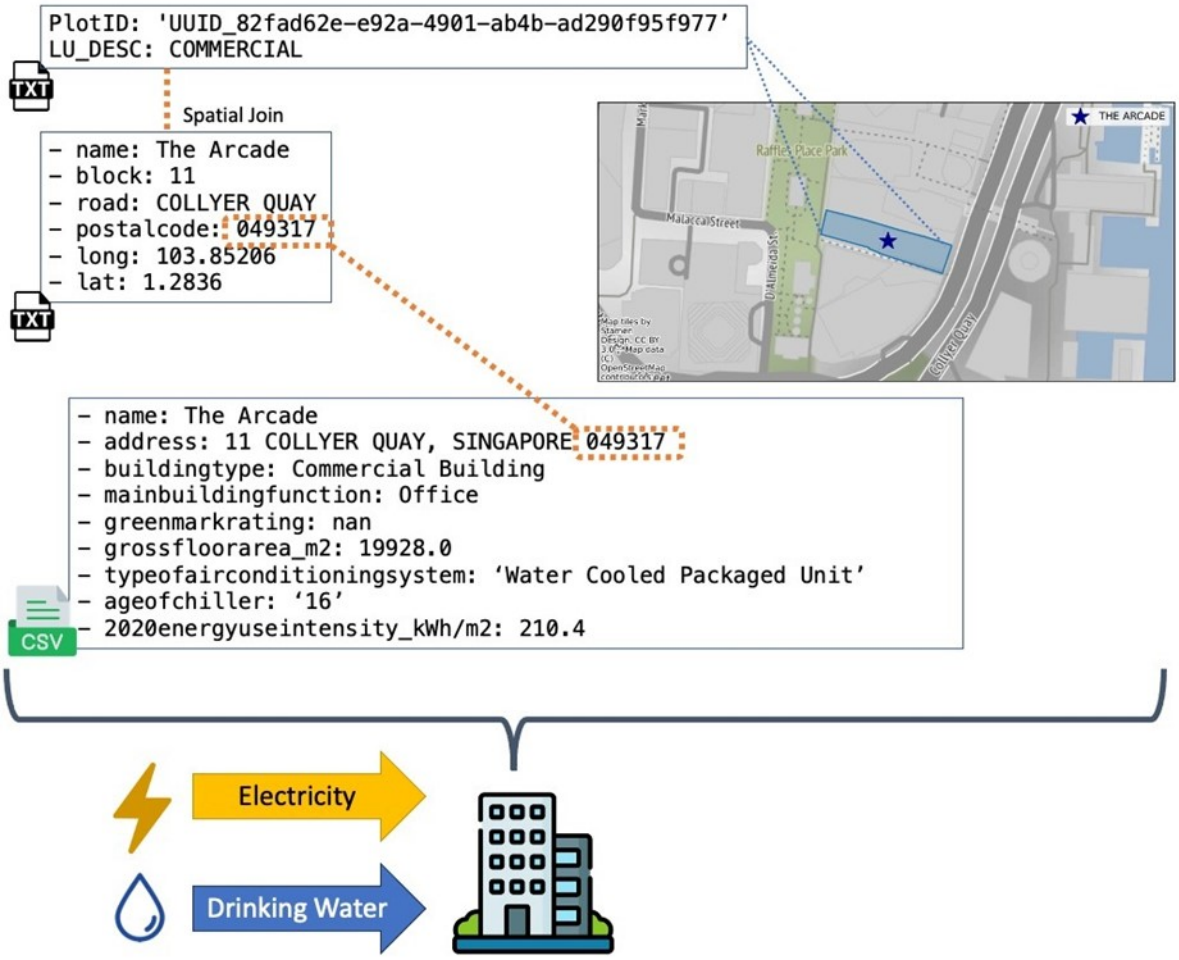


Figure 7.3: General framework to show data from plots and buildings, together with other relevant datasets. It is assumed that each plot is characterised by an urban metabolism.

represented in the ontologies OntoBIM and OntoCityGML, respectively (Figure 7.4). This distinguishes the geometry from other semantic properties, improving the flexibility and maintenance of application systems, as new properties can be directly linked to the central building concept without affecting the underlying geometric representation. Different geometric features can also be linked simultaneously to one building representation, enabling users to retrieve various levels of detail or modelling standards for the same building, as required.

Mr Yi-Kai TSAI (Software Developer, CARES), **Mr Wilson ANG (Software Developer, CARES)**, Mr Quek and Dr Mosbach have revised and extended the urban building energy modelling and master planning ontology (OntoUBEMMP) for representing building utility and solar energy concepts, which the City Energy Analyst agent utilises to represent its outputs.

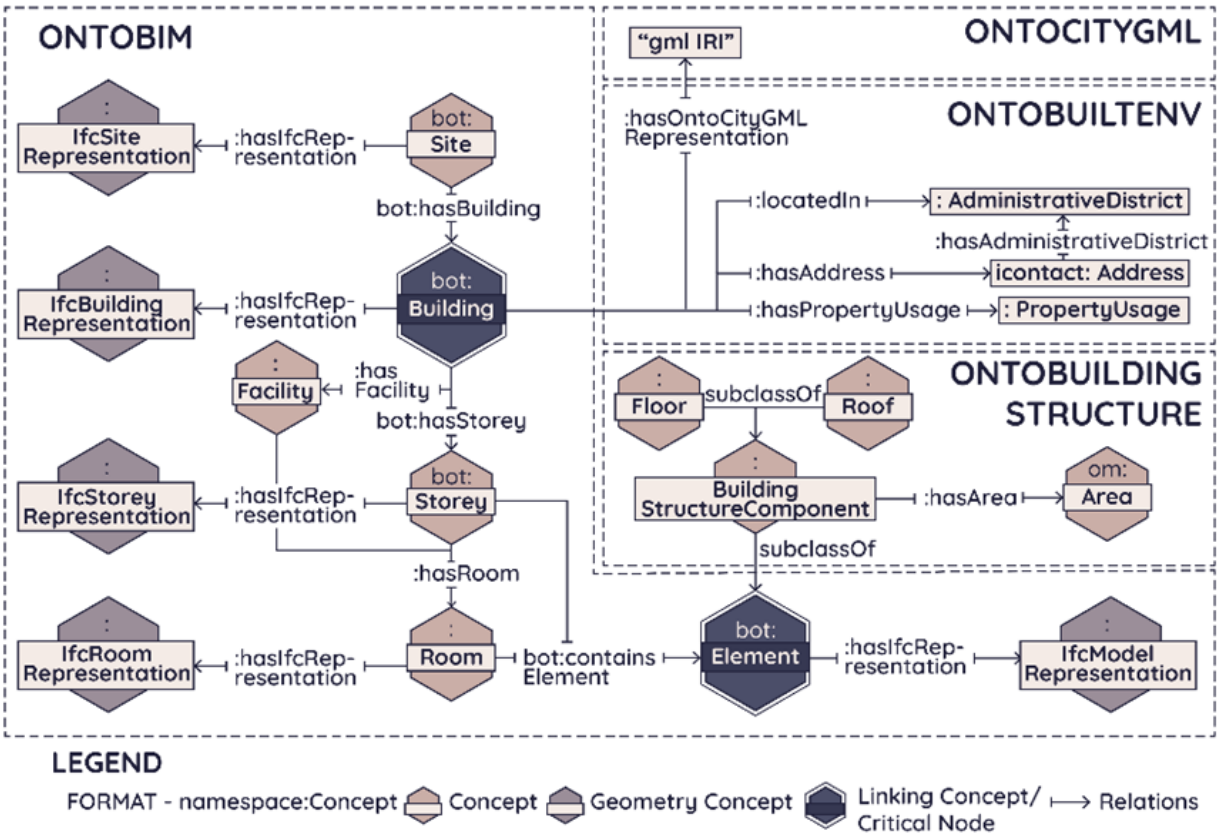


Figure 7.4: An extract of the modular ontology design connecting Building Information Modelling (BIM) and Geographic Information System (GIS) features of buildings.

Update on work package 2

Developing the knowledge graph's architecture

The paper entitled '*Semantic 3D city interfaces – Intelligent interactions on dynamic geospatial knowledge graphs'*, led by **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, was published in *Data-Centric Engineering* Volume 4 in September 2023. It presents a system architecture and a set of interfaces that can build scalable information systems capable of large city modelling based on dynamic geospatial knowledge graphs to avoid pitfalls of Web 2.0 applications while blending artificial and human intelligence during the knowledge enhancement processes. The architecture and its components are illustrated in the example of various intelligent autonomous agents demonstrating various capabilities.

Firstly, the City Export agent processes geospatial data into a suitable form to provide city object visualisation and interactions on the augmented 3DCityDB-Web-Map-Client. Non-geospatial and contextual knowledge, such as the one concerning city regulations, is provided to the 3DCityDB-Web-Map-Client by the City Information agent. The capability of interactions between agents is demonstrated on the example of enrichment of such contextual information by City Energy Analyst (CEA) agent that automatically estimates energy demands for city model members. The Distance agent can track interactions with the model members on the web, calculate distances between objects of interest, and add new knowledge to CKG. Lastly, the Thematic Surface Discovery agent automatically upgrades the model's level of detail to interact with thematic parts of city objects by other agents.

The logical foundations of the underlying representation and CityGML-based conceptual schema used to describe cities in terms of the OntoCityGML ontology, together with the system of intelligent autonomous agents, make systems built upon such architecture capable of assessing and maintaining ground truths with certainty. This new era of GeoWeb 2.5 systems lowers the risk of deliberate misinformation within geography web systems used for modelling critical infrastructures.

Mr Yi-Kai TSAI (Software Developer, CARES) prepared the latest release for the CKG project. This release included updates to the CEA agent, aiming to improve the accuracy of building energy demands and solar potentials simulation results. Mr Tsai improved the CEA agent to retrieve terrain and weather data from the knowledge graph, to use as inputs to the CEA simulation. Mr Tsai also updated the agent to use the latest version of the OntoUBEMMP ontology described in Work Package 1.

Update on work package 3

Developing agents to operate software and integrate data

Mr Yi-Kai TSAI (Software Developer, CARES) developed the Open Meteo agent to instantiate historical weather data retrieved with the Open-Meteo Application Programming Interface (API).

Mr Tsai improved the City Energy Analyst (CEA) agent to work in conjunction with the Open Meteo agent to retrieve realistic weather data for locations across the globe, replacing the weather data assumptions in the CEA. Mr Tsai has also updated the CEA agent to query for and process raster data to use as terrain input to CEA, replacing the CEA default assumption of fixed elevation terrain. Retrieving realistic input data from the knowledge graph improves the accuracy of CEA simulations of building energy demands and solar energy generation. Mr Tsai also refactored the CEA agent code and documentation to improve the ease of use for users and developers.

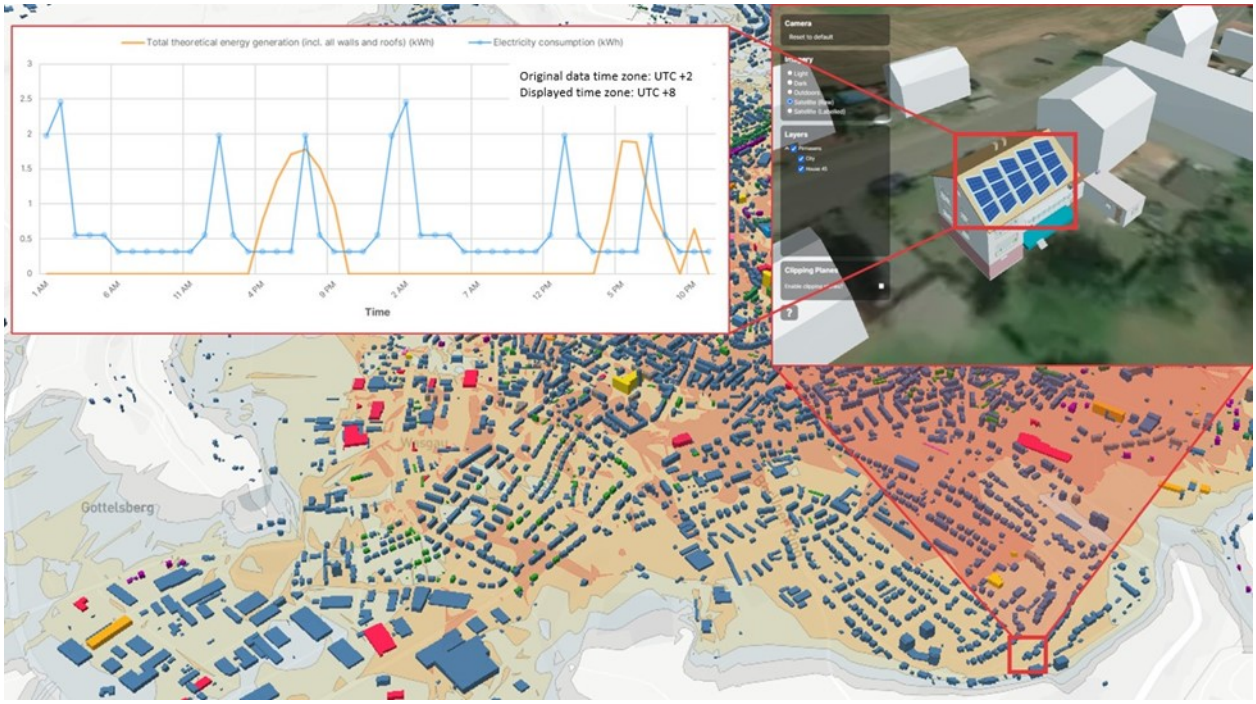


Figure 7.5: Using the City Energy Analyst (CEA) agent to simulate building energy demands and calculate theoretical solar energy generation for a building. The graph shows (in kWh) the total theoretical energy generation (including all walls and roofs) as orange and electricity consumption as blue against time throughout the day.

Mr Shin Zert PHUA (Software Developer, CARES) and Mr Tsai further developed the Open Street Map (OSM) agent which extracts building data tags from OSM and categorises them into building usage instances. This agent can also match the OSM data with the corresponding 3D buildings instantiated in the knowledge graph. The building usages and usage share (for buildings with mixed usage) are used as inputs to improve the simulation results of the CEA agent.

Mr Phua also designed the Traffic Routing agent, which supports strategic planning for smart cities and disaster recovery efforts. Mr Phua has developed use cases supporting both tactical and strategic decision-making across three major cities: Singapore, King's Lynn (United Kingdom) and Pirmasens (Germany), enabling cross-domain issues to be addressed.

