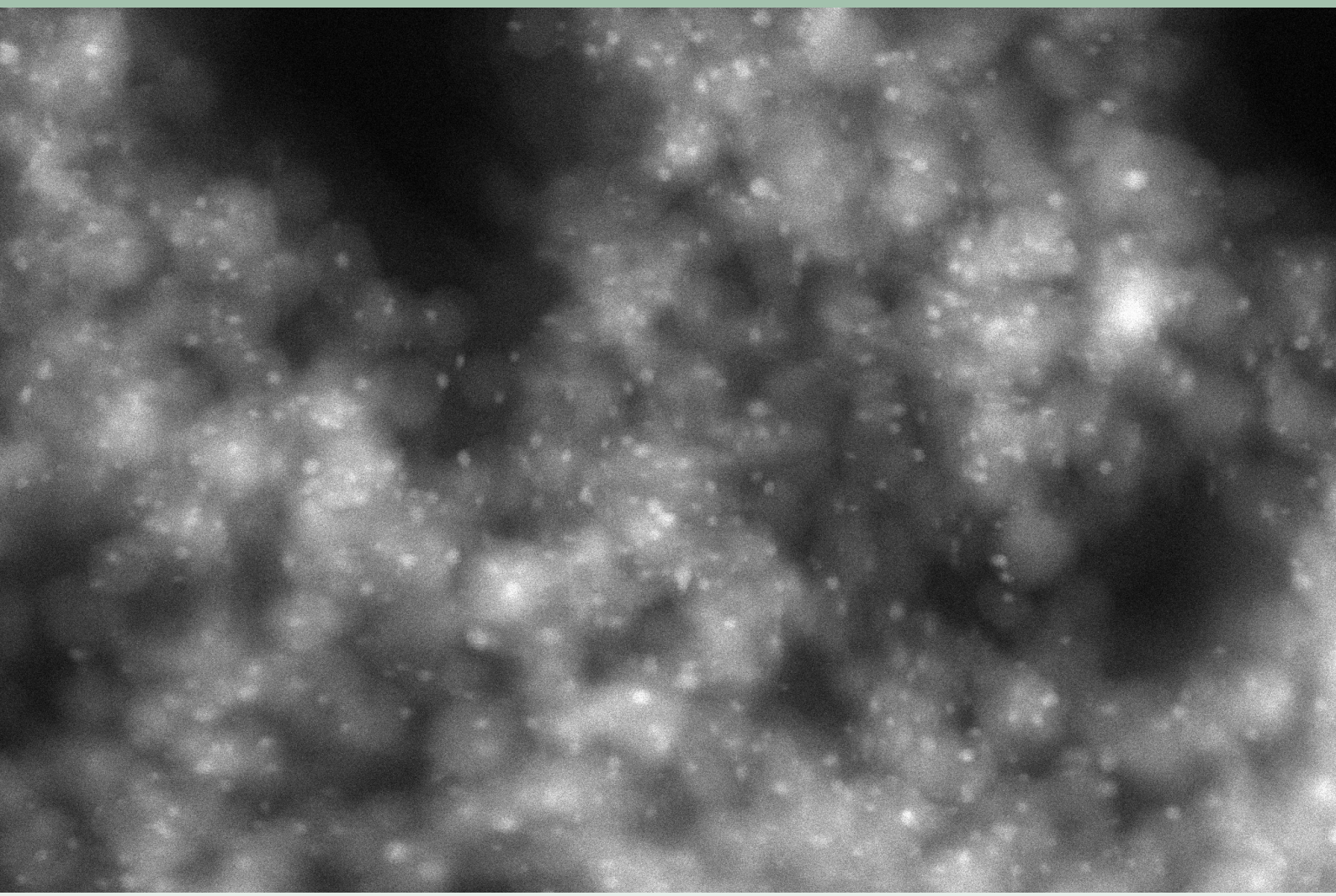
CAMBRIDGE **CARES**

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



Biannual Research Report

October 2021 - March 2022

CAMBRIDGE
CARES

CAMBRIDGE CENTRE
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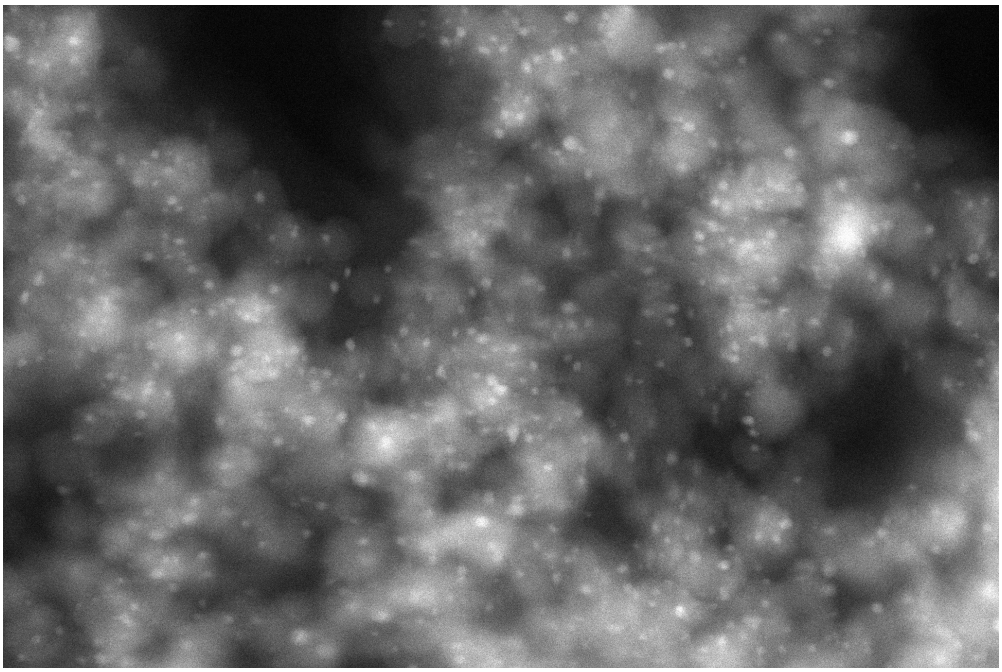
Cover image



TEM images (dark field) of Pt-decorated TiO_2 nanoparticles prepared from the one-step flame synthesis.

Image by Dr Manoel MANUPUTTY (Research Fellow, IRP 3). *See more on page 59.*

Note on the photographs in this report: Many of the photographs of CARES researchers were taken prior to the pandemic and therefore show researchers unmasked. CARES researchers currently comply fully with local guidance for safe working, including mask wearing.

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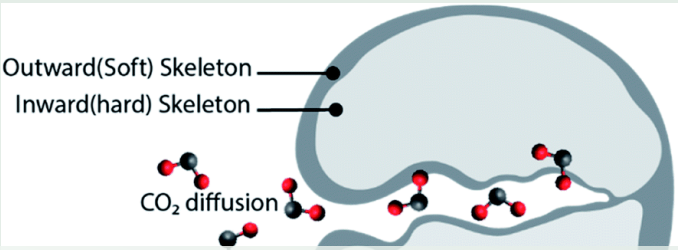
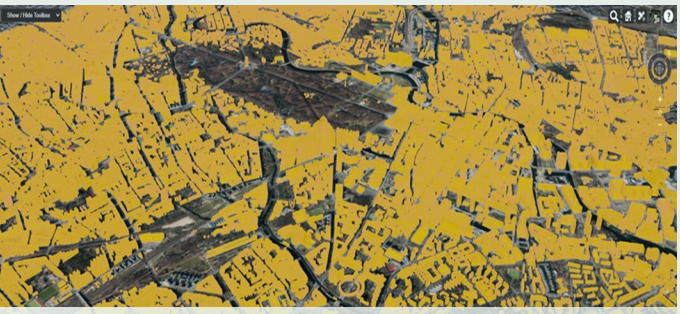
8
Focus on Fundamental Science



12
Scientific Highlights



23
Programme Updates

148
Publications

Contents

Highlights

Programme Updates

Facts and Figures

FOREWORD

I am very pleased to present the 16th Biannual Research Report for the Cambridge Centre for Advanced Research and Education in Singapore (CARES). In contrast to the past two years, we are starting to see strong signs of recovery from the pandemic which has been invigorating. The last few months have seen a gradual return to workplace arrangements and in-person events at CARES. The ease in travel restrictions has also allowed our researchers to start presenting at in-person conferences and made international hiring practical again, both of which help us to increase our international visibility and collaborations across all the programmes.