Mr Phua integrated his work with the Traffic Incident agent, developed by **Mr Xinyu SUN (Project Officer Intern, CARES)**. The agent retrieves data from Singapore Land Transport Au-

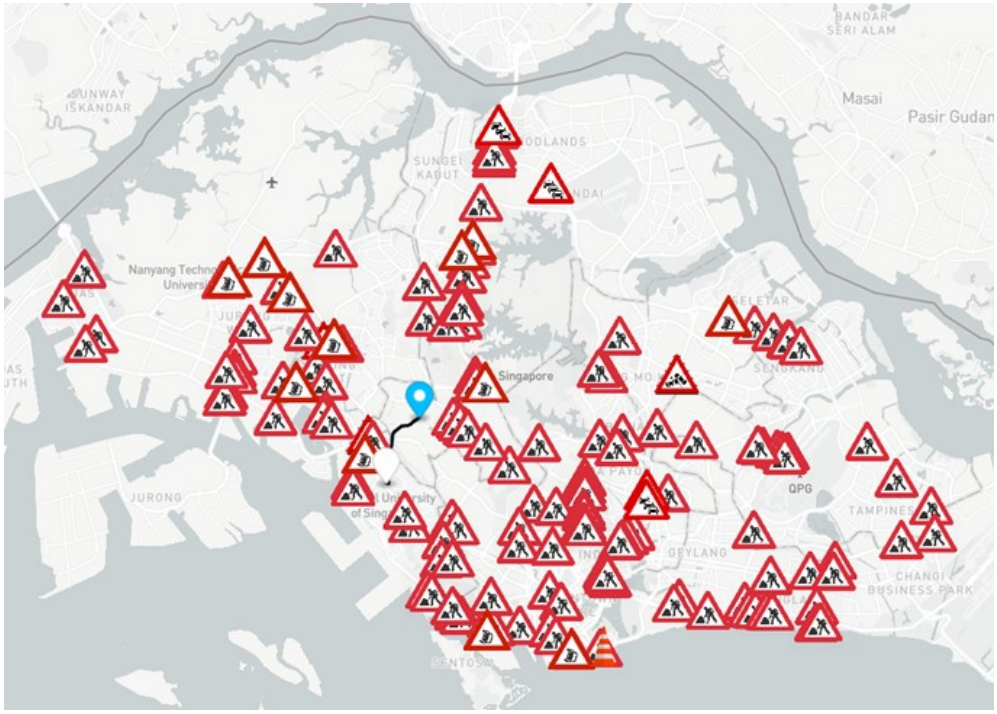


Figure 7.6: Traffic Routing agent determines the shortest path avoiding obstacles such as road works to address traffic challenges.

thority's DataMall API, assesses the status of traffic incidents and instantiates this data into the knowledge graph. This enables the Traffic Routing agent to determine the shortest route between two points while avoiding obstacles such as road incidents, addressing traffic challenges for the city.

Mr Phua integrated his work with the Traffic Incident agent, developed by **Mr Xinyu SUN (Project Officer Intern, CARES)**. The agent retrieves data from Singapore Land Transport Authority's DataMall API, assesses the status of traffic incidents and instantiates this data into the knowledge graph. This enables the Traffic Routing agent to determine the shortest route between two points while avoiding obstacles such as road incidents, addressing traffic challenges for the city.

In King's Lynn, where data are readily and publicly available, Mr Phua integrated the Traffic Routing agent with insights such as flood depth level, location of user in distress, travelling time required and vehicle type into its routing calculations to demonstrate intelligent navigation around flooded areas. This also includes determining minimum rescue times under flooded road conditions. The Traffic Routing agent can further retrieve the location of critical infrastructure from the knowledge graph and calculate the reachable area from these locations, to determine the area and the share of population who are likely unreachable as shown in Figure 7.7, assisting in strategising emergency service coverage.

Mr Phua also developed a transportation network criticality analysis function to identify which roads should be prioritised for repair or kept clear from traffic due to flood waters, to foster flood resilience and post-disaster recovery.

Lastly, Mr Phua utilised the information instantiated by the OSM agent to generate isochrones from buildings with certain amenities, such as pharmacies, thereby enabling effective city planning.

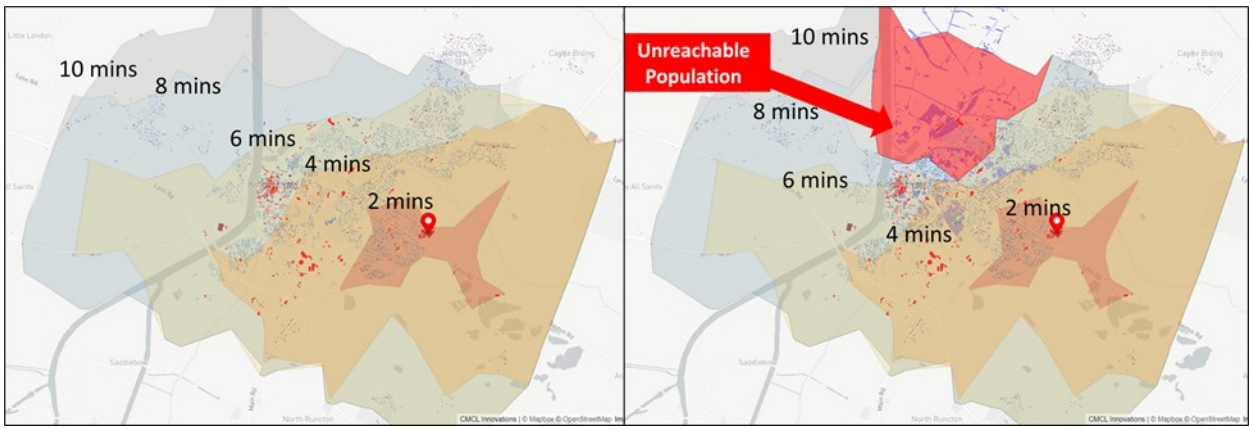


Figure 7.7: The Traffic Routing agent can create isochrone maps from hospitals. (Left) The isochrone maps in 2-minute intervals from Queen's Elizabeth Hospital during unflooded condition. (Right) The isochrone maps under flooded conditions and the unreachable population area outlined.

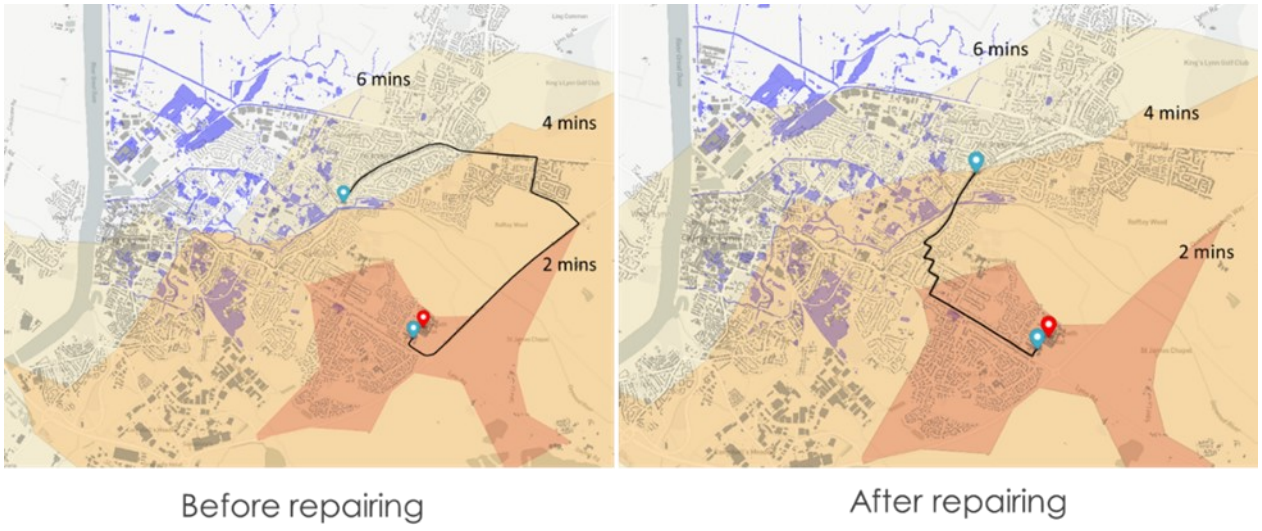


Figure 7.8: Transportation network criticality analysis: Before and after repairing the critical bridges – achieving more area of reach and shorter travelling time.

Update on work package 4

Developing interfaces and planning libraries for the CKG

Ms Shiying LI (Software Engineer, SEC) developed an interface to retrieve relevant information about all the plots within a search area, using the geospatial search functionality provided by Blazegraph as part of the Suitable Site Selector demonstrator. For each chosen plot, the centre of the plot is retrieved and used for creating the search boundary, which is described as a string containing coordinates of the bounding box. The search area is user-specified, and within each search area, the relevant information is retrieved and displayed in the comparison boxes to compare 'present' and 'future' scenarios.

Dr Jingya YAN (Research Fellow, CARES) developed two agents to link and instantiate geometric and non-geometric data related to building representations. The Data Integration agent uses spatial matching with data in Open Street Map to link building attributes such as building names and addresses to the 3D building geometries. The Building Linking agent then links the 3D building geometries, along with the names and addresses, to their non-geospatial attributes, such as building energy demands and solar potentials, using a fuzzy matching algorithm, which uses the building names and addresses as the common links between the two datasets. This process allows the 3D building data to be linked to various other datasets to provide a holistic overview of cities.

Dr Yan also processed the visualisation of the 3D building data in a web-based map tool, Mapbox, by extracting the building footprints and heights from the 3D building geometries. This process included considering buildings with clearly defined thematic surfaces as well as those without. The result of this process is shown in Figure 7.9 for the town of Pirmasens, Germany, where data are readily and publicly available.

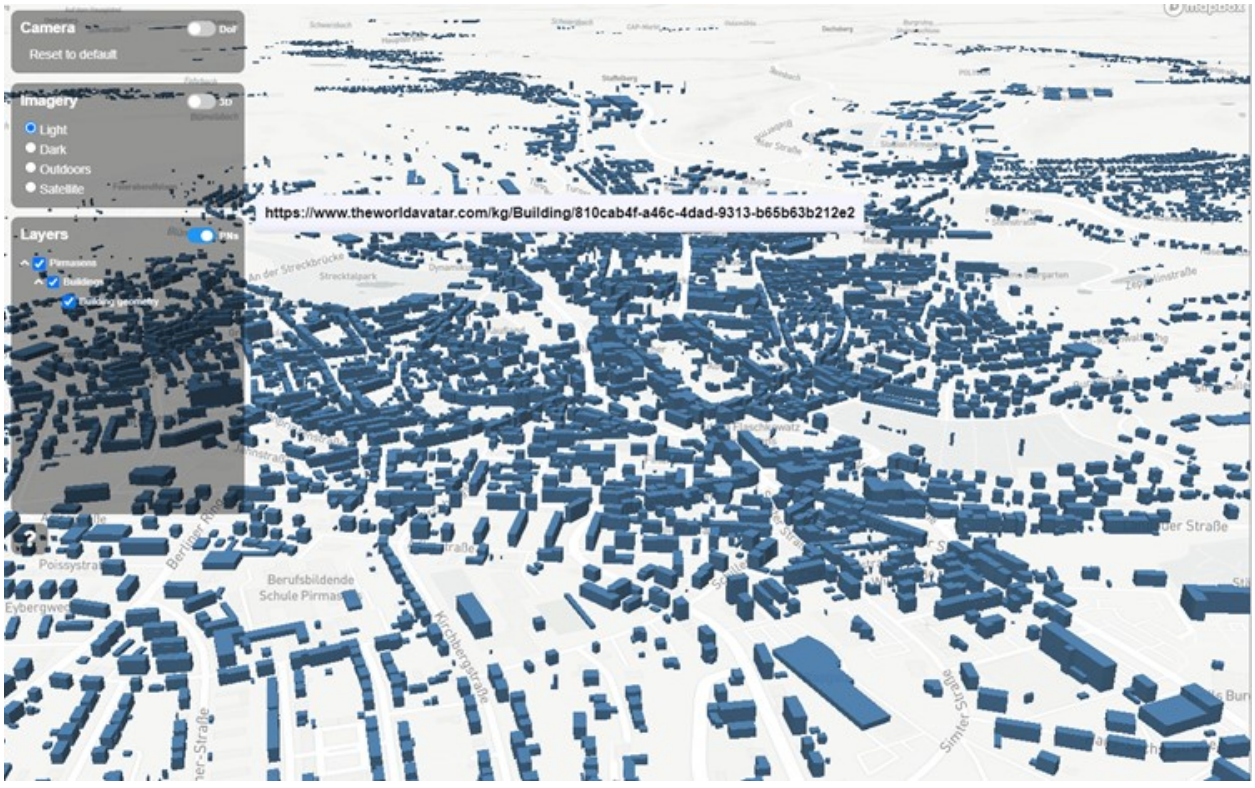


Figure 7.9: 3D building geometries in Pirmasens, Germany, visualised in Mapbox.

Update on work package 5

Developing Design Informatics Functions

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES), in collaboration with **Dr Pieter HERTHOGS (Senior Researcher, SEC)** and **Ms Shiying LI (Software Engineer, SEC)** developed a knowledge administration panel for CKG with the aim to provide an intuitive user interface to manage ontologies and rules of inference within dynamic geospatial knowledge graphs.

Mr Chadzynski and Dr Herthogs defined initial use cases and roles for the panel based on the system requirements determined from exchanges with the Urban Redevelopment Authority (URA). A high-level overview of the cases is presented in Figure 7.10. There are two expected roles within the application: Semantic City Planner and City Knowledge Manager. The Semantic City Planner has access to the knowledge stored within the CKG and can geolocate instances of concepts defined in ontologies that are part of it. The City Knowledge Manager can perform logical and empirical validation of the knowledge stored within the CKG, which includes operations such as checking for consistency, conciseness, adherence to standards and best practices as well as domain coverage, correctness, and answers to competency questions.

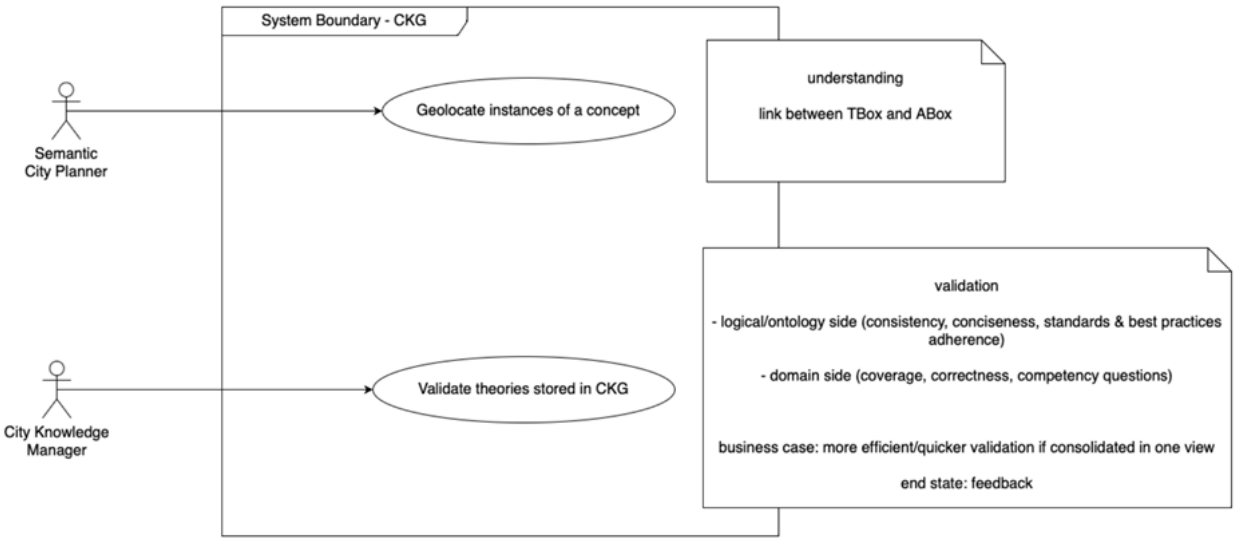


Figure 7.10: Use case diagram for the CKG web knowledge management panel.

Mr Chadzynski implemented and presented the set of capabilities necessary to support the first use case within WebProtégé. As illustrated in Figure 7.11, Mr Chadzynski extended the existing application to support concurrent knowledge management and geo-visualisation by multiple city planners accessing the same dynamic knowledge graph. He implemented a set of extensions to store ontology concepts in Resource Description Framework (RDF) stores. He also implemented capabilities allowing the application to support concurrent editing of the TBoxes stored this way to constitute fully dynamic knowledge graphs.

For the geo-visualisation, Mr Chadzynski annotated concepts with Internationalized Resource Identifiers (IRIs) that redirect to a Web Map Client showing instances of a particular concept on a map. To support this work and demonstrate using a Web Map Client, Ms Li extended the 3DCityDB-Web-Map-Client to accept IRIs corresponding to taxonomies stored within CKG. This development supports city planners in their daily work by allowing them to relate city planning knowledge to the geolocated objects presented on a map.

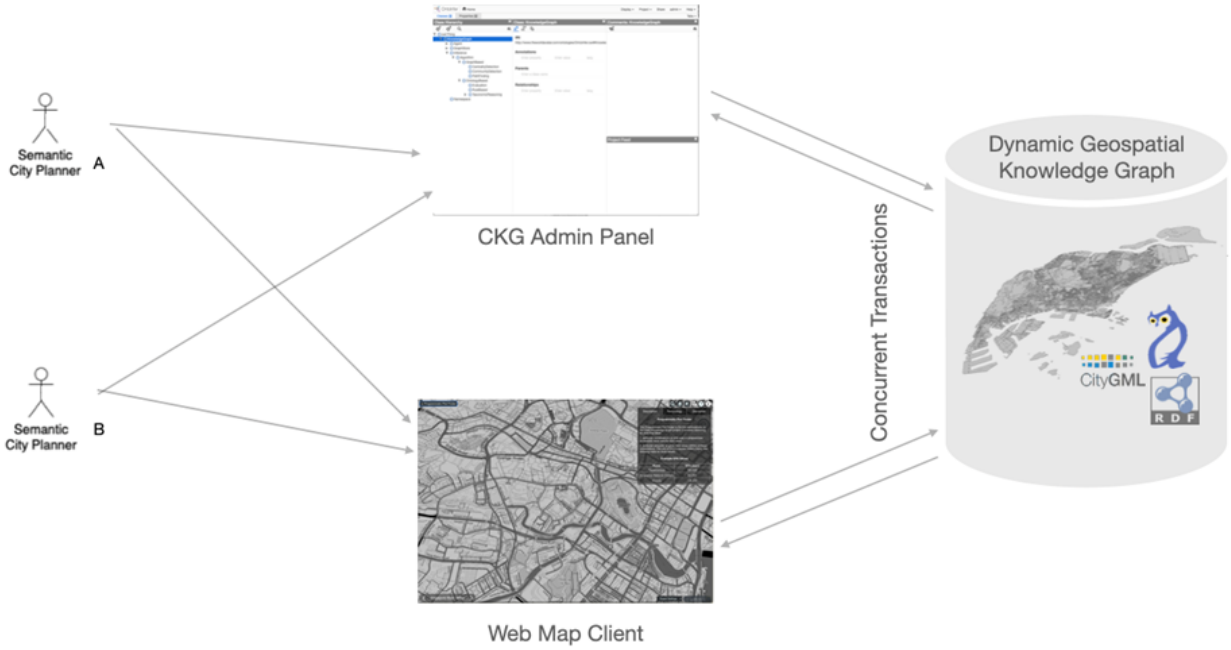


Figure 7.11: Overview of concurrent interactions between the knowledge administration panel, a Web Map Client and the Resource Description Framework (RDF) store.

Update on work package 6

Demonstrators: horizontal and vertical use cases

This work package aims at developing use cases showcasing horizontal (island-wide, strategic) and vertical (plot-based, built-form-related) planning synthesis support to demonstrate the potential applications and extensibility of the CKG approach. The demonstrators show how CKG supports three planning meta-practices: representation, evaluation, and projection.

The development of the first demonstrator, the Programmatic Plot Finder (PPF) (demonstrating Representation and Search), was led by **Dr Pieter HERTHOGS (Senior Researcher, SEC)** and developed by **Ms Shiying LI (Software Engineer, SEC)**, **Ms Ayda GRIŠIŪTĖ (PhD Researcher, ETH Zürich)** and **Ms Heidi SILVENNOINEN (Researcher, SEC)**, with inputs from the entire CKG team. The team continued to improve this demonstrator based on feedback from the Urban Redevelopment Authority (URA).

Dr Herthogs also led the development of the second demonstrator, the Suitable Site Selector (SSS), with the implementation done by Ms Li, Ms Grisiute, **Dr Andrea BARTOLINI (Postdoctoral Researcher, SEC), Dr Chenyi CAI (Researcher, SEC)** and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**. This demonstrator extends the PPF, enabling the user to compare multi-domain information and evaluations for up to five selected plots. The information design was driven by the need to integrate impact assessments to support site selection tasks, and the need to integrate agencies' strategies into the selection procedure. As such, the final design of the plot comparison panels differentiates between 'present' and 'future' data, computes deltas between the 'present' and 'future', provides land use statistics, and does this for both the selected plots and their immediate contexts. To allow for a fast user experience for the demonstrator, the team defined the default context as all plots within a 500 m distance, representing a '7.5-minute city' (similar to the '15-minute city' concept popular in contemporary urban planning) that can be computed with minimal delays.

Figure 7.12 illustrates the plot comparison panels for each selected plot. The users can select up to five plots and trigger the search engine. During the search, the centre of each chosen plot is retrieved from the knowledge graph and used for

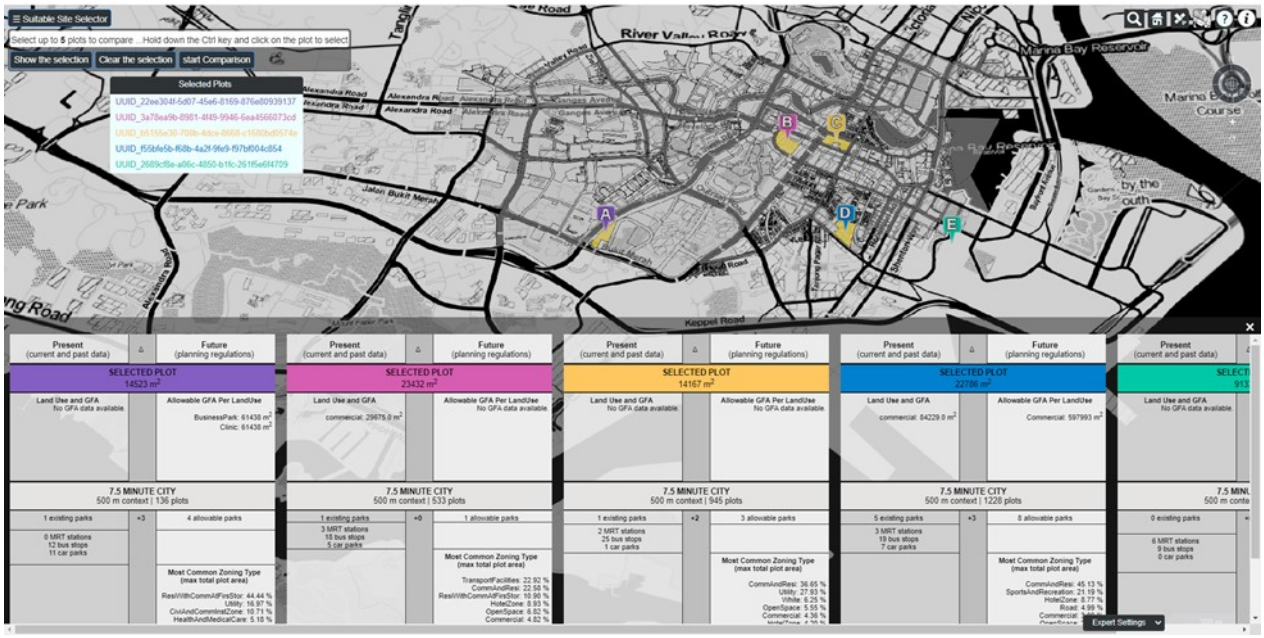
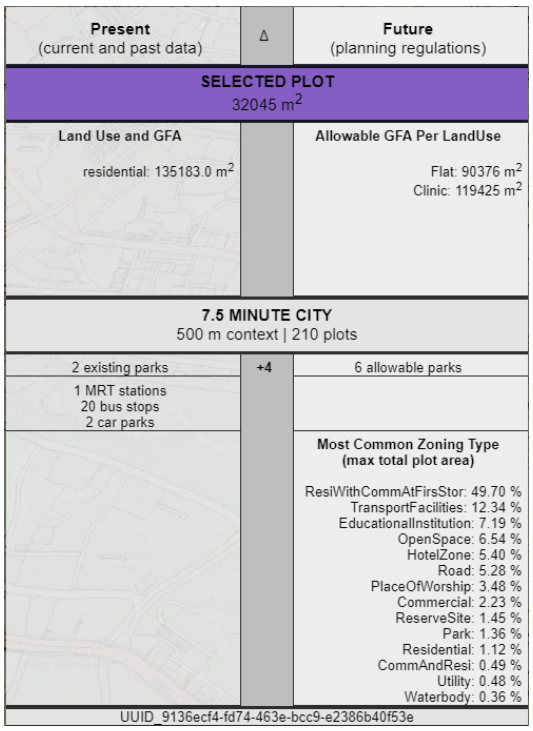
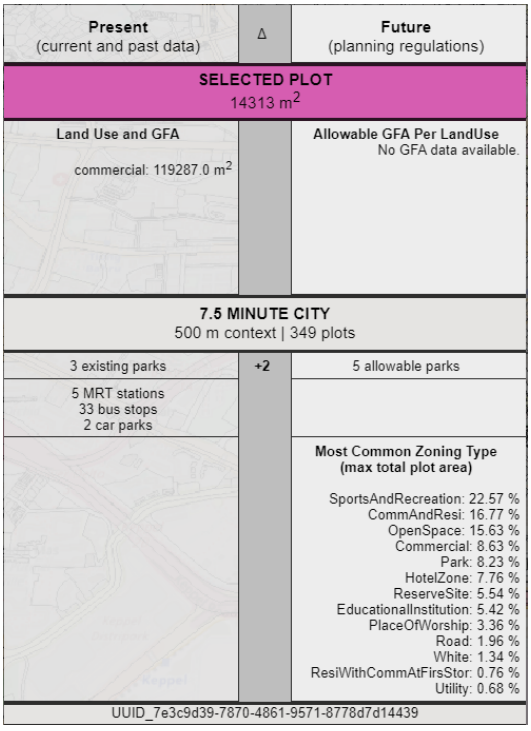


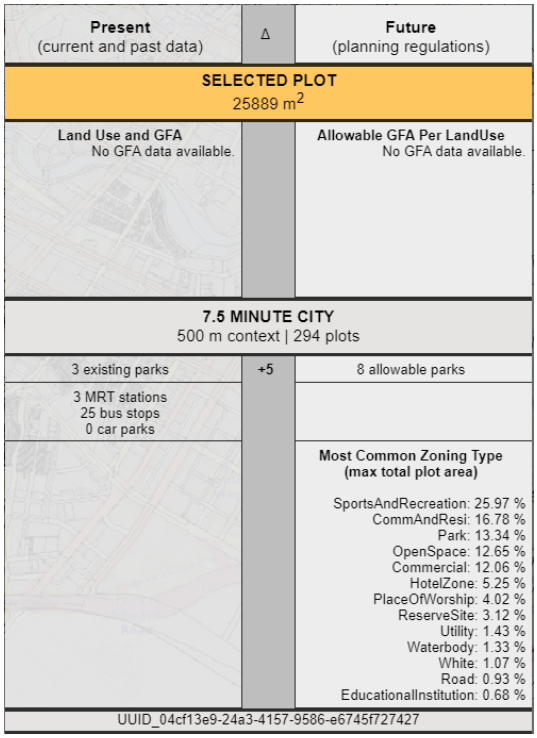
Figure 7.12: The Suitable Site Selector (SSS) demonstrator illustrating the plot comparison panels for five selected plots. See the enlarged coloured boxes on the next page.

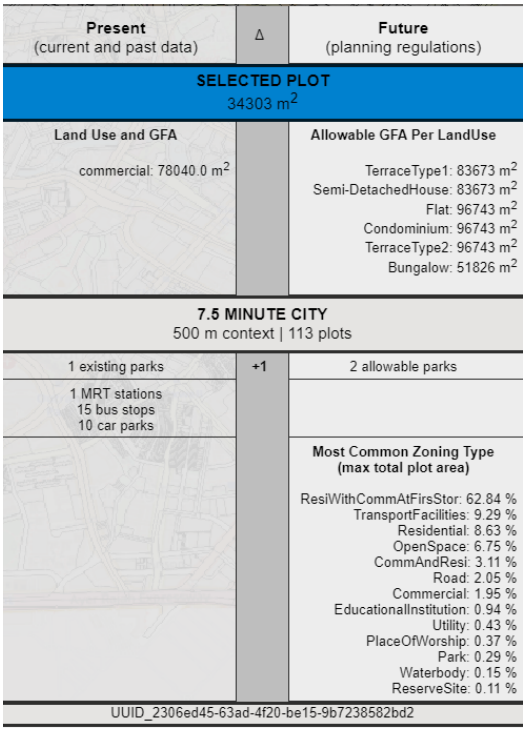
creating the search boundaries. Figure 7.13 illustrates a single information panel comparing the 'present' and 'future' scenarios. The top half of the panel displays allowed Gross Floor Area (GFA) values for different land uses that are part of the selected plot. The bottom half of the panel displays information about the plots within a 500 m distance representing the '7.5-minute city', such as the number of bus stops and the common zoning types in the search area.

For the development of this demonstrator, Ms Li implemented an interface that utilises the geospatial search functionality provided by Blazegraph, to retrieve required information within a given bounding box. As the comparative analyses require extensive database queries, Ms Li further optimised the query construction to improve the speed of the demonstrator.









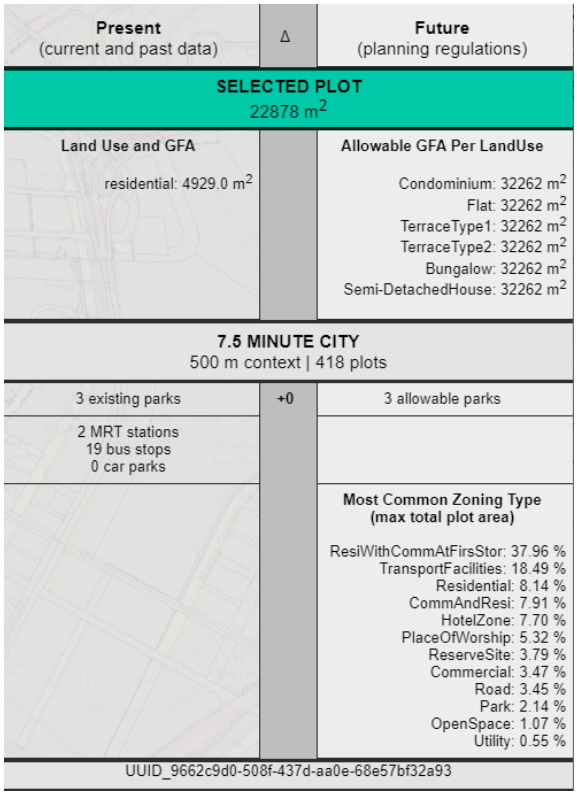


Figure 7.13: Comparison between 'present' and 'future' scenarios for the selected plot, as part of the Suitable Site Selector (SSS) demonstrator.