CLOSING PROJECTS

Two of our smaller projects recently completed in March 2022. Despite happening entirely during the pandemic, the Intra-CREATE seed-funded project "Consumer Energy Usage Data in Smart City Development" (CEUS) was able to deliver some important groundwork on use of intelligent systems in the consumer energy field and helped to further build up our valued collaboration with the Singapore-ETH Centre (SEC). CARES also supported Judge Business School (University of Cambridge) in establishing a South-East Asia hub of the Cambridge Alternative Finance Collaboration Network (CAFCN). The project has put CARES in an excellent position to support similar Cambridge efforts in South-East Asia in the future. Looking forward, 2022 will also see the completion of the first two Pharmaceutical Innovation Programme Singapore (PIPS) projects hosted by CARES. We are excited by the promising results from these projects and our colleagues in the PIPS office at A*STAR have recently announced the launch of the PIPS 2 funding stream that we are already having productive discussions on.

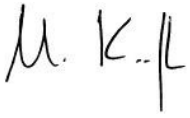
CLIC SCIENTIFIC ADVISORY COMMITTEE

In December 2021, our CLIC programme (Centre for Lifelong Learning and Individualised Cognition) had its first progress meeting with its independent and international Scientific Advisory Committee. I am delighted to report that the Committee commended the programme's early progress and particularly noted the innovative adjustments made by the team to continue human subjects research during the extraordinary challenges of the pandemic. The CLIC team are now preparing for their first phase assessment meeting and funding renewal decision in late 2022/early 2023.

RINGS SPIN-OFF INTO AMPLE

We will soon be starting a new project "An accelerated, manufacturing platform for engineered nanomaterials" (AMPLE) that materialised from the impactful results of "Rapid Industrialization of Next Generation Materials" (supported by the SMART Innovation Centre Innovate Grant). AMPLE will aim to create a market-ready technology platform for the rapid, scalable and cost-effective manufacture of nanomaterial technologies, which will then be made commercially available via a spin-off company in Singapore.

I hope I have encouraged you to read more about CARES' latest work and achievements in this report. As ever, please do get in touch if you would like to know more about our work or have ideas for collaboration.



Professor Markus Kraft, CARES Director
March 2022

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 integrate materials design and selection (i.e. for adsorbents and catalysts) with advances in process design to achieve improved selectivity and conversion. Such improvements will provide a reduced carbon footprint and energy demand for both established and new processes. Lowering the cost of CO_2 capture, and technologies and strategies for waste heat utilisation are also underlying drivers in the research. 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.

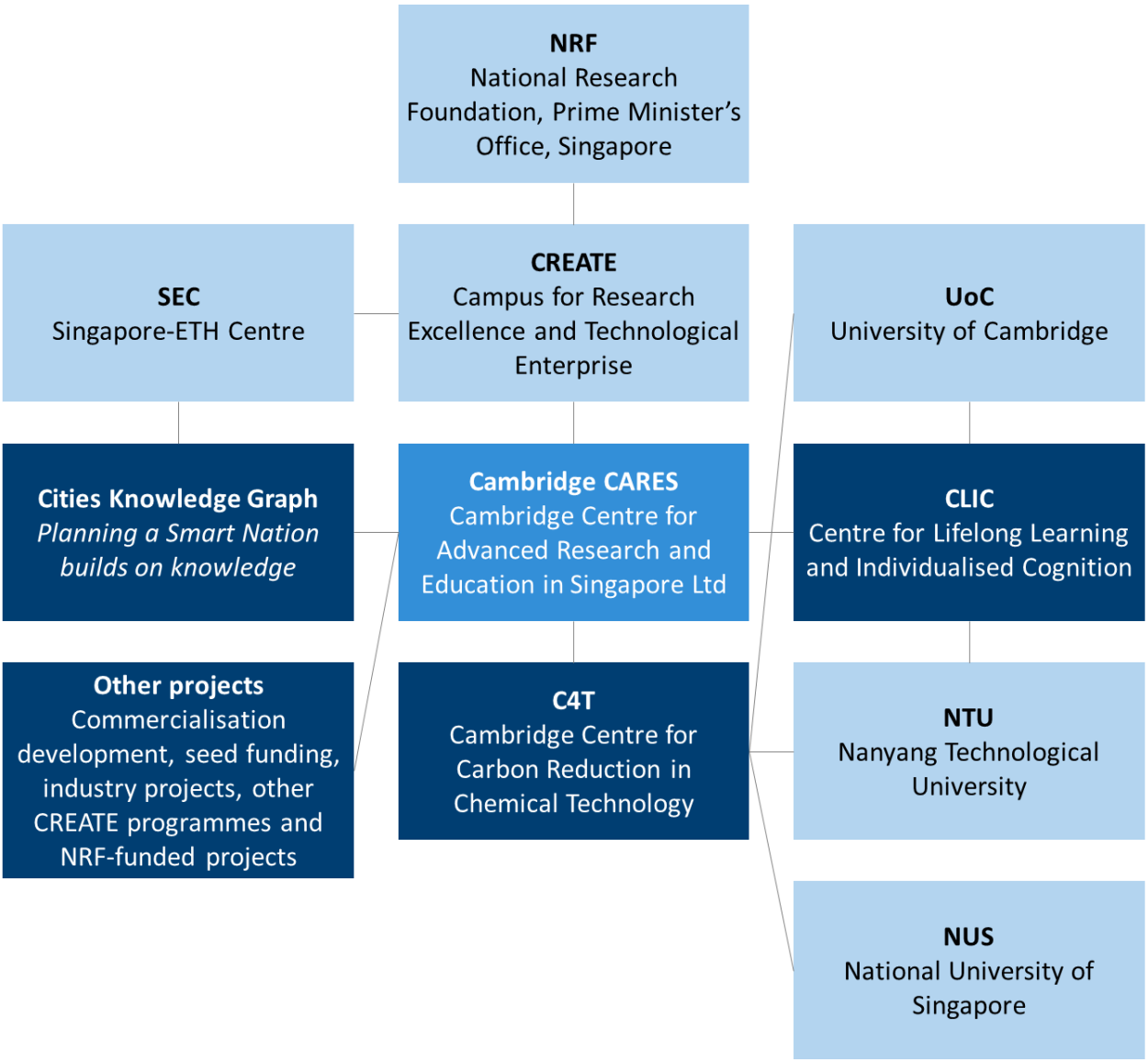
A second large CREATE-funded programme, the Centre for Lifelong Learning and Individualised Cognition (CLIC), began in October 2020. CLIC is a collaboration between University of Cambridge and NTU and focuses on the neuroscience of learning, a new research area for CARES.