The SSS allows urban planners to retrieve multi-domain information using a knowledge graph and conduct comparative analyses, removing the need for extensive document checks and manual evaluations of each site according to different criteria. The knowledge graph improves the interoperability of data from different domains with various representations, allowing for complex cross-domain analyses.

As demonstrations of projective planning meta-practices, the team automated simulation tools and equations to estimate resource usage scenarios for current urban areas and future urban planning proposals.

Dr Bartolini investigated urban metabolism scenarios concerning the estimation of electricity and drinking water metabolisms (demands) of given plots of land in Singapore over a year, according to the 'present' and potential 'future' built environment. The 'future' built environment for a given plot is calculated based on the assumption that all the available buildable space is used for new developments, drawing on GFA estimates represented using the OntoBuildableSpace ontology.

To perform the metabolism estimation for a given plot, Dr Bartolini used different data sources such as information about the built environment within the plot (building GFA, number of residential units), information about the plot itself (assigned land use), and information about building energy consumption (declared energy use intensity) of the actual buildings within the plot. For the estimation of 'future' metabolisms, Dr Bartolini followed a similar approach, with the only differences being in the origin of the data sources: the GFA is computed according to calculations performed with OntoBuildableSpace, and the energy use intensity follows the distribution of typical intensities for the same type of building end-use. In both the 'present' and 'future' scenarios, the electricity and water metabolisms are computed using the consumption rate of the appropriate resource based on the size of the built environment within the plot expressed by its GFA. An example of the procedure applied to a sample plot is shown in Figure 7.14.

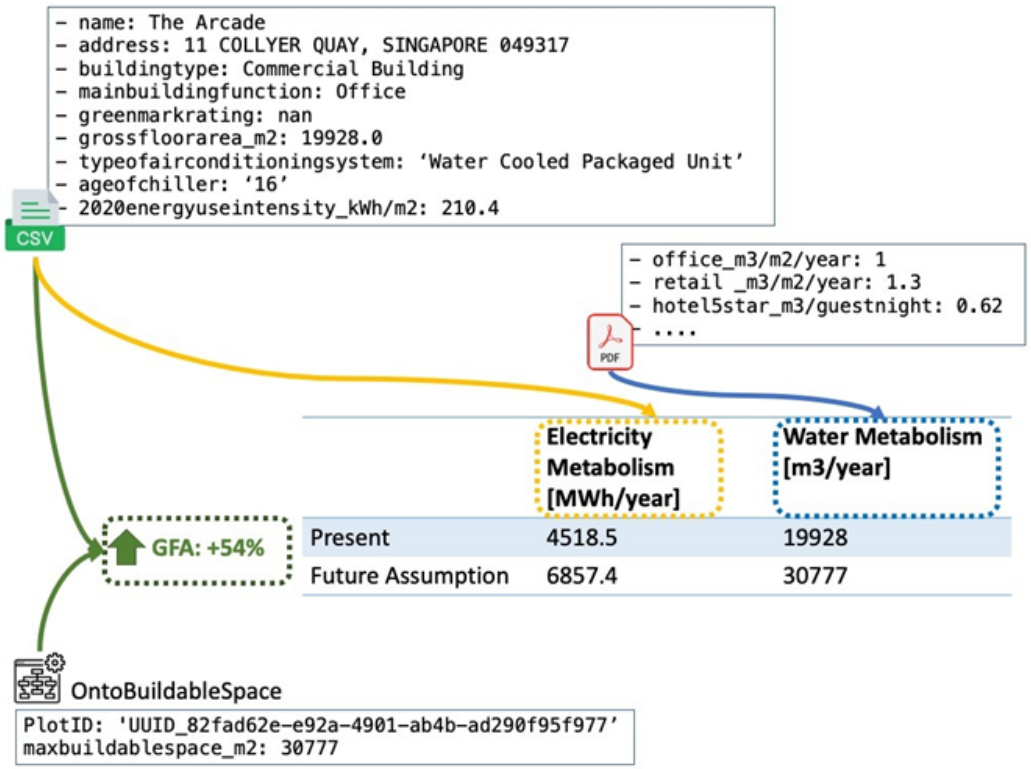


Figure 7.14: Example of estimation of urban metabolism in a plot. Data from different sources and results from other models are combined in computing urban metabolism in terms of electricity and water demand over a given plot.

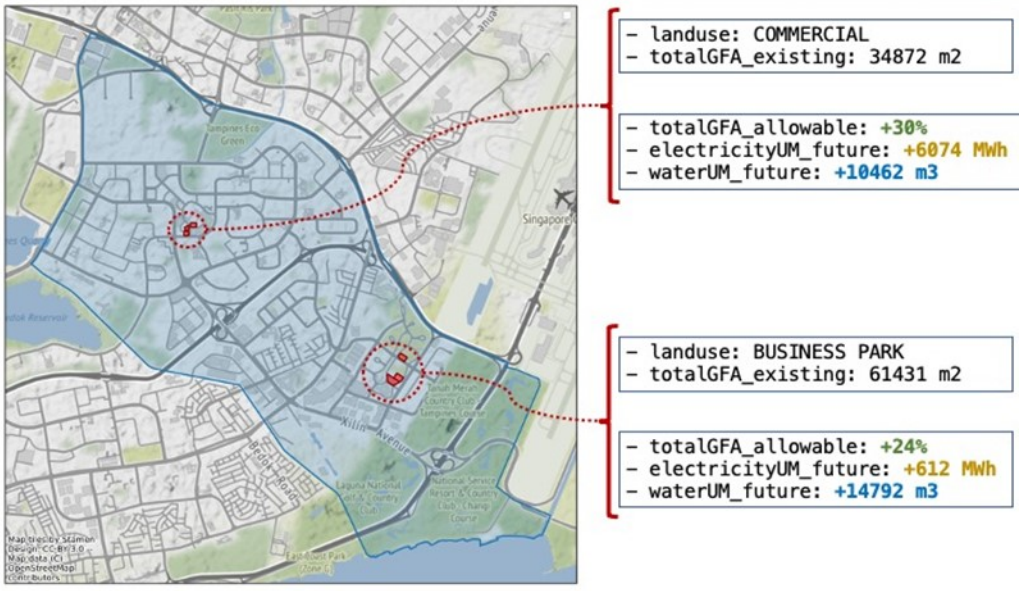


Figure 7.15: Extension of the urban metabolism estimation approach to larger areas. Plots in different areas with different assigned land uses, with projections in future metabolism following allowable buildable space.

Mr Yi-Kai TSAI (Software Developer, CARES) investigated the building energy demands and solar potentials of buildings at the Nanyang Technological University in Singapore using the City Energy Analyst (CEA) agent described in Work Package 3. Given a target building, the CEA agent queries for its geometry, its usage, the surrounding buildings' geometry, the historical weather data at the building's location and the terrain information around the building from the knowledge graph. The agent passes the various queried information to CEA to run the energy simulations and obtain the results, as displayed in Figure 7.16.

Figure 7.16: Building energy demands and solar potentials for the School of Physical and Mathematical Sciences in Nanyang Technological University, determined using the City Energy Analyst (CEA) agent.

Other activities and achievements

As part of the stakeholder engagement strategy, we have continued outreach activities towards academia, industries of urban project consultants and developers, and government agencies. In April and May 2023, officers from Singapore's Urban Redevelopment Authority (URA) internally reviewed, tested, and validated the three URA-specific ontologies developed by the project (OntoZoning, OntoPlanningRegulations, and OntoBuildableSpace) and the project's Programmatic Plot Finder application, a demonstrator of a regulatory search engine supporting site search tasks in city planning.

In May 2023, with support from the National Research Foundation (NRF) and the Smart Nation and Digital Government Office (SNDGO), the team organised a workshop for representatives from multiple government agencies to present the project and discuss how the CKG approaches and results could support agency use cases. We were joined by representatives from the SNDGO, NRF, the URA, the Ministry of National Development (MND), JTC Corporation, the Housing & Development Board (HDB), the Singapore Land Authority (SLA) and the Singapore University of Technology and Design (SUTD).

In September 2023, the team organised the hybrid CKG Completion Event, to celebrate the completion of the project, widely share its results, and allow attendees to try out various demonstrators. The event was hosted by **Prof Markus KRAFT (PI, CAM)**, **Dr Pieter HERTHOGS (Co-I, SEC)**, and **Dr Aurel VON RICHTHOFEN (Team Leader Cities, Arup Germany)**. A live demonstration of the Programmatic Plot Finder and Suitable Site Selector was performed by **Ms Shiying LI (Software Engineer, SEC)**, **Dr Andrea BARTOLINI (Postdoctoral Researcher, SEC)**, and **Dr Chenyi CAI (Researcher, SEC)**. In addition, various aspects of the World Avatar were demonstrated. **Mr Mingchuan TIAN (Software Developer, CARES)** showed a knowledge-graph-based digital twin of the Nanyang Technological University campus. **Mr Markus HOFMEISTER (PhD Student, CARES)** showed a representation of cross-domain data in King's Lynn. **Mr Shin Zert PHUA (Sofware Developer, CARES)** demonstrated a routing agent for disaster-resilient cities. **Mr Hou Yee QUEK (Research Associate, CARES)** and **Ms Sandra DENG (Software Developer, CARES)** demonstrated the augmented CARES laboratory. **Mr Dan TRAN (Software Developer, CARES)** and **Dr Aleksandar KONDINSKI (Research Fellow, CARES)** showed a question-answering system for chemistry. Dr Cai and Dr Herthogs, with inputs from Ms Li, Dr Bartolini and **Mr Genki UNNO (SEC Visiting Scholar, Takenaka Corporation)**, developed a final video for the CKG project, presenting a tangible overview of the project and its results.

The team also presented results from the project at several events over the last six months. In June 2023, Ms Li, Dr Bartolini, Dr Cai, and Mr Unno presented the project and its demonstrators to the Swiss National Council President and his delegation, during their visit to the Singapore-ETH Centre. In July 2023, Dr Bartolini presented the project during the CREATE Symposium as part of the information booth of SEC's Future Cities Laboratory (FCL) Global programme. Also in July 2023, **Ms Ayda GRIŠIŪTĖ (PhD Researcher, ETH Zürich)** presented a paper titled *'A Semantic Spatial Policy Model to Automatically Calculate Allowable Gross Floor Areas in Singapore'*, describing the initial workflow and preliminary allowable Gross Floor Area (GFA) results for Singapore's River Valley area at the Computer-aided Architectural Design (CAAD) Futures 2023 conference in Delft, The Netherlands. In September 2023, Ms Li and Dr Bartolini presented the project to a high-level delegation of Singapore's Land Transport Authority (LTA) visiting the Singapore-ETH Centre. Also in September 2023, Mr Unno presented his work on CKG in an FCL Global Seminar at SEC.

In September 2023, Dr Herthogs presented the project on the fourth day of the inaugural Urban Science Workshop Series, a week-long event series organised by the Centre for Liveable Cities (CLC). Ms Li, Dr Bartolini, and Dr Cai organised a hands-on demonstration session on the same

day. Mr Phua also presented his work on the Traffic Routing agent in the hands-on demonstration session.

Dr Bartolini's work on urban metabolism is accepted for presentation at the CLC's Science of Cities Symposium, part of the Urban Solutions and Sustainability R&D Congress 2023, organised by Singapore's MND, taking place in October 2023.

The team also engaged in various industrial networking events in the last six months. In June 2023, Mr Unno presented work on a thematic evaluation framework for Smart Circular City projects and visions at the New York - Livable Cities 2023 conference. In August 2023, Dr Herthogs and Mr Unno presented the project and Mr Unno's work to a delegation from Takenaka Corporation to discuss potential next steps.

Photos from the CKG Completion Event. (Top) From left to right are Dr Aurel von Richthofen, Dr Pieter Herthogs, and Prof Markus Kraft describing a dystopian future city – "Neotropolis" – saved by their knowledge graph technology. (Bottom) Attendees enjoying the interactive aspect of the demonstrators.

SMALL PROJECTS

OTHER CARES-FUNDED PROJECTS

In addition to C4T and CLIC, CARES hosts a number of other projects. These give our researchers an opportunity to explore new areas, develop technologies for commercialisation or build relationships with new industry partners or public sector collaborators.

The current CARES small projects include An Accelerated Manufacturing Platform for Engineered Nanomaterials (AMPLE) supported by the NRF Central Gap Fund, Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables (an Intra-CREATE seed collaboration grant), 'Digital Workflow and Continuous Processing in Pharmaceuticals', a member-specific project with Pfizer as part of the Pharmaceutical Innovation Programme Singapore (PIPS), and two further PIPS projects. CARES is now collaborating with the Singapore-ETH Centre on Cooling Singapore 2.0 and an update on this work is included.

These projects also provide a good opportunity for interns (such as Mr Hans GOH and Mr Seungjan CHA, pictured above working for AMPLE) to have a novel experience of research and technology development not easily available during their undergraduate degrees. This section also includes updates on the ten projects under the C4T Emerging Opportunities Fund, which was created to support exciting new ideas that have arisen since the start of C4T Phase 2.

An Accelerated Manufacturing Platform for Engineered Nanomaterials (AMPLE)

Central Gap Fund

AMPLE (An Accelerated Manufacturing Platform for Engineered Nanomaterials), a direct result of C4T's IRP1 research in WP1, began in June 2022. The S$6.5M funded project seeks to translate annular flow microreactor technology to 100 kg/day scale production, utilising machine learning and an agile product development methodology. By pushing the technology to a TRL7/8 level, the team will overcome the scale-up "gap" for industrialisation of new material technologies.

The key deliverables of Phase 1 (the first year) of AMPLE are 1) commissioning of the pilot plant in C4T's lab and 2) securing of industry partners for trials in Phase 2.

The period of April to September has seen a flurry of activity in AMPLE as the team, led by **Dr Nicholas JOSE (Project Lead, AMPLE)** and **Dr Mikhail KOVALEV (Product Development Manager, AMPLE)**, managed to reach their Phase

Figure 8.1: (Top left image) Showcasing of AMPLE and Accelerated Materials at TechConnect in Washington DC; (top right image) and the Advanced Materials Show in the US. (Bottom image) Finalised Pilot Room following completion of commissioning. From left to right: Dr Nicholas Jose, Dr Alvin Lim, Dr Susithra Lakshmanan, Ms Faye Ng, and Ms Kencha Satya

1 deliverables on time and pass towards Phase 2 of the project. In Phase 1 (ending June 2023), they successfully commissioned their 100 kg/day functional pilot facility within the C4T pilot lab. Working together with industry partners they created specifications for their new product family, ZARMOUR, a broadband nano-ZnO additive for antimicrobial and ultraviolet light protection, to be used in applications from air filtration to cosmetics.

AMPLE launched this at trade shows in the US and UK in June and garnered positive reception. As a result of their product and business development efforts, they have secured agreements with both local and MNC industrial partners to trial ZArmour at the multi-kilogram scale in Phase 2. Throughout June to September, they have been busy testing and upgrading the facility, and are currently serving sample requests from potential clients. For the next 6 months, they are focusing on experimental trials with the pilot facility and securing commercial agreements for the spinoff of an Accelerated Materials manufacturing facility in Singapore.

Other activities and achievements

Dr Nicholas JOSE (Project Lead, AMPLE) presented a poster entitled "Accelerating Autonomous Experimentation with Flab" at the 6th Machine Learning and AI in Bio(Chemical) Engineering Conference in Cambridge, UK from 6 – 7 July 2023. This presentation highlighted the group's work on automated laboratories and attracted potential partners for commercialisation.