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

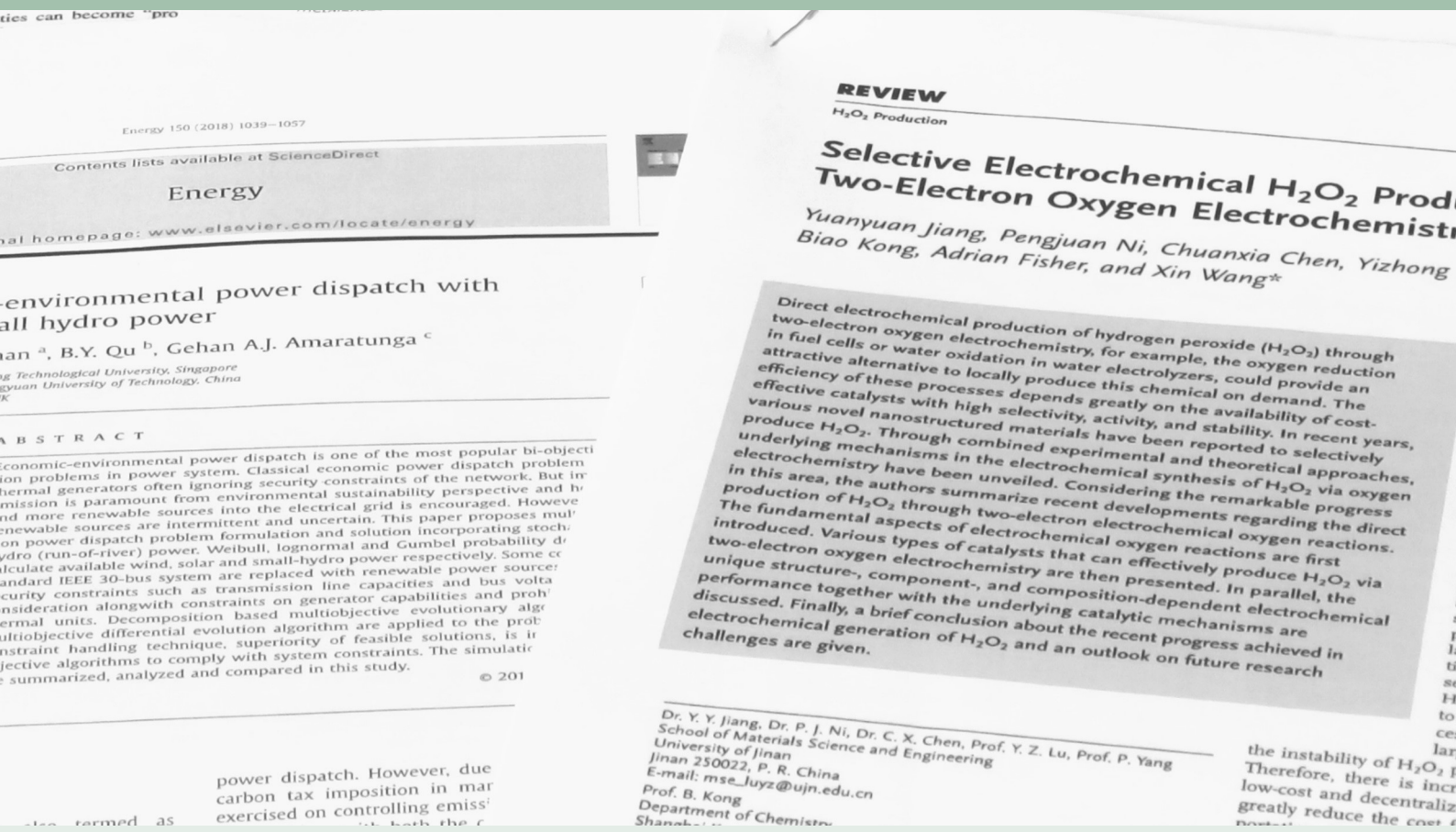
University of Cambridge and ETH Zürich to harness rapidly growing and diversifying data streams to improve the planning and design of cities. Cities Knowledge Graph will do this by developing an innovative digital platform designed to combine data and share knowledge about cities, and to inject new precision and responsiveness to static instruments of planning, such as the city master-plan.

As well as these large Intra-CREATE grants, CARES has several smaller projects and spin-offs ongoing. There is one seed-funded, CARES-hosted Intra-CREATE project between University of Cambridge and the Singapore-ETH Centre (Consumer Energy Usage Data in Smart City Development) which ended on March 2022, and three further projects under the Pharmaceutical Innovation Programme Singapore (PIPS) that involve industry funding. 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 129.

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 on carbon reduction.



OUTSTANDING WORK FROM THE LAST SIX MONTHS OF CAMBRIDGE CARES RESEARCH



FOCUS ON
FUNDAMENTAL SCIENCE

The World Wide Web is dead. Long live The World Avatar.

Dr Andrew BREESON, Science Communication Officer, C4T JPS

The invention of the World Wide Web changed everything. It revolutionised business, education, government, healthcare, and even how we interact with loved ones. But some, including its inventor, are dreaming of something bigger and better.

Sir Tim Berners-Lee, the creator of the World Wide Web, has emphasised the importance of a "Semantic Web" for over 20 years. The problem with the World Wide Web, he says, is that it is set out for humans to read. Whereas a Semantic Web would be understandable to machines.

This web of machine-readable data would be the next technological leap forward. For example, today, when you ask Google a question, it instantly presents you with a list of relevant documents for you to find your answer. However, imagine if machines actually understood the data in their repositories; they could instantly give you a detailed answer to literally any question you ask, from "what is the temperature of this room?" to "how likely am I to have a heart attack?".

The World Avatar will aim to create a living digital "avatar" of the real world.

But that's not all. The true power of a Semantic Web will be realised when people create many programmes that collect Web content from diverse sources, process the information and exchange the results with other programmes. A Semantic Web promotes this synergy: even software agents that were not designed to work together can transfer data among themselves when the data come with semantics.

Enter the World Avatar. Starting in 2013, researchers at CARES began working on the World Avatar project to connect data and software agents to create a living digital "avatar" of the real world. It started with the J-Park Simulator – a digital twin of Singapore's Jurong Island industrial park – but its scope has broadened considerably and it is now used for projects in Cambridge and Germany.

The World Avatar is a dynamic knowledge graph based on Semantic Web technology. It can represent every aspect of the real world, extending the idea of "digital twins" to consider the possibility of representing any abstract concept or process. Within it, there is a "base world" that describes the current state of the real world and "parallel worlds" that can ask what-if questions to see how they change the base world. Essentially, the base world can solve real-world control problems, and the parallel worlds can perform scenario analysis to address real-world design problems.

This is not just theoretical. The World Avatar is alive and working today, performing everything from quantum mechanical calculations to flood damage predictions and optimisations of district heating networks. As the wealth of the base world increases, its performance will only improve, and it will only limited by what is conceptual. What's certain is we have only scratched the surface of what the World Avatar is capable of.

For more information: A related paper to this novel technology is "Universal Digital Twin - A Dynamic Knowledge Graph" (DOI: 10.1017/dce.2021.10) published in *Data-Centric Engineering* by researchers from Cambridge CARES, University of Cambridge, and Nanyang Technological University.

Developments on J-Park Simulator (JPS) and the World Avatar project can be found on pg77.

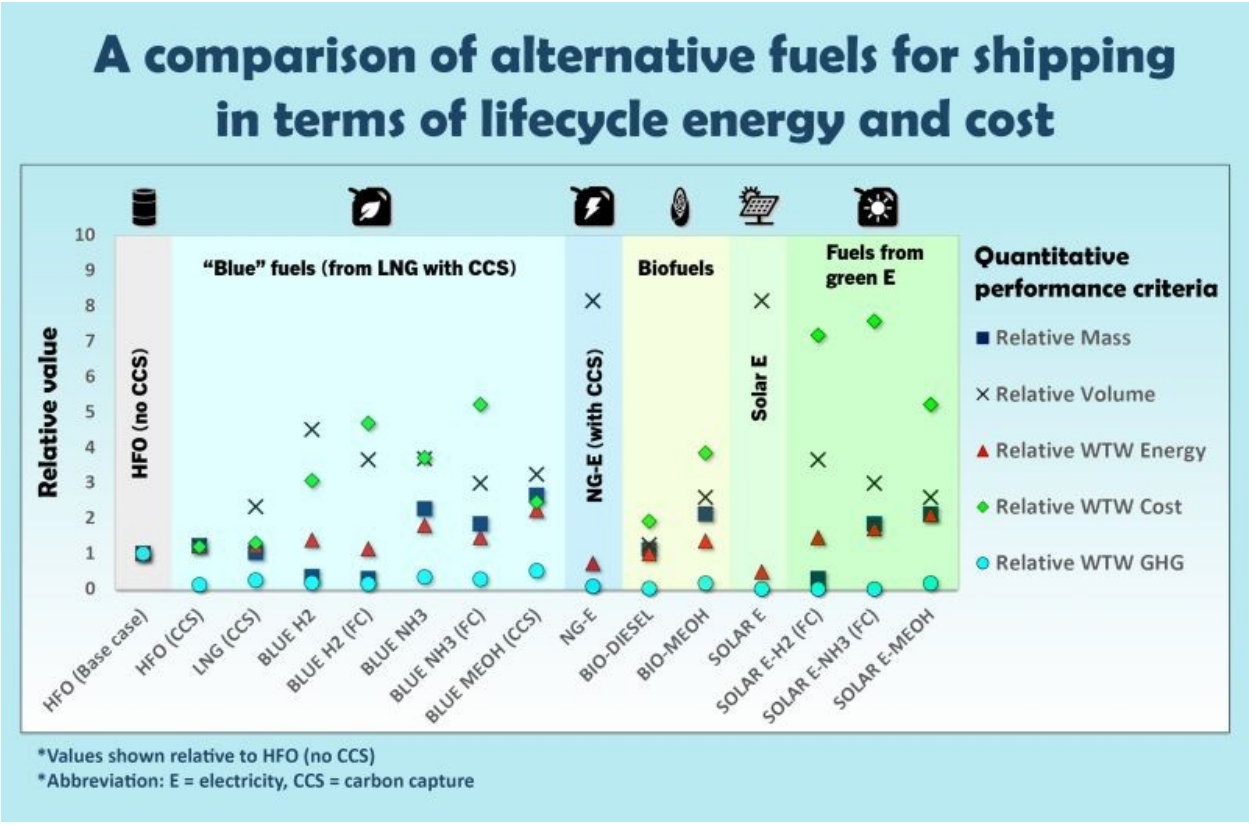
Dr Andrew Breeson is a Science Communication Officer for Cambridge CARES. After completing his MSc and PhD in chemistry at University College London (UCL), he began his career as a science communicator for Cambridge-based life science marketing company, BioStrata. He then moved to Singapore in 2018 to become a Science Communication Manager for the National University of Singapore (NUS) where he oversaw NUS Research News. He joined CARES in July 2021.

Picking the right fuel for future shipping

Dr LAW Li Chin, Research Engineer, C4T EOF

For a long time, heavy fuel oil (HFO) has monopolised the shipping industry as the main marine fuel, which leads to nearly 3% of global carbon emissions. Decarbonisation of shipping is prudent, and the most straightforward approach is the replacement of HFO with a low-carbon alternative fuel. The potential alternative fuels is determined by many factors, for instance, technology reliability, energy consumption, price, and availability. A high potential marine fuel should have low mass and volume, low cost, low energy requirement for its production, and importantly, low carbon throughout the lifecycle from the well-to-tank (WTT) and the tank-to-wake (TTW) stages.

Propositions include biodiesel, bio-methanol, hydrogen, ammonia, and electricity produced from different primary energies. How to choose? There is no one solution for all kinds of ships and different parties are trying to discover the suitability of different fuels for maritime applications. But which fuel would be the winner? To resolve this, the various alternative fuels must be compared consistently and as quantitatively as possible. To contribute to this global issue, we have produced a scoring system



A comparison of alternative fuels for shipping in terms of lifecycle energy and cost.

that compares various fuels to HFO using six quantifiable parameters: (i) fuel mass, (ii) fuel volume, (iii) life cycle (Well-To-Wake—WTW) energy intensity, (iv) WTW cost, and (v) WTW greenhouse gas (GHG) emission, and (vi) non-GHG emissions, and four qualitative parameters: (i) fuel scalability, (ii) fuel safety, (iii) availability of regulations and, (iv) technological readiness. Our summary and analysis methods have been presented in our latest publication.

The highlight of this research is presented in the figure above, which shows the relative value of five quantifiable parameters for 15 fuel pathways. HFO as the reference fuel has a relative value of 1 for all parameters. From this figure, we conclude that all the selected fuels can achieve at least a 50% carbon reduction compared to HFO, however, how much energy and cost need to be paid? Is the fuel suitable for a ship with mass and space constraints? The numbers, as shown in the chart, can help engineers and policymakers make well-founded decisions. We believe that in this way, all stakeholders in shipping can make the right choice of fuel for their vessels, and a low-carbon shipping industry is within reach.

For more information: The paper related to this research, "A Comparison of Alternative Fuels for Shipping in Terms of Lifecycle Energy and Cost" (DOI: 10.3390/en14248502) is published in *Energies* by researchers from Cambridge CARES, Universiti Sains Malaysia, and the University of Cambridge. The abstract can be found in our Research Highlights on pg17.

Dr. Law Li Chin obtained her bachelor degree and Doctor of Philosophy in chemical engineering at University Science of Malaysia. Her expertise is in the field of techno-economic analysis of carbon capture. She is a member of Board of Engineering Malaysia. Having worked in the shipbuilding industry for five years, Dr. Law has experience in the process design of the topsides and living quarters of vessels. She was involved in the deliveries of the Floating Production Storage and Offloading (FPSO) project including Libra FPSO and Johan Castberg FPSO with Sembcorp Marine Shipyard as process and piping engineer. She was also appointed as a lead piping engineer during her period of service. Her experience and knowledge in ship design and building made her competent for the research related to maritime decarbonisation. Currently, Dr. Law is working with Cambridge CARES under Cambridge Centre for Carbon Reduction in Chemical Technology (C4T).

Highlighted research outputs from October 2021 - March 2022

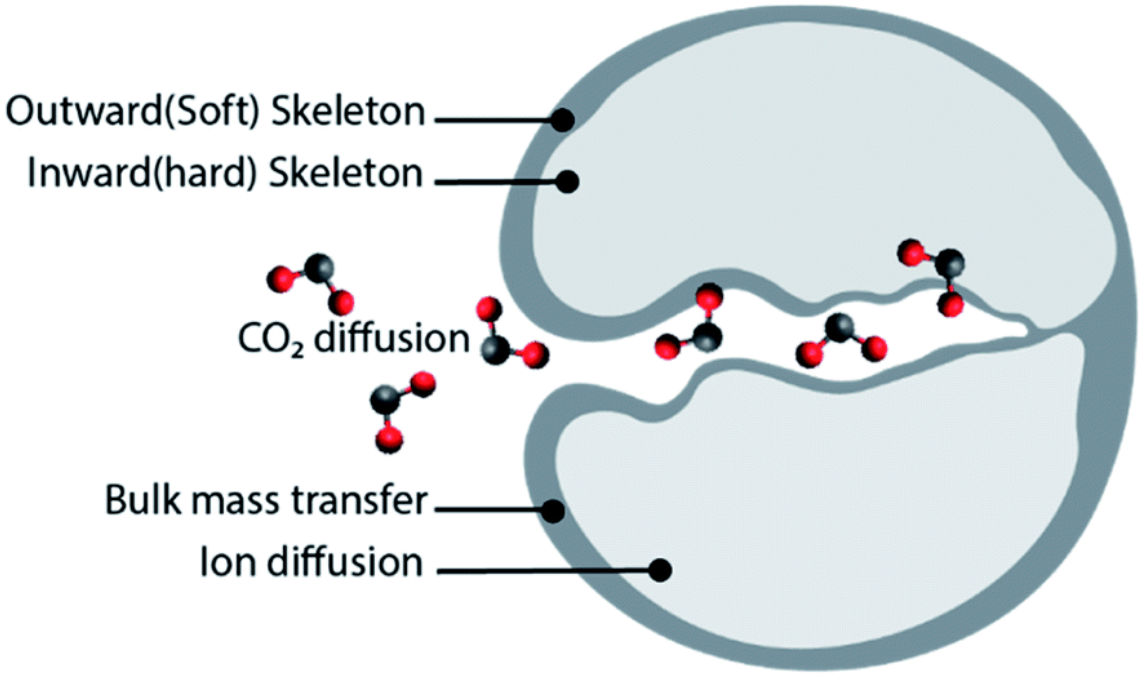
A selection of publications from across our programmes.

C4T IRP 1: Synthetic solid oxide sorbents for CO_2 capture: state-of-the art and future perspectives

Ribooga Chang, Xianyue Wu, Ocean Cheung, and Wen Liu, *Journal of Materials Chemistry A*

DOI: 10.1039/D1TA07697C

Abstract: Carbon capture is an important and effective approach to control the emission of CO_2 from point sources such as fossil fuel power plants, industrial furnaces and cement plants into the atmosphere. For an efficient CO_2 capture operation, many aspects of the CO_2 capture steps need to be carefully considered. Currently the most mature CO_2 capture technology is liquid amine scrubbing. Alternatively, solid sorbents can be used to effectively capture CO_2 while alleviating the disadvantages associated with liquid amine sorbents. In this review, we critically assess solid metal oxide CO_2 sorbents, especially oxides of group 1 (Li, Na and K) and group 2 (Mg, Ca, Sr and Ba) metals, for capturing CO_2 at moderate to high temperatures. In particular, we focus on the recent advances in developing synthetic metal oxide sorbents, and the correlation between the design, synthetic approaches and their cyclic CO_2 capture performance, which are characterised by CO_2 uptake capacity, rate of carbonation and cyclic stability. The state-of-the-art, challenges, opportunities and future research directions for these metal oxide sorbents are discussed. By devoting more research effort to address the issues identified, there can be great potential to utilise Group 1 and 2 metal oxides as cost-effective, highly efficient sorbents for CO_2 capture in a variety of carbon capture applications.