AMPLE have secured a number of partnership agreements with industry collaborators following successful product development trials in AMPLE phase 1. These include:

- A Memorandum of Understanding with Corning AFR (CN/US) to jointly explore large-scale manufacturing expansion.
- A Research Collaboration Agreement with LivinWall (i.e., Gush Paints) (SG) to develop ZArmour formulations for interior paints.
- A Memorandum of Understanding with Kowa Company (SG/JP) to explore a distribution partnership for specialty nanomaterials supply.
- A Research Collaboration Agreement with Purafy (SG) to develop next-generation air filter media with ZArmour.

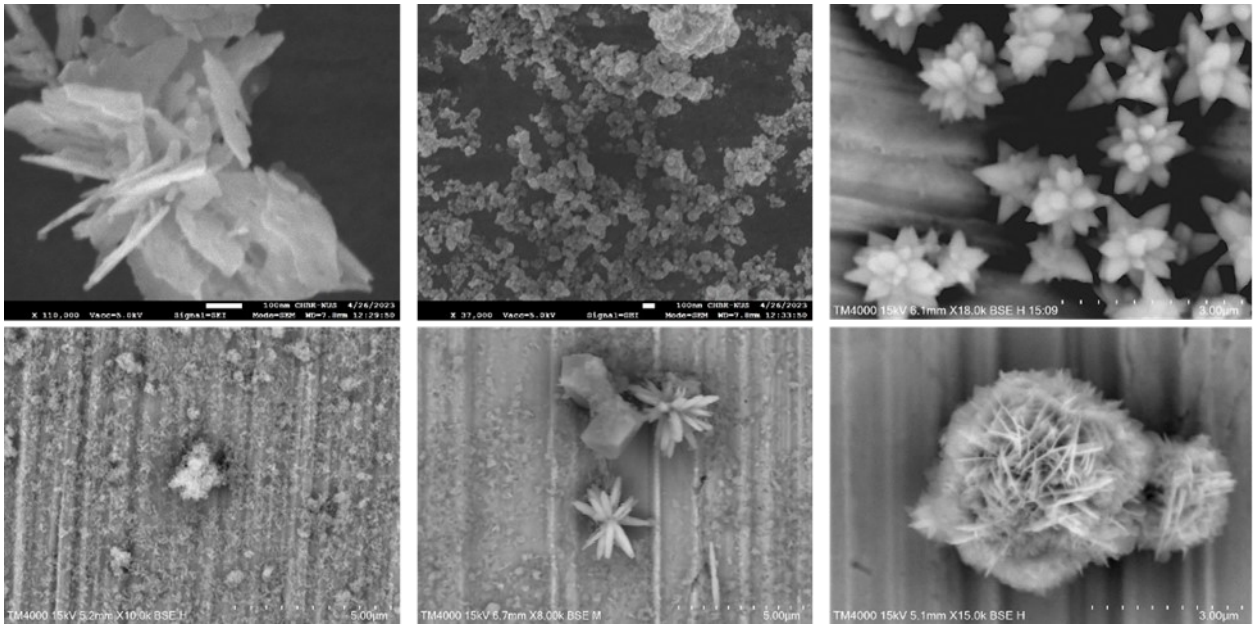


Figure 8.2: Various morphologies of nano zinc oxide formed during the product development trials.

Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables

Intra-CREATE seed collaboration grant

The project aims to develop an energy market framework that leverages the benefits of a dynamic knowledge graph for efficient peer-to-peer (P2P) energy trading between prosumers while satisfying the stable and secure operation of the distribution grid. This is an 18-month project that commenced in October 2022.

In this reporting period, **Dr Casper LINDBERG (PI, CARES)**, **Mr Mingchuan TIAN (Software Developer, CARES)**, and **Ms Qi ZHOU (Project Officer Intern, CARES)** have worked on ontology development, instantiation and agent development in the context of two test cases. The first test case aims to develop a digital twin of the NTU campus with 3D building data, building usage, solar photovoltaics (PVs), building load and voltage data, and details of the electrical network topology. The instantiated NTU test case currently includes historical load data for thirteen buildings, estimated solar PV placement and a hypothetical 15-bus power network topology. Agents can estimate solar generation in real time using live meteorological data and run Optimal Power Flow (OPF) calculations for the network. The second test case is based on a microgrid at the NTU Clean Energy Research Lab (CERL). The microgrid avoids the challenges associated with obtaining sufficient real building power consumption and network data and serves as the testbed for the P2P framework.

Mr Tian instantiated the NTU power network topology and specifications, historical power readings, solar panel specifications, and historical weather data. He also developed and refined agents such as the HistoricalNTUEnergyAgent (energy data instantiation), OpenMeteoAgent

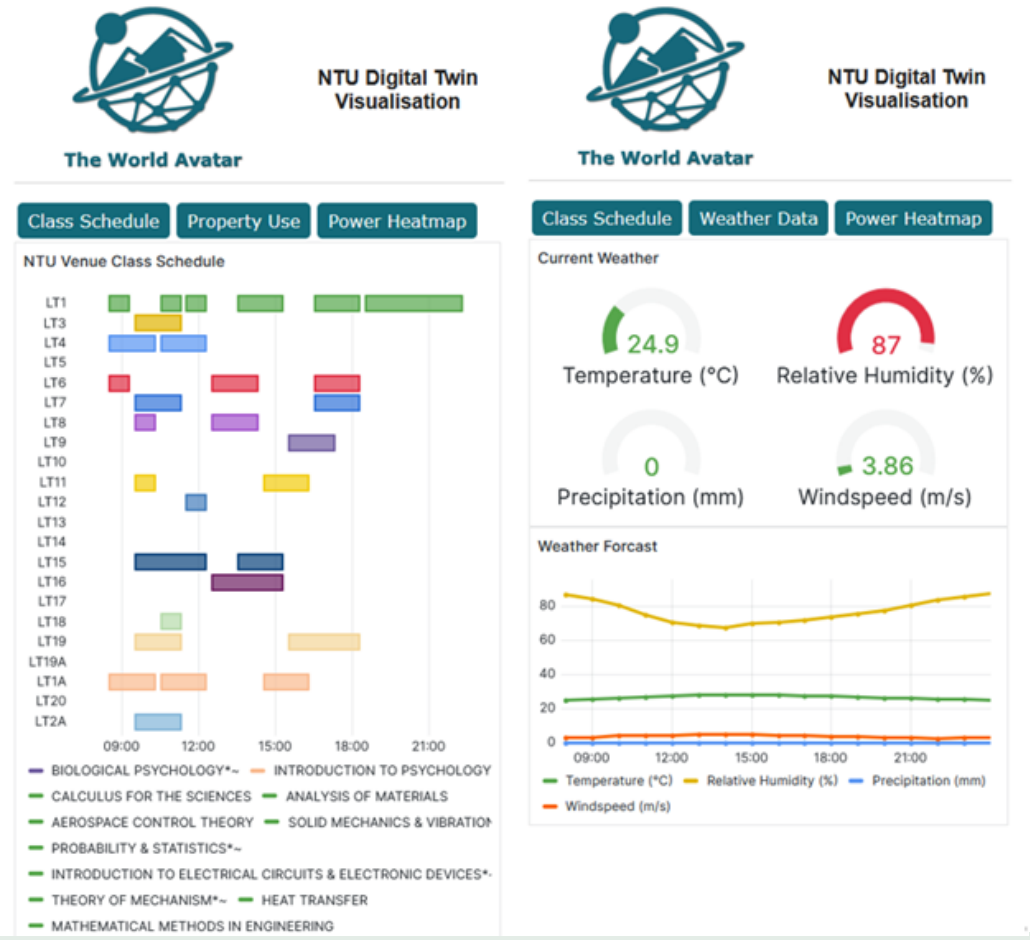


Figure 8.3: Dashboard visualisation of class schedules at NTU and weather data.

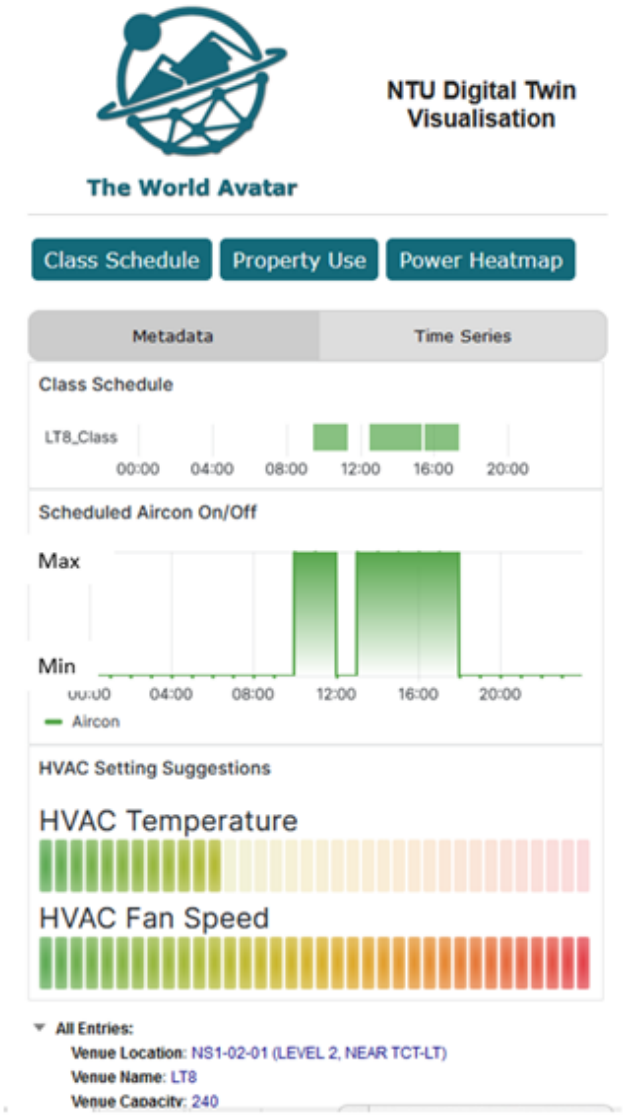


Figure 8.3 (cont'd): Dashboard visualisation of class schedules at NTU and weather data

(weather data instantiation), OPFAgent (OPF calculation), PVLibAgent (PV output calculation), and NNClusterAgent (neural network-based OPF prediction). Additionally, Mr Tian introduced a dynamic heatmap to the visualisation that reflects the building's voltage level based on data from the knowledge graph, facilitating system control and management. He further improved the user interface by integrating power branch topologies, employing distinct colour schemes to categorise building usages, and adding labels for individual building names. Mr Tian also retrieved the current semester's class schedule data from the NTU website, which (when integrated with the power system representation) can address energy challenges at NTU. A dashboard visualising this data and sample HVAC settings for energy savings (including scheduled air-conditioning period, optimal temperature settings, and fan speed) based on this data is displayed in Figure 8.3.

Ms Zhou completed the development of the OPFAgent by wrapping PYPOWER, a Python port of the MATPOWER package, as an agent to perform OPF calculations. The OPFAgent queries the knowledge graph for details of the electrical network, power load and solar generation, runs the power flow calculations and then updates the knowledge graph with the results of the calculations.

Ms Zhou also developed a SmartMeterAgent to retrieve microgrid smart meter readings from a database, process the data and update the associated time series instances in the knowledge graph. The processing step down samples the

data and filters out unwanted or invalid data (e.g., devices turned off or lost data). This completes the first step in combining the knowledge graph with the energy trading framework.

Dr Hung NGUYEN (PI, NTU) and **Dr Veerapandiyan VEERASAMY (Research Fellow, NTU)** set up the P2P energy trading framework in a hardware testbed consisting of the 0.4 kV microgrid at the NTU CERL and also implemented the framework in a Hardware-In-the-Loop (HIL) system using an OPAL-RT simulator. They carried out a simulation to create the solar PV and wind prosumers that participate in the trading. The P2P trading is implemented in a blockchain platform in order to secure the transactions among peers against adversarial attacks. Furthermore, an adaptive fractional-order-based recurrent neural network-based controller has been developed for the microgrid system to regulate the system frequency during P2P trading. The next stage will work on wrapping the prosumer and consumer framework as computational agents in the knowledge graph.

Dr Nguyen and Dr Veerasamy are currently analysing the knowledge graph-driven voltage stability of power systems through an artificial neural network (ANN)-based power flow. This is achieved by creating a bubble neural network to identify the feasibility of bus voltages that operate in either low-voltage, normal or high voltage regions. Based on the voltage profile from the ANN -based power flow and graphical location, they are developing a fuzzy clustering algorithm to identify the probability of a bus belonging to a particular region of clusters.

In the future, P2P trading will be enabled to trade the energy from the high voltage regions to low voltage regions to bring the system to the stable region. This will be tested with a microgrid setup at CERL and with the NTU test system.

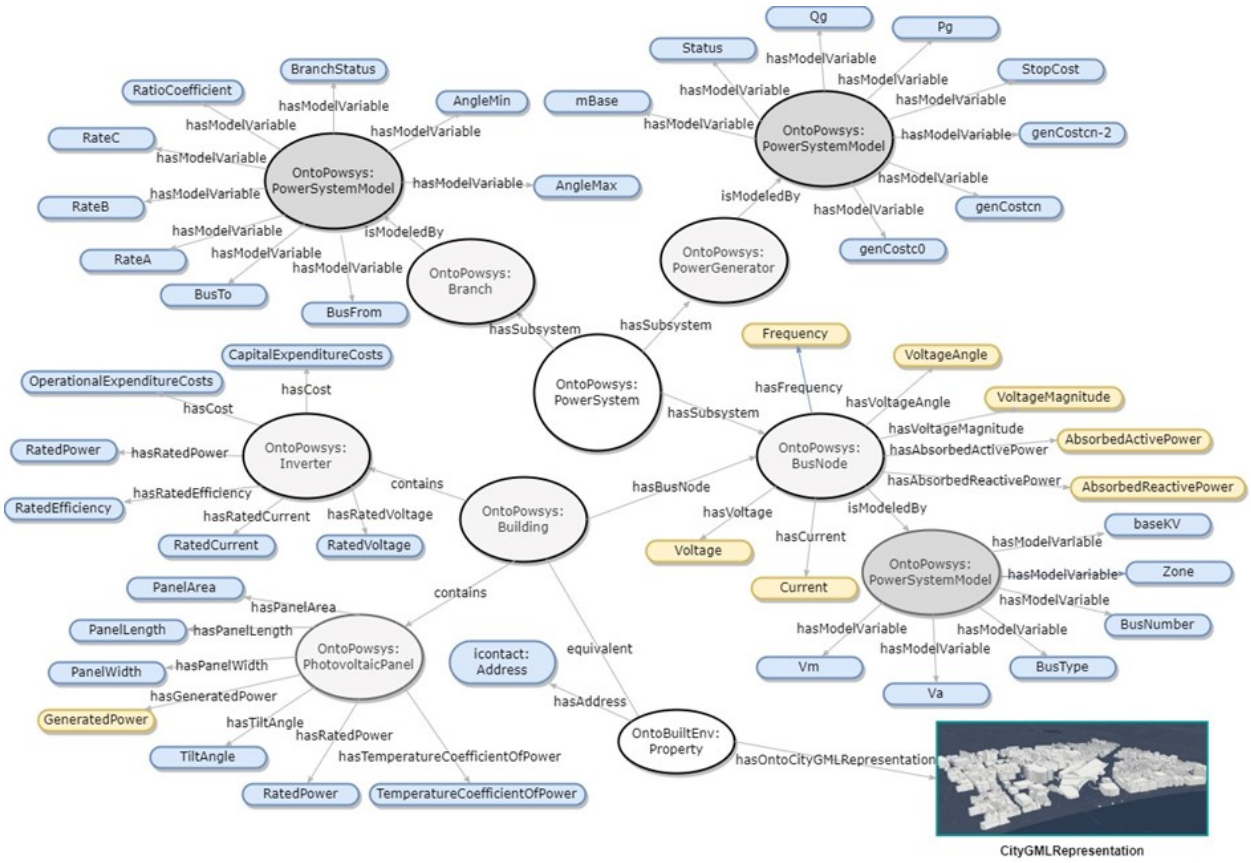


Figure 8.4: Power system ontology and link to building concepts and OntoCityGML representation. Yellow shading indicates quantities with time series representation.