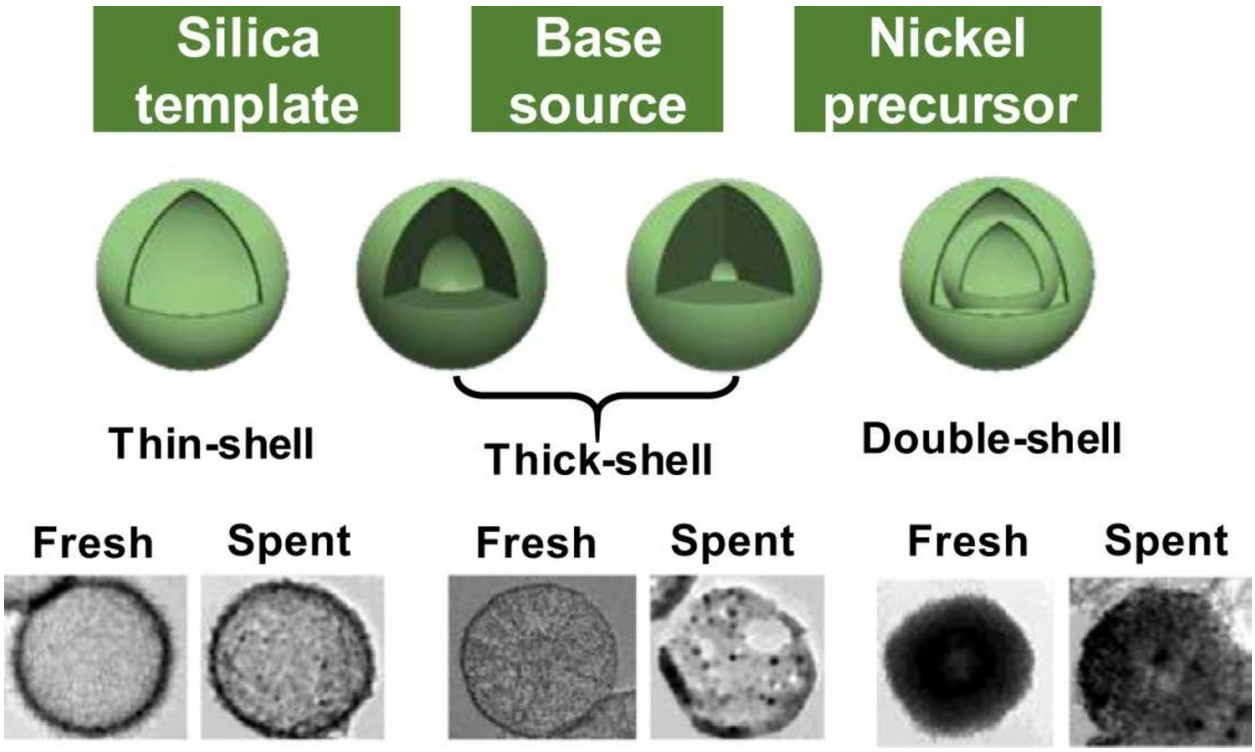


C4T IRP 1: Strong coke-resistivity of spherical hollow Ni/SiO_2 catalysts with shell-confined high-content Ni nanoparticles for methane dry reforming with CO_2

Mohammadreza Kosari, Saeed Askari, Abdul Majeed Seayad, Shibo Xi, Sibudjing Kawi, Armando Borgna, Hua ChunZeng, *Applied Catalysis B: Environmental*

DOI: 10.1016/j.apcatb.2022.121360

Abstract: Hollow nanocatalysts, which are vehemently researched for their delimited cavity and enclosed shell, could manifest tunable focal properties besides well-defined active sites, thus enhancing the catalytic functionality. Herein, nickel-silicate hollow spheres (NHSs) with varied shell thickness and interior cavity size were commensurately designed. Distinction between various NHSs-derived Ni/SiO_2 with identically mimicked morphologies was realized by examining their catalytic performance for methane dry reforming (DRM) reaction with sweeping pre- and post-reaction characterizations (TEM, XPS, XANES, in-situ DRIFTS). Besides facilitating the DRM reaction up to its thermodynamic limit, it was revealed that optimal NHS conformation is beneficial as a potential natural barrier against sintering and coking bottlenecks. Furthermore, a fine-tuned shell composition could endow improved Ni-sintering resistivity and enhanced reactivity to the NHS nanocatalysts. Our findings prove that the hollow interior space with a conducive shell thickness positively influences the reactant conversion and coking hindrance during the DRM reaction.

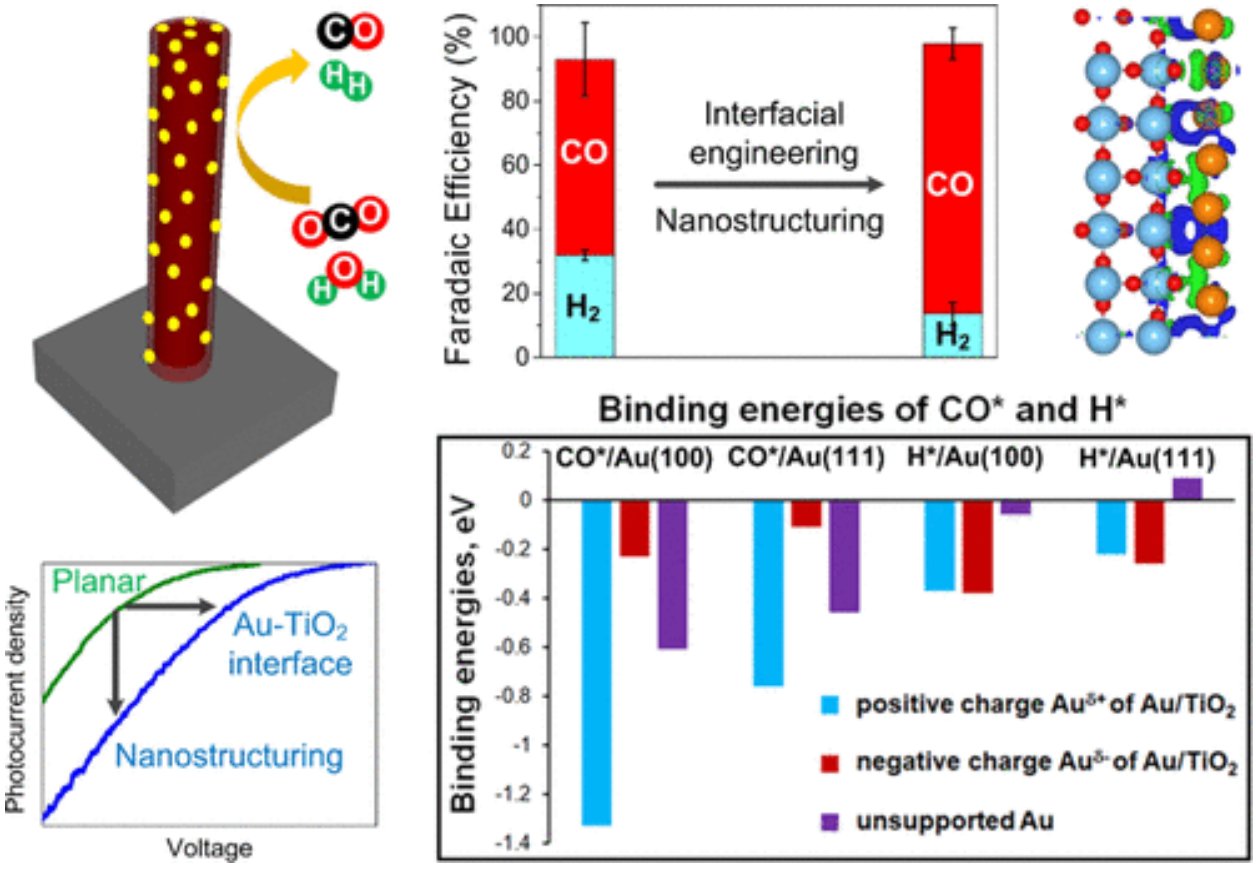


C4T IRP 1 and IRP 3: Manipulating Intermediates at the Au–TiO_2 Interface over InP Nanopillar Array for Photoelectrochemical CO_2 Reduction

Guanyu Liu, Parvathala Reddy Narangari, Quang Thang Trinh, Wenguang Tu, Markus Kraft, Hark Hoe Tan, Chennupati Jagadish, Tej Choksi, Joel Ager, Siva Karuturi, and Rong Xu, *ACS Catalysis*

DOI: 10.1021/acscatal.1c02043

Abstract: Photoelectrochemical (PEC) reduction of CO_2 with H_2O is a promising approach to convert solar energy and greenhouse gas into value-added chemicals or fuels. However, the exact role of structures and interfaces of photoelectrodes in governing the photoelectrocatalytic processes in terms of both activity and selectivity remains elusive. Herein, by systematically investigating the InP photocathodes with Au–TiO_2 interfaces, we discover that nanostructuring of InP can not only enhance the photoresponse owing to increased light absorption and prolonged minority carrier lifetime, but also improve selectivity toward CO production by providing more abundant interfacial contact points between Au and TiO_2 than planar photocathodes. In addition, theoretical studies on the Au–TiO_2 interface demonstrate that the charge transfer between Au and TiO_2, which is locally confined to the interface, strengthens the binding of the CO* intermediate on positively charged Au interfacial sites, thus improving CO_2 photoelectroreduction to form CO. An optimal Au–TiO_2/InP nanopillar-array photocathode exhibits an onset potential of +0.3 V vs reversible hydrogen electrode (RHE) and a Faradaic efficiency of 84.2% for CO production at −0.11 V vs RHE under simulated AM 1.5G illumination at 1 sun. The present findings of the synergistic effects of the structure and interface on the photoresponse and selectivity of a photoelectrode provide insights into the development of III–V semiconductor-based PEC systems for solar fuel generation.