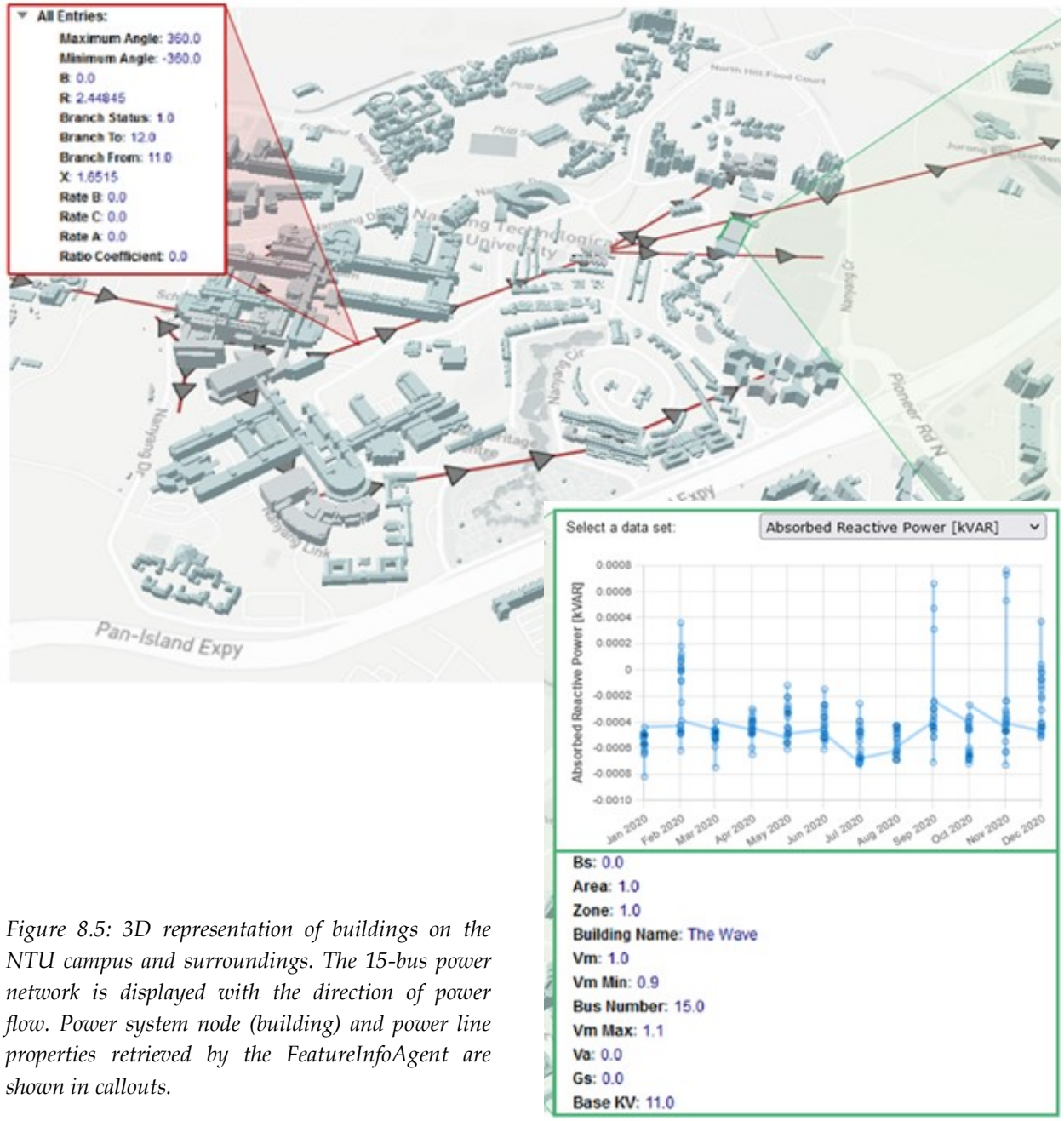


Figure 8.5: 3D representation of buildings on the NTU campus and surroundings. The 15-bus power network is displayed with the direction of power flow. Power system node (building) and power line properties retrieved by the FeatureInfoAgent are shown in callouts.

Digital Workflow and Continuous Processing in Pharmaceuticals Manufacturing

With funding from Pfizer as part of the Pharma Innovation Programme Singapore (PIPS)

Dr Dogancan KARAN (Research Fellow, CARES) is currently working on an industrially relevant multistep (2-step) process for the synthesis of an active pharmaceutical ingredient. The project involves developing automated continuously flow reactors and gaining process understanding via machine learning. In the last 6 months, he finished the development of the flow chemistry platform and machine learning workflow to gain a process understanding of Step 2 of the process. The flow chemistry platform allowed Dr Karan to precisely control the process parameters (temperature, residence time and stoichiometry) and enabled robust and reliable data collection to train a machine learning algorithm. A Bayesian multi-objective optimisation algorithm TSEMO (Thompson Sampling Efficient Multi-Objective Optimization) was used to optimise the process parameters and to build process knowledge. The algorithm successfully identified

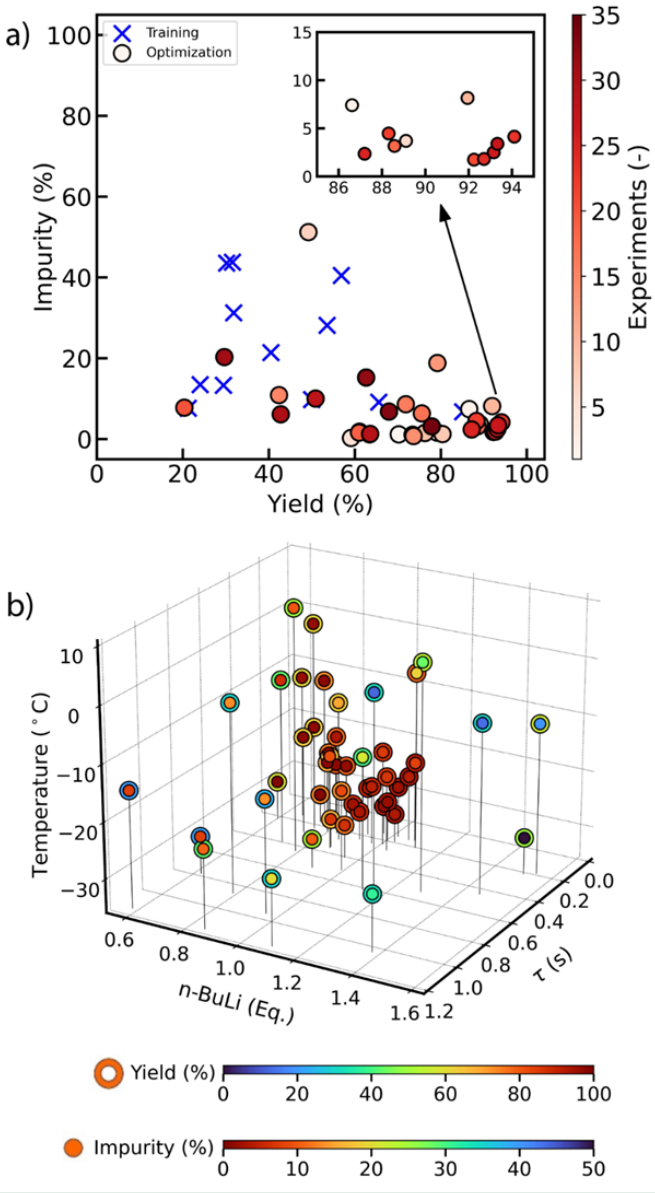


Figure 8.6: (a) Plot of yield vs impurity for experiments related to optimisation of Step 2. The initial training set experiments and optimisation experiments combine to form a Pareto plot to highlight the trade-off between the two objectives. The tip of the Pareto plot is magnified in the inset plot for visual clarity. (b) Plot of the experimental conditions executed during the optimisation with the reaction profiles. The shell color of each point denotes the yield (%) whereas the core color of each point denotes the impurity (%).

a set of optimal conditions corresponding to the trade-off between yield and impurity in different optimisation campaigns. The machine learning workflow has proven to be robust and data-efficient, revealing rich information about the reaction studied compared to single-objective, OFAT and DoE approaches.

Currently, Dr Karan is working on developing a novel machine learning algorithm for Step 1 of the process where catalyst deactivation occurs during the course of the reaction. New machine learning algorithms will allow us to learn the change in the catalyst state during the reaction and will result in better predictions than the conventional machine learning algorithms. Once the algorithm is established, the performance of the algorithm will be experimentally tested.

In addition, as a part of the project, a group of scientists from Pfizer came to Singapore for a technology transfer workshop. Dr. Karan presented all the details of the project to Pfizer, demonstrated how to apply machine learning workflows to optimise process parameters and gain process knowledge on various chemical systems, and answered questions. This workshop opened up various interesting ideas for potential future research collaborations.

Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes

With funding from Pharma Innovation Programme Singapore (PIPS), via A*STAR

Automated Evaluation of Environmental Impacts of Pharma Manufacturing Processes is a three-year project that started in July 2023 funded by the Pharma Innovation Programme (PIPS 2) programme and led by **Prof Alexei LAPKIN (CAM)**.

CARES has sub-contracted the research and development work on this project to its spin-off company Chemical Data Intelligence (CDI) Pte Ltd. CDI works with proprietary data, is set-up to productise software for application in the chemical industry, and hence is ideally positioned to deliver this project. The project has an ambitious target to create best-in-class solutions for rapid evaluation of environmental impacts in the complex setting of production of medicines. This work will combine data-driven modelling, first principles models, and hybrid models to create a predictive tool for life cycle impacts.

From Digital Twins to Real Time AI-supported Plant Operation

With funding from Pharma Innovation Programme Singapore (PIPS), via A*STAR

This project is funded under the Pharma Innovation Programme Singapore (PIPS) programme and led by **Prof Alexei LAPKIN (CAM)**, **Prof Markus KRAFT (CAM)**, and **Dr Lianlian JIANG (A*STAR)**. This is a 2-year project that commenced in July 2023 and aims to demonstrate a methodology of management and development of physical models-based digital twins for pharmaceutical process development, operation and management.

The first stage of this project focuses on a literature review of the process ontologies that could potentially align with the data, models, physical setup, and software intended for use in this project.

Mr Jiaru BAI (PhD student, CAM) and **Dr Jiyizhe ZHANG (Research Associate, CAM)** reviewed different sections of the OntoCAPE ontology, which is used to represent concepts in the

domain of Computer Aided Process Engineering (CAPE). Mr Bai investigated into three aspects of OntoCAPE: *ChemicalSpecies,* which reflects the intrinsic characteristics of species, *Material,* which is part of the phase system which describes macroscopic thermodynamic behaviour, and *MaterialAmount,* which refers to a concrete occurrence of an amount of matter in the physical world. Mr Bai also explored concepts in the areas of kinetic modelling, and laboratory automation.

Dr Zhang reviewed the OntoCAPE ontology in the context of phenomena-based modelling. Process models are usually generated based on multi -scale phenomena. The model structure and phenomena can be defined using the OntoCAPE *MathematicalModel* module. For real applications, models must be calibrated before use and need experiment information and data, which can be represented in the OntoCAPE *Material* module. Dr Zhang also reviewed related software and packages for ontology generation, model equation solving, and parameter estimation.

Dr Shuyuan ZHANG (Research Fellow, CARES) has been reviewing the ontologies related to continuous pharmaceutical reactors, such as an oscillatory baffled reactor, for constructing operable physical models. To optimise the model construction procedure, Dr Shuyuan Zhang is also investigating the *Python* and *Julia* packages for ontology reasoning, parameter estimation, and process simulation.

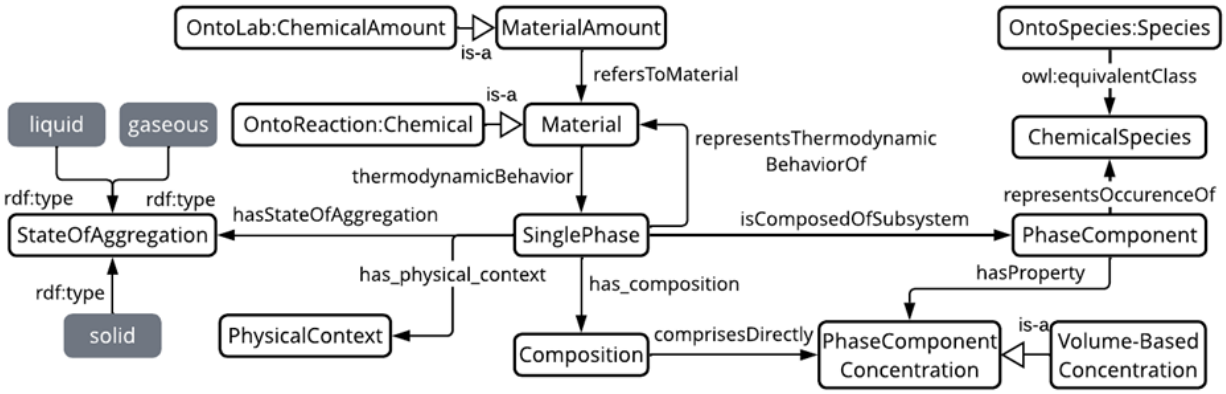


Figure 8.7: Concepts from OntoCAPE re-used for chemical representation in the World Avatar.

Cooling Singapore 2.0

In collaboration with the Singapore-ETH Centre

Cooling Singapore 2.0 aims to construct a Digital Urban Climate Twin (DUCT) for Singapore. This platform integrates several computational models (environmental, land surface, industrial, traffic, building and energy) and climate models to investigate ways to reduce Singapore's urban heat and mitigate its effects. In addition, the DUCT will allow researchers to trial various scenarios and predict their impact on urban heating.

CARES' contribution to Cooling Singapore 2.0 is to evaluate anthropogenic heat emissions from industrial activity in Jurong Island, Singapore, by developing computational energy models using the World Avatar (TWA) Knowledge Graph. The results of these models constitute the input for DUCT. CARES will also perform sensitivity analysis to investigate the impact of the anthropogenic heat emissions from industrial activity in Jurong Island on Singapore.

Dr Karthik NAGARAJAN (Software Developer, CARES) and **Dr Hansong XUE (Research Fellow, CARES)** collected information to estimate the heat emissions of Jurong Island companies. They estimated heat emissions using publicly available data on specific energy consumption, greenhouse gas emissions intensity, production capacity, electricity consumption, revenue, and number of employees. They then instantiated this data and the geospatial information of the associated physical structures in the knowledge graphs to calculate the locations and heights of the heat sources. They developed a Java program to retrieve this information and prepare the input file for DUCT.