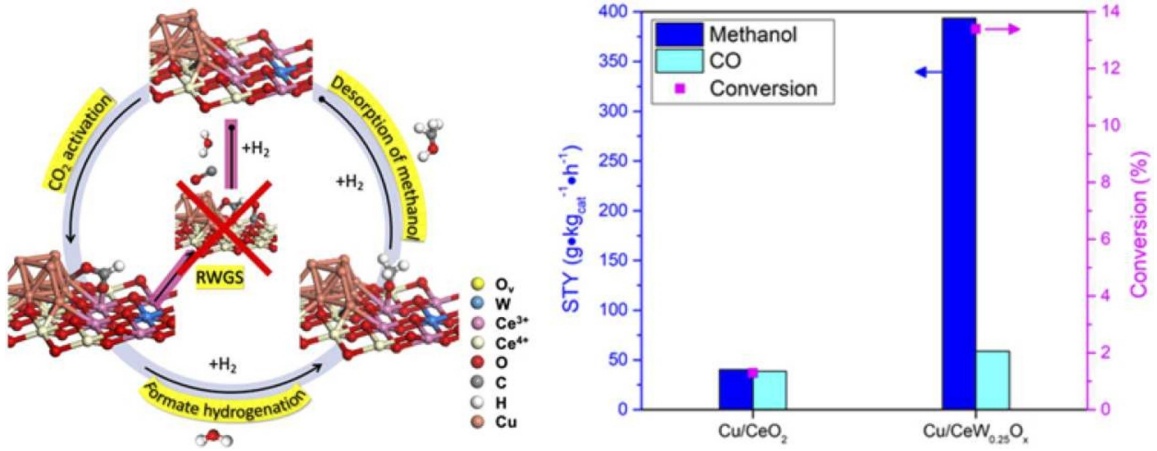


C4T IRP 1: CO2 hydrogenation to methanol on tungsten-doped Cu/CeO2 catalysts

Yong Yan, Roong Jien Wong, Zhirui Ma, Felix Donat, Shibo Xi, Syed Saqline, Qianwenhao Fan, Yonghua Du, Armando Borgna, Qian He, Christoph Müller, Wei Chen, Alexei Lapkin, Wen Liu, *Applied Catalysis B: Environmental*

DOI: 10.1016/j.apcatb.2022.121098

Abstract: The catalytic hydrogenation of CO_2 to methanol depends significantly on the structures of metal-oxide interfaces. We show that doping a high-valency metal, viz. tungsten, to CeO_2 could render improved catalytic activity for the hydrogenation of CO_2 on a $Cu/CeW_{0.25}O_x$ catalyst, whilst making it more selective towards methanol than the undoped Cu/CeO_2. We experimentally investigated and elucidated the structural-functional relationship of the Cu/CeO_2 interface for CO_2 hydrogenation. The promotional effects are attributed to the irreversible reduction of Ce^{4+} to Ce^{3+} by W-doping, the suppression of the formation of redox-active oxygen vacancies on CeO_2, and the activation of the formate pathway for CO_2 hydrogenation. This catalyst design strategy differs fundamentally from those commonly used for CeO_2-supported catalysts, in which oxygen vacancies with high redox activity are considered desirable. °C.

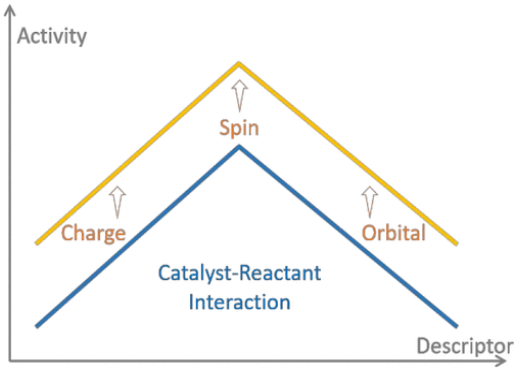


C4T IRP 2: Catalytically Influential Features in Transition Metal Oxides

Yuanmiao Sun, Gao Chen, Shibo Xi, and Zhichuan J. Xu, *ACS Catalysis*

DOI: 10.1021/acscatal.1c04393

Abstract: The development of efficient catalysts is critical in advancing electrocatalysis techniques. While tremendous progress has been made on the perspective of optimizing the catalyst–reactant interaction, the influence from other properties has received relatively less attention to date. These properties are normally originated from the intrinsic solid-state properties and can be circumstantially influential on the reaction activity and reaction mechanism. In particular, transition metal oxides (TMOs) possess complex inherent features that enable a wide variety of catalytically influential properties. Therefore, understanding the inherent features in TMOs and mastering the strategies to take full advantage of them will bring opportunities for further advances. Here we provide an overview of the inherent features in TMOs and conceptually discuss how they can alter the catalytic behaviors in electrocatalysis. Perspectives to take full advantage of these features are also proposed for a better design of TMO-based electrocatalysts.

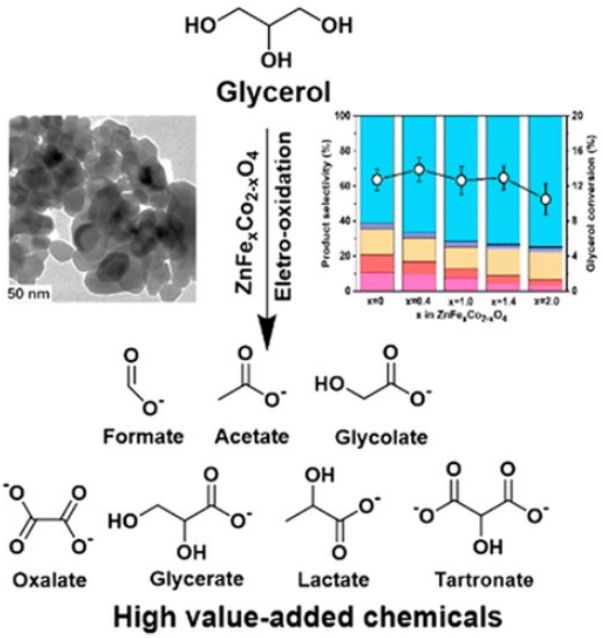


C4T IRP 2: Electro-Oxidation of Glycerol to High-Value-Added C1–C3 Products by Iron-Substituted Spinel Zinc Cobalt Oxides

Haibo Wan, Chencheng Dai, Liujun Jin, Songzhu Luo, Fanxu Meng, Gao Chen, Yan Duan, Chuntai Liu, Qingfeng Xu, Jianmei Lu, and Zhichuan J. Xu, *ACS Applied Materials & Interfaces*

DOI: 10.1021/acsami.2c02215

Abstract: Glycerol is a byproduct of biodiesel production and can be a low-cost source for some high-value C1–C3 chemicals. The conversion can be achieved by photo-, thermo-, and electrocatalysis methods. The electrocatalytic oxidation method is attractive due to its moderate reaction conditions and high electron to product efficiency. Most reported catalysts are based on noble metals, while metal oxides are rarely reported. Here, we investigated the electro-oxidation of glycerol on a series of ZnFexCo2–xO4 (x = 0, 0.4, 1.0, 1.4, and 2.0) spinel oxides. Seven types of value-added C1–C3 products including formate, glycolate, lactate, and glycerate can be obtained by this approach. The selectivity and Faraday efficiency toward these products can be tuned by adjusting the Fe/Co ratio and other experimental parameters, such as the applied potential, glycerol concentration, and electrolyte pH.