The heights, locations and emissions of heat sources in Jurong Island are shown in Figure 8.8. The heat emission values, ranging from 2.6×10^{-3} to 5.1×10^{2} MW, reflect the diversity of chemical processes and variation in production volumes of the various chemical plants. Most of the heat sources are located in the East of Jurong Island, with relatively few emitting points in the Southwest. This is because most of Jurong Island's petrochemical plants are located in the East, and the Southeast part of Jurong Island is primarily reserved for logistics facilities without significant heat emissions. The heights of the heat sources range from 2 to 105 metres, reflecting the presence of both ground and stack flares. Ground flares typically emit heat 2-3 metres above ground level and are enclosed within a heat shield to protect people in the vicinity from high levels of radiation. On the other hand, stack flares have heights ranging from 10 to over 100 metres. Dr Nagarajan and Dr Xue have prepared a technical report to summarise their work.

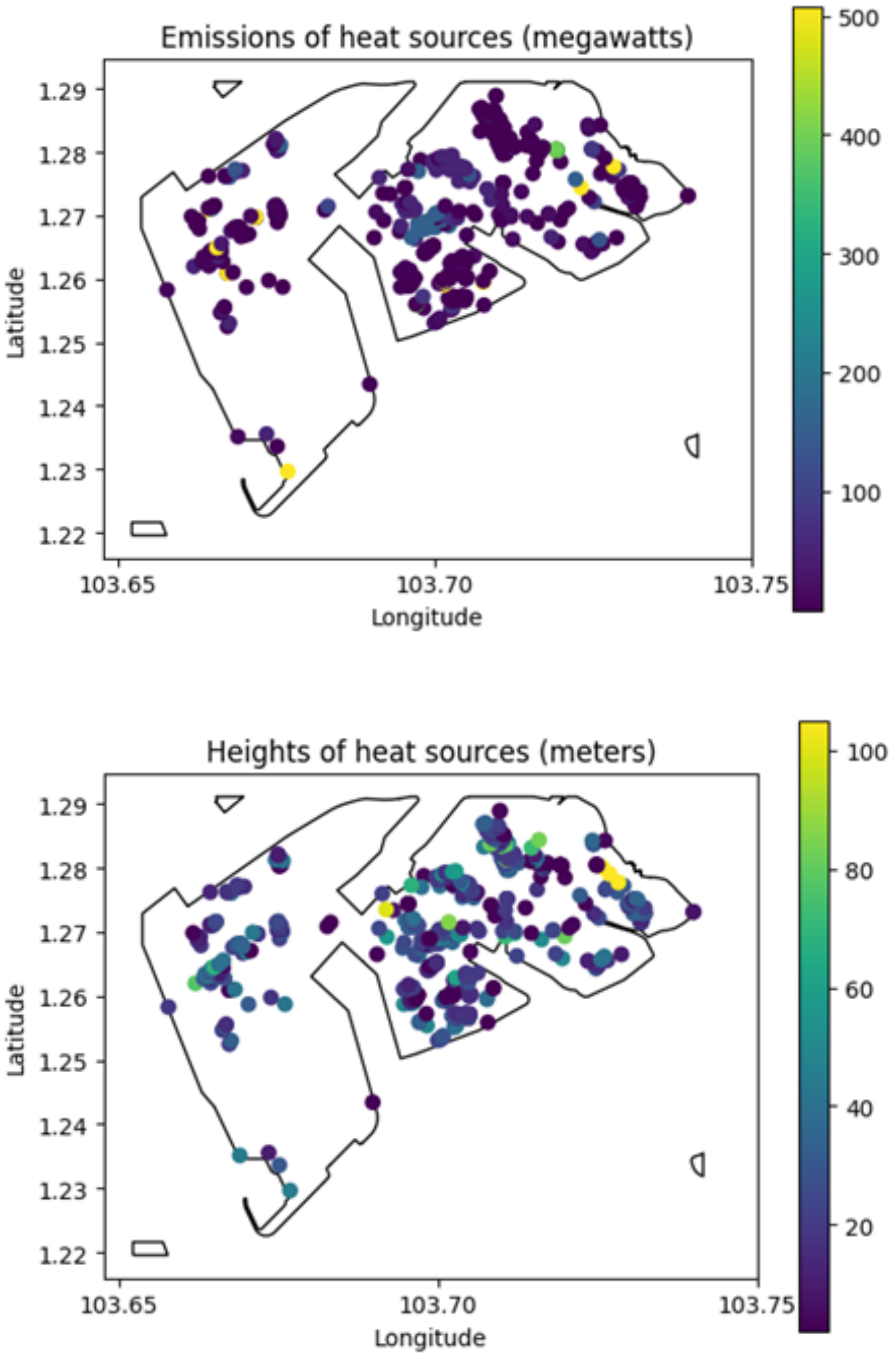


Figure 8.8: Spatial distribution of anthropogenic heat emission points and its sensible heat range in Jurong Island for the baseline case.

C4T Emerging Opportunities Fund

1) Brown carbon laser characterisation and light-absorbing property

Prof Markus KRAFT and Dr Yichen ZONG

The majority of this research was conducted in collaboration with researchers from the Department of Environmental Engineering at the National University of Singapore (NUS). The key findings have been published in *Atmospheric Environment X*. This paper investigates brown carbon (BrC) from engine combustion emissions and provides insights into how blending fuels impact the chemical and optical properties of both black carbon (BC) and BrC.

2) Chemical farming

Assoc Prof Ning YAN and Prof Alexei LAPKIN

The team led by **Assoc Prof Ning YAN (PI, NUS)** and **Prof Alexei LAPKIN (PI, CAM)** have studied the reaction mechanism of renewable organonitrogen compound formation and have submitted a paper with their results on the enhanced product yield using a fed batch operation. This paper has been accepted and published in the journal *ChemSusChem*.

3) Impact of Singapore's shipping activities on urban air quality

Prof Markus KRAFT and Ms Mei Qi LIM

This project aims to assess how emissions from shipping activities affect the air quality in Singapore while also showcasing the application of knowledge graph technology in a multi-domain context. The generation and dispersion of the pollutants is influenced by a highly diverse range of geospatial factors. Hence, the data required to simulate the dispersion of pollutants are highly heterogeneous, resulting in a demand for data interoperability.

Dr Kok Foong LEE (Software Developer, CARES) is currently working on integrating a dispersion model, AERMOD, into The World Avatar agent framework, jointly developed with IRP 4. The model estimates pollutant dispersion using data from different domains, including elevation, buildings, weather, and pollutant emission rates. This project demonstrates the knowledge graph's ability to link data from different domains and the power of intelligent agents to update the knowledge graph dynamically.

Dr Lee worked with **Dr Karthik NAGARAJAN (Software Developer, CARES)** on refining the integration of building data and elevations data into the knowledge graph and ensuring that the AERMOD agent can operate in any part of the world based on the provided inputs.

Dr Lee and Dr Nagarajan designed the visualisation to function separately from the AERMOD agent. They refined ontologies to ensure outputs from the AERMOD simulation can be properly marked up and queried by the visualisation independently. They based the visualisation framework on a web-based map tool, Mapbox. They also developed several additional features to enhance the visualisation experience, particularly the ability to swap the displayed layers based on a user-specified selection, including the simulation, pollutant type, and time step. Figure 8.9 shows the current state of the visualisation where users can select the simulation, pollutant, and time step via the dropdowns on the bottom left corner.

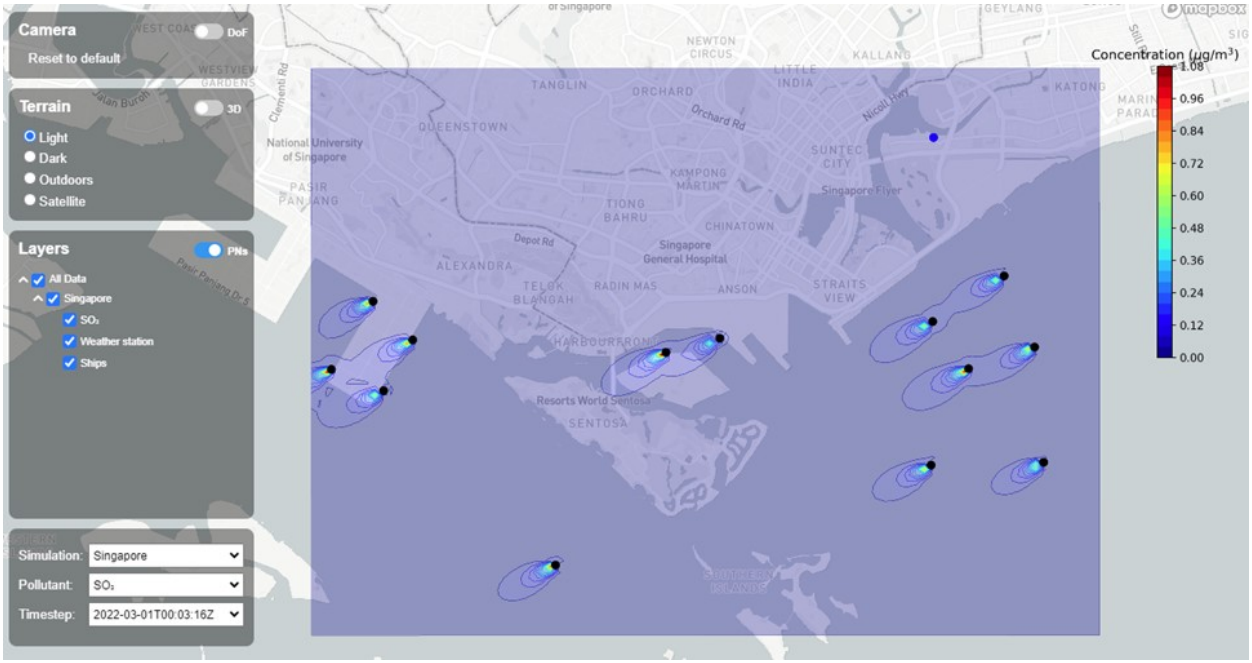


Figure 8.9: Dispersion of SO_2 emitted from ships around Singapore.

4) Ignition systems for natural gas engines

Prof Epaminondas MASTORAKOS and Dr B HARIKRISHNAN

Dr B HARIKRISHNAN (Research Fellow, CARES) has developed the solver dcmc-Converge, which combines the CFD solver Converge with 3D doubly conditional moment closure (DCMC), which is an advanced turbulent combustion closure. Large eddy simulations (LES) is chosen as the turbulence model. The researcher was testing the capabilities of the LES-DCMC solver with some canonical problems.

A constant volume lean-burn chamber (Figure 8.10) with CH_4/air mixture is taken as the problem for study. The pre-chamber (PC) has stoichiometric composition of $\phi = 1.0$, while the main chamber (MC) has a lean composition of $\phi = 0.5$. The initial pressure is 1 atm and the walls are adiabatic.

$$\frac{\partial Q_\alpha}{\partial t} + \underbrace{\nabla \cdot (Q_\alpha \langle \mathbf{u}|\eta,\zeta\rangle)}_{T_1} = \underbrace{Q_\alpha \nabla \cdot (\langle \mathbf{u}|\eta,\zeta\rangle)}_{T_2} - \underbrace{\frac{1}{\bar{\rho}\tilde{p}} \nabla \cdot (\bar{\rho}\tilde{p}\,[\langle \mathbf{u} Y_\alpha|\eta,\zeta\rangle - Q_\alpha \langle \mathbf{u}|\eta,\zeta\rangle])}_{T_3}$$

$$+ \underbrace{\frac{1}{\bar{\rho}\tilde{p}} \nabla \cdot (\bar{\rho}\tilde{p}\langle D\nabla Y_\alpha|\eta,\zeta\rangle)}_{T_4} + \underbrace{\langle N_\xi|\eta,\zeta\rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2}}_{T_5} + \underbrace{2\langle N_{\xi c}|\eta,\zeta\rangle \frac{\partial^2 Q_\alpha}{\partial \eta \partial \zeta}}_{T_6} + \underbrace{\langle N_c|\eta,\zeta\rangle \frac{\partial^2 Q_\alpha}{\partial \zeta^2}}_{T_7} + \underbrace{\langle \dot{\omega}_\alpha|\eta,\zeta\rangle}_{T_8} - \underbrace{\langle \dot{\omega}_c^*|\eta,\zeta\rangle \frac{\partial Q_\alpha}{\partial \zeta}}_{T_9}$$

[Eqs 1]

$$\frac{\partial Q_h}{\partial t} + \nabla \cdot (Q_h \langle \mathbf{u}|\eta,\zeta\rangle) = Q_h \nabla \cdot (\langle \mathbf{u}|\eta,\zeta\rangle) - \frac{1}{\bar{\rho}\tilde{p}} \nabla \cdot (\bar{\rho}\tilde{p}\,[\langle \mathbf{u}h|\eta,\zeta\rangle - Q_h \langle \mathbf{u}|\eta,\zeta\rangle])$$

$$+ \frac{1}{\bar{\rho}\tilde{p}} \nabla \cdot (\bar{\rho}\tilde{p}\langle a\nabla h|\eta,\zeta\rangle) + \langle N_\xi|\eta,\zeta\rangle \frac{\partial^2 Q_h}{\partial \eta^2} + 2\langle N_{\xi c}|\eta,\zeta\rangle \frac{\partial^2 Q_h}{\partial \eta \partial \zeta} + \langle N_c|\eta,\zeta\rangle \frac{\partial^2 Q_h}{\partial \zeta^2} - \langle \dot{\omega}_c^*|\eta,\zeta\rangle \frac{\partial Q_h}{\partial \zeta} + \langle \frac{1}{\rho}\frac{\partial p}{\partial t}|\eta,\zeta\rangle$$

[Eqs 2]

Equations 1 and 2 are the governing equations for the conditional scalars in the conserved space. Figure 8.11 elucidates the flame initiation from PC to MC. Figure 8.12 shows the contour plot of temperature in $\eta - \zeta$ space at the DCMC cell located in the main chamber and at time t = 1.5 ms. Also, it includes the contour plots of temperature, mixture fraction, and velocity magnitude in the physical space at the same time step. A series of such plots at every time step and at every DCMC cell location gives interesting insights into the influence of different terms in the Eqs [1] and [2], and how it interacts with the flow field. For instance, the effect of a high scalar dissipation rate of mixture fraction near the nozzle exit can be visualised in both conserved space and physical space giving deep insight into the flame structure.

As a next phase, the researcher will work on applying the solver to dual fuel marine engines with various alternate fuels/fuel blends, such as ammonia, methanol, methane, etc., and will study their combustion and emission characteristics. In parallel, efforts will be taken to enable the adaptive mesh refinement (AMR) capabilities on CFD and DCMC sides.

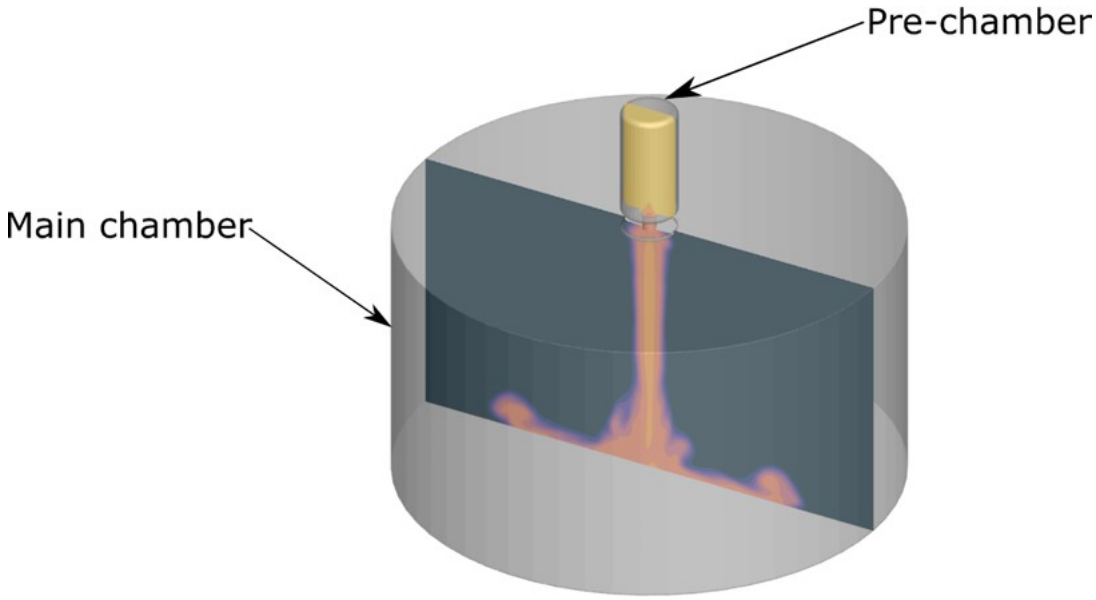


Figure 8.10: Geometry of the constant volume chamber.

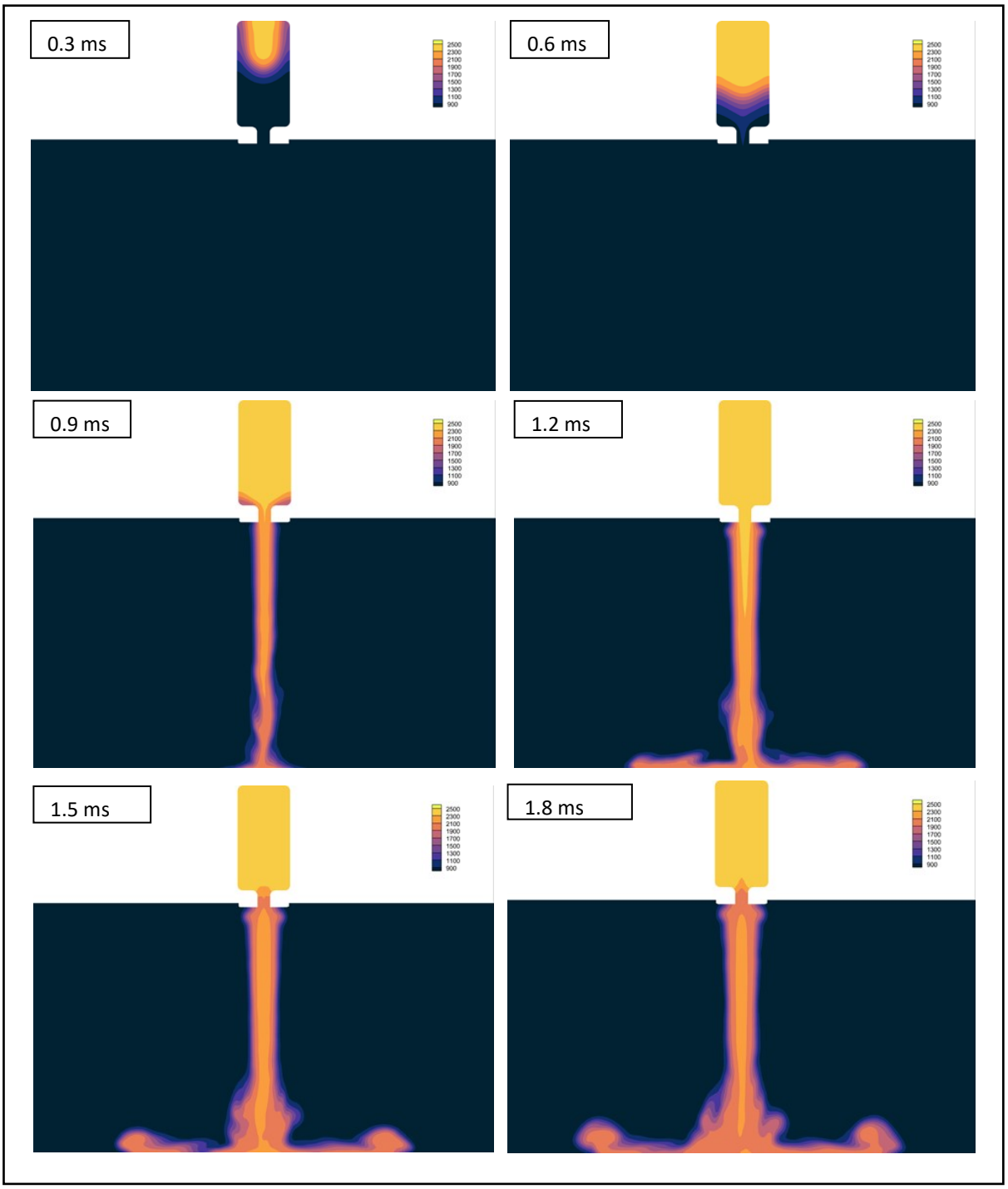
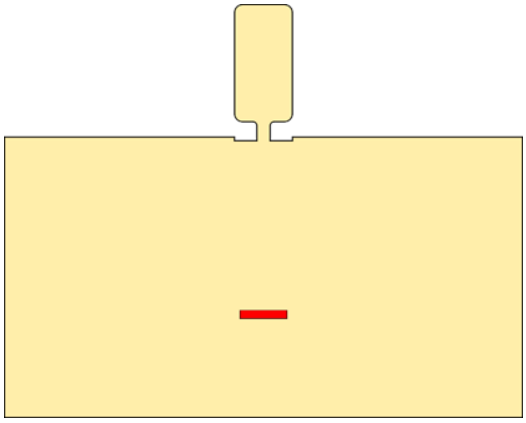
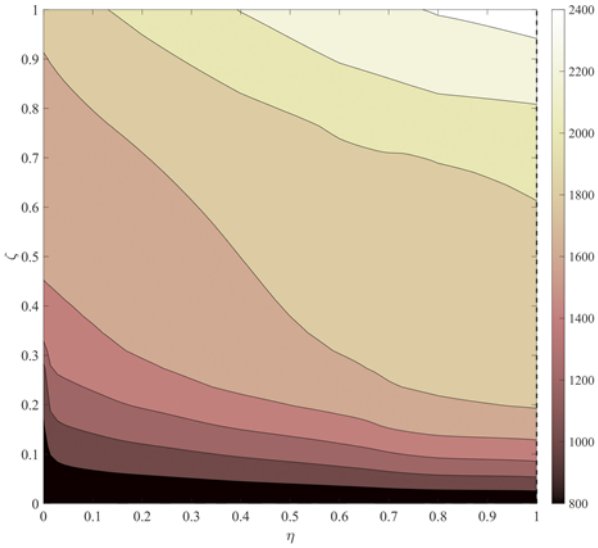


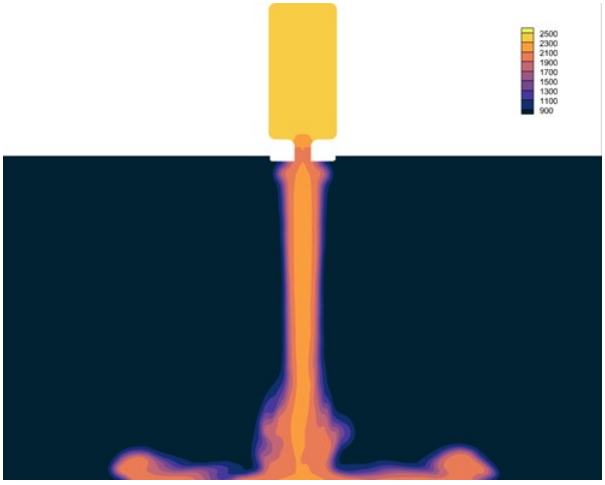
Figure 8.11: Snapshots of evolution of the temperature field from 0.3ms to 1.8ms.



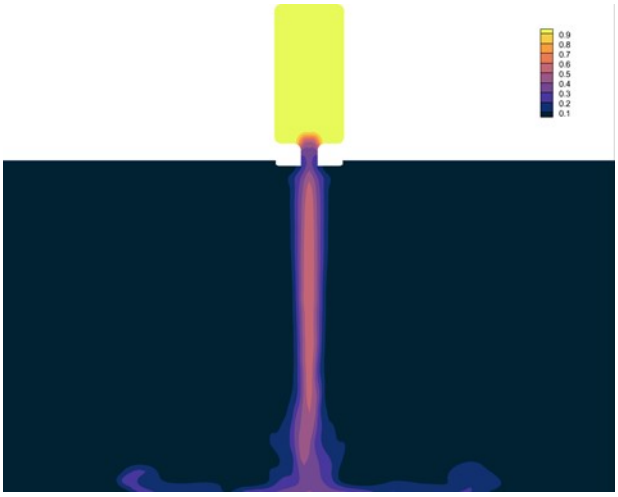
a) Position of the DCMC cell



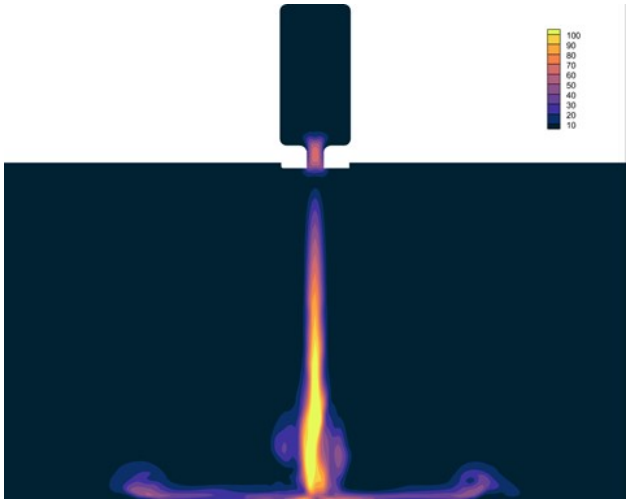
b) Temperature contour in the $\eta - \zeta$ space



c) Temperature contour in the physical space



d) Mixture fraction contour in the physical space



e) Velocity magnitude contour in the physical space

Figure 8.12: Contours in the conserved scalar space and the physical space at time 1.5 ms.

5) Future marine economy

Prof Epaminondas MASTORAKOS, Prof Steve EVANS and Dr Li Chin LAW

This project was initiated with the aim of addressing the gaps in marine fuel assessment by consistently and systematically quantifying the lifecycle energy, cost, and greenhouse gas emissions associated with a range of low-carbon alternatives. In the subsequent phase, the analysis expanded to include ship design factors when powered by these alternative fuels. To facilitate the dissemination of these valuable findings, the project has developed the https://www.lowcarbonship.com website, serving as a hub for sharing the extensive outcomes of the study and to aid in decision-making. Three papers related to this research have been published in *Energies* and *Energy Reports.*

6) Carbon reduction strategies of top chemical companies

Prof S. VISWANATHAN, Dr Abhiruchi GADGIL

Dr Abhiruchi GADGIL (Research Fellow, NTU) and **Prof S. VISWANATHAN (PI, NTU)** have analysed the Oil and Gas sector and have a manuscript ready titled "Decarbonization in the Oil and Gas sector". They will be submitting it soon to a journal. The paper reviews different technology-related strategies that the firms in the oil and gas sector are claiming to employ currently and, the ones they are aiming to, in the future, according to their sustainability reports. In the paper, this data is also assessed against actions by the sector so far towards decarbonisation.

7) Decarbonisation of Singapore by 2050

Asst Prof Paul LIU and Prof Markus KRAFT

Dr Hui Ling TAN (Research Fellow, NTU) has prepared a manuscript discussing the various decarbonisation scenarios (e.g. CCSU-centric, green hydrogen-centric, green electron-centric, biofuel-centric, etc). The manuscript is currently at the final stage of review by the PIs.

8) Reaction Pathways of Formic Acid Conversion

Asst Prof Tej CHOKSI, Asst Prof Paul LIU and Dr Ari FISCHER

The group continues development of a rigorous kinetic model for formic acid decomposition on low-dimensional titanium boride films supported on Pd. The group considered > 10+ active site motifs and used first-principles methods to evaluate the reaction pathways for formic acid dehydrogenation to hydrogen on this dynamically changing catalyst. These reaction pathways were reconciled with experimental findings from **Asst Prof Paul LIU's (PI, NTU)** group. Such findings reveal how the structure of active sites influences the reaction mechanism and rate, providing vital insights into catalyst design. Finally, the group developed a workflow to evaluate the performance of next-generation chemical reactors that use triggers beyond temperature gradients to drive chemical reactions. Focussing on sonochemical reactors, the group developed multiscale models to quantify the yield of free radicals and understand the sensitivity of this free radical yield to a multitude of operating variables.

9) Electrified Chemical Production

Prof Jason Zhichuan XU and Prof Adrian FISHER

Dr Yubo CHEN (past-Research Fellow, NTU) and **Dr Chencheng DAI (Research Fellow, NTU)** have been collaborating on applying the self-synthesised mesoporous IrO_xH_y catalyst in proton exchange membrane water electrolyser (PEMWE) for hydrogen production at current densities of ampere level. They synthesized BM-Ir_4+O_xH_y catalyst through the chemical leaching of Sr_4IrO_6 followed by ball milling. The BM-Ir_4+O_xH_y catalyst exhibits superior performance compared with the commercial Alfa Aesar IrO_xH_y, especially at high current density regions through the enhanced mass transport. To achieve a current density of 4A cm^2, the BM-Ir_4+O_xH_y PEMWE only requires a cell voltage of 1.833V. In addition, the long-term stability test suggests excellent stability at 1A cm^2 over 1000 hours. This invention developed an efficient and robust electrocatalyst for decentralised water electrolysis for industrial applications. The invention has been filed on 10 May 2023 and accorded Singapore provisional patent application number 10202301308V.

10) Electrolysis for renewable carbon utilisation

Prof Xin WANG

This research project has successfully completed.

ALL C4T PUBLICATIONS WITH CREATE ACKNOWLEDGEMENT

The following list includes all the C4T publications from the beginning of Phase 2 (November 2018). Those in bold are new for this reporting period. For a full record of Phase 1 publications (April 2013 – October 2018) please visit our Publications page on the CARES website: www.cares.cam.ac.uk/publications/

C4T joint IRP publications

IRP 1 and IRP 2

- **Li, Xiaogang, Wenjie Xu, Luan Q. Le, Shuangming Chen, Li Song, Tej S. Choksi, and Xin Wang. 2023. 'Sulfur-Modulated Isolated NiNx Sites toward Electrocatalytic Hydrogen Peroxide Generation'. Chem Catalysis, August, 100724. https://doi.org/10.1016/j.checat.2023.100724.**

IRP 1 and IRP 3

- **Hu, Xiaochun, Qianwenhao Fan, Mingwu Tan, Yuqing Luo, Xianyue Wu, Manoel Y. Manuputty, Jie Ding, et al. 2023. 'Investigating the Impact of Dynamic Structural Changes of Au/Rutile Catalysts on the Catalytic Activity of CO Oxidation'. Carbon Energy, September, e412. https://doi.org/10.1002/cey2.412.**

IRP 3 and IRP JPS

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IRP 3 and eCO_2EP

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