C4T IRP 2 and C4T Emerging Opportunities Fund: Surface Reconstruction of Perovskites for Water Oxidation: The Role of Initial Oxides' Bulk Chemistry

Haiyan Li, Yubo Chen, Justin Zhu Yeow Seow, Chuntai Liu, Adrian Fisher, Joel Ager, Zhichuan J. Xu, *small science*

DOI: 10.1002/smsc.202100048

Abstract: Developing highly active electrocatalysts for oxygen evolution reaction (OER) is crucial for the scalable production of renewable hydrogen fuels by water electrolysis. Perovskite oxides are extensively studied as OER catalysts as they can have high activity and also offer considerable flexibility in composition and structure. Recently, there are increasingly numerous reports regarding dynamic surface reconstruction of perovskite oxides under OER conditions, with claims that the reconstruction-derived species are the actual catalysts responsible for the measured OER activity. To enable rational design of perovskite oxides as precatalysts to generate actual active components in situ, gaining essential understanding of their reconstruction behaviors is crucial. This perspective discusses the roles of initial bulk chemistry in the surface evolution process of perovskite oxides during OER, including the dependency of surface stability on electronic structure of the precatalyst and the possibility of occurrence of lattice oxygen evolution reaction and cation leaching on the surface of a perovskite oxide precatalyst. It is reasonably argued that tailoring the bulk properties of perovskite precatalysts, such as electronic structure, crystallographic structure, and ion stoichiometry, can influence the occurrence of surface reconstruction and the formation of actual active surface species.

C4T IRP 3: Understanding the particulate formation process in the engine fuelled with diesel/Jet A-1 blends

Qiren Zhu, Yichen Zong, Wenbin Yu, Wenming Yang, and Markus Kraft, *Fuel*

DOI: 10.1016/j.fuel.2021.122675

Abstract: Jet fuel has been recognized as a potential alternative for traditional diesel engines because of its ability to reduce particulate matter (PM) emissions while retaining engine power output. In this study, the particulate formation process has been studied in detail using diesel/Jet A-1 blends with evenly staggered ratios. The number concentration of the accumulation mode particle decreases exponentially when additional Jet A-1 is introduced to the blends under 30% engine load, as more fuel and particle precursors are oxidized. Additionally, the comparison of PM emissions with pilot-main and single main two injection strategies is conducted to better understand the particle formation process. The phenomenon of 'particle saturation' of nucleation mode particles is observed using the pilot-main injection strategy. With these supporting findings, we strengthen the point that the pilot-injection strategy has the potential weaken the oxidation process during the combustion process. Furthermore, this research quantifies the impact of Jet A-1 on combustion and gas emission characteristics by extracting the change rate from the data. In general, Jet A-1 tends to delay the ignition and shorten the combustion duration. The results also reveal that the rise in NOx emissions is due to a higher proportion of premixed combustion, while the increase in HC emissions is attributed to a longer ignition delay and shorter combustion time.

C4T IRP 4 and C4T IRP BB: A Comparison of Alternative Fuels for Shipping in Terms of Lifecycle Energy and Cost

Li Chin Law, Beatrice Foscoli, Epaminondas Mastorakos, and Stephen Evans, *Energies*

DOI: 10.3390/en14248502

Abstract: Decarbonization of the shipping sector is inevitable and can be made by transitioning into low- or zero-carbon marine fuels. This paper reviews 22 potential pathways, including conventional Heavy Fuel Oil (HFO) marine fuel as a reference case, "blue" alternative fuel produced from natural gas, and "green" fuels produced from biomass and solar energy. Carbon capture technology (CCS) is installed for fossil fuels (HFO and liquefied natural gas (LNG)). The pathways are compared in terms of quantifiable parameters including (i) fuel mass, (ii) fuel volume, (iii) life cycle (Well-To-Wake—WTW) energy intensity, (iv) WTW cost, (v) WTW greenhouse gas (GHG) emission, and (vi) non-GHG emissions, estimated from the literature and ASPEN HYSYS modelling. From an energy perspective, renewable electricity with battery technology is the most efficient route, albeit still impractical for long-distance shipping due to the low energy density of today's batteries. The next best is fossil fuels with CCS (assuming 90% removal efficiency), which also happens to be the lowest cost solution, although the long-term storage and utilization of CO_2 are still unresolved. Biofuels offer a good compromise in terms of cost, availability, and technology readiness level (TRL); however, the non-GHG emissions are not eliminated. Hydrogen and ammonia are among the worst in terms of overall energy and cost needed and may also need NOx clean-up measures. Methanol from LNG needs CCS for decarbonization, while methanol from biomass does not, and also seems to be a good candidate in terms of energy, financial cost, and TRL. The present analysis consistently compares the various options and is useful for stakeholders involved in shipping decarbonization.

C4T IRP JPS: The World Avatar—A World Model for Facilitating Interoperability

Mei Qi Lim, Xiaonan Wang, Oliver Inderwildi, and Markus Kraft, *Intelligent Decarbonisation, Chapter 4*

DOI: 10.1007/978-3-030-86215-2_4

Abstract: Digitalisation enhances communication and therefore offers new ways to achieve efficiency gains in science, technology and society at large. However, there are still many open questions around how digitalisation can contribute to a more sustainable environment and lifestyle. We believe that knowledge graph technology is a promising candidate with which this can be achieved. In this chapter, we present the World Avatar, a dynamic knowledge graph (dKG), and explain the main underlying concepts and principles. Using several use cases, two key fundamentally different aspects—control and design—are introduced and illustrated. In addition, we show how the World Avatar can improve interoperability between heterogeneous data formats as well as software, and thus enable cross-domain applications in wider contexts. Moreover, we highlight how the Parallel World framework can consider different scenarios and hence facilitate time-dependent what-if scenario analysis. All use cases show how interoperability between multiple domains involved in the complex decarbonisation process can contribute to CO_2 abatement of digitalisation.

C4T IRP JPS: Universal Digital Twin: Land use

Jethro Akroyd, Zachary Harper, David Soutar, Feroz Farazi, Amit Bhave, Sebastian Mosbach, and Markus Kraft, *Data-Centric Engineering*

DOI: 10.1017/dce.2021.21

Abstract: This article develops an ontological description of land use and applies it to incorporate geospatial information describing land coverage into a knowledge-graph-based Universal Digital Twin. Sources of data relating to land use in the UK have been surveyed. The Crop Map of England (CROME) is produced annually by the UK Government and was identified as a valuable source of open data. Formal ontologies to represent land use and the geospatial data arising from such surveys have been developed. The ontologies have been deployed using a high-performance graph database. A customized vocabulary was developed to extend the geospatial capabilities of the graph database to support the CROME data. The integration of the CROME data into the Universal Digital Twin is demonstrated in two use cases that show the potential of the Universal Digital Twin to share data across sectors. The first use case combines data about land use with a geospatial analysis of scenarios for energy provision. The second illustrates how the Universal Digital Twin could use the land use data to support the cross-domain analysis of flood risk. Opportunities for the extension and enrichment of the ontologies, and further development of the Universal Digital Twin are discussed.

C4T IRP JPS and PIPS: From Platform to Knowledge Graph: Evolution of Laboratory Automation

Jiaru Bai, Liwei Cao, Sebastian Mosbach, Jethro Akroyd, Alexei Lapkin, and Markus Kraft, *Journal of the American Chemical Society*

DOI: 10.1021/jacsau.1c00438

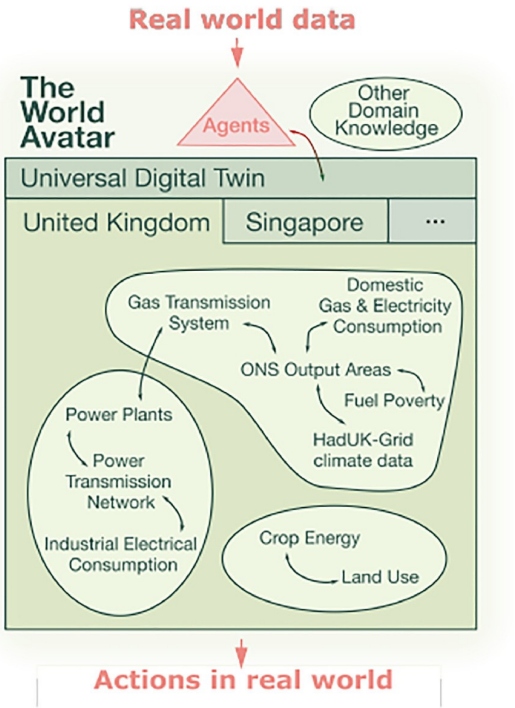
Abstract: High-fidelity computer-aided experimentation is becoming more accessible with the development of computing power and artificial intelligence tools. The advancement of experimental hardware also empowers researchers to reach a level of accuracy that was not possible in the past. Marching toward the next generation of self-driving laboratories, the orchestration of both resources lies at the focal point of autonomous discovery in chemical science. To achieve such a goal, algorithmically accessible data representations and standardized communication protocols are indispensable. In this perspective, we recategorize the recently introduced approach based on Materials Acceleration Platforms into five functional components and discuss recent case studies that focus on the data representation and exchange scheme between different components. Emerging technologies for interoperable data representation and multi-agent systems are also discussed with their recent applications in chemical automation. We hypothesize that knowledge graph technology, orchestrating semantic web technologies and multi-agent systems, will be the driving force to bring data to knowledge, evolving our way of automating the laboratory.

C4T IRP JPS and CEUS: Universal Digital Twin – the impact of heat pumps on social inequality

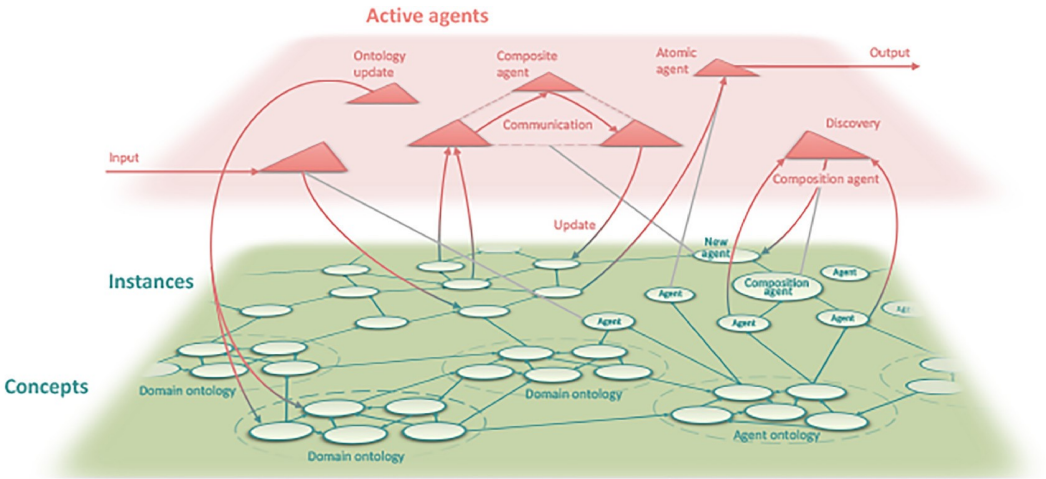
Thomas Savage, Jethro Akroyd, Sebastian Mosbach, Michael Hillman, Franziska Sielker, and Markus Kraft, *Advances in Applied Energy*

DOI: 10.1016/j.adapen.2021.100079

Abstract: This paper investigates how using heat pumps for domestic heating would impact fuel poverty and social inequality. The analysis integrates a geospatial description of climate observations, gas and electricity infrastructure, energy consumption and fuel poverty from the base world of a Universal Digital Twin based on the World Avatar knowledge graph. Historic temperature data were used to estimate the temporal and geospatial variation of the performance of air source heat pumps in the UK. The corresponding change in gas and electricity consumption that could be achieved using heat pumps instead of gas for domestic heating was estimated. The geospatial impact of the heat pumps was assessed in terms of CO2 savings, and their effect on fuel cost and fuel poverty. Whilst heat pumps would reduce emissions, it is predicted that they would increase fuel costs. It was shown that both local and regional areas of high fuel poverty would experience some of the largest increases in fuel cost. This illustrates the potential for the transition to sustainable heating to exacerbate social inequality. The analysis suggests that existing regional inequalities will increase, and that it comes down to a political choice between investments to support the most effective use of heat pumps, and delayed investments to counter social inequality. The ability of the World Avatar to integrate the models and data necessary to perform this type of holistic analysis provides a means to generate actionable information, for example, to enable local policy interventions to address the tension between social and environ-



(b) Schematic showing the relationship between selected data from the base world of the World Avatar.



(a) The design of the World Avatar dynamic knowledge graph [23]. Image reproduced under a CC BY 4.0 licence.

CLIC: Age-specificity and generalization of behavior-associated structural and functional networks and their relevance to behavioral domains

Junhong Yu, Nastassja Lopes Fischer, *Human Brain Mapping*

DOI: 10.1002/hbm.25759

Abstract: Behavior-associated structural connectivity (SC) and resting-state functional connectivity (rsFC) networks undergo various changes in aging. To study these changes, we proposed a continuous dimension where at one end networks generalize well across age groups in terms of behavioral predictions (age-general) and at the other end, they predict behaviors well in a specific age group but fare poorly in another age group (age-specific). We examined how age generalizability/specificity of multimodal behavioral associated brain networks varies across behavioral domains and imaging modalities. Prediction models consisting of SC and/or rsFC networks were trained to predict a diverse range of 75 behavioral outcomes in a young adult sample (N = 92). These models were then used to predict behavioral outcomes in unseen young (N = 60) and old (N = 60) subjects. As expected, behavioral prediction models derived from the young age group, produced more accurate predictions in the unseen young than old subjects. These behavioral predictions also differed significantly across behavioral domains, but not imaging modalities. Networks associated with cognitive functions, except for a few mostly relating to semantic knowledge, fell toward the age-specific end of the spectrum (i.e., poor young-to-old generalizability). These findings suggest behavior-associated brain networks are malleable to different degrees in aging; such malleability is partly determined by the nature of the behavior.

CLIC: A New Remote Guided Method for Supervised Web-Based Cognitive Testing to Ensure High-Quality Data: Development and Usability Study

Victoria Leong, Kausar Raheel, Sim Jia Yi, Kriti Kacker, Vasilis Karlaftis, Chrysoula Vassiliu, Kastoori Kalaivanan, Annabel Chen, Trevor Robbins, Barbara Sahakian, and Zoe Kourtzi, *Journal of Medical Internet Research*

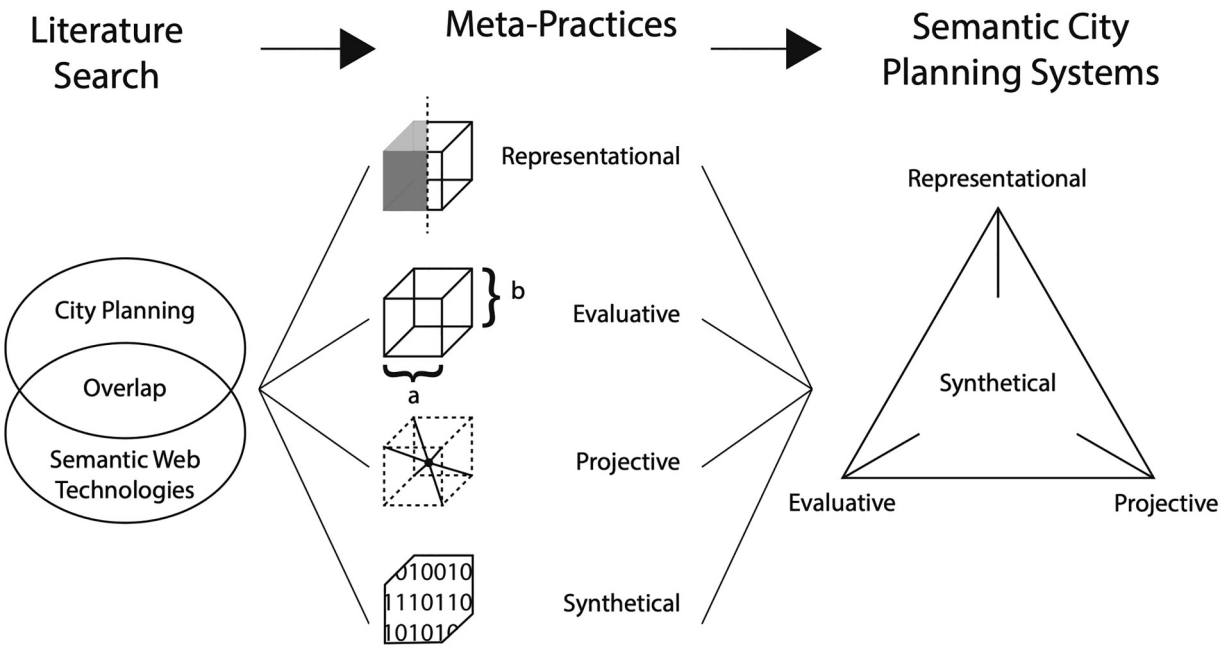
DOI: 10.2196/28368

Abstract: The global COVID-19 pandemic has triggered a fundamental reexamination of how human psychological research can be conducted safely and robustly in a new era of digital working and physical distancing. This study examines the opportunities and challenges afforded by the societal shift toward web-based testing and highlights an urgent need to establish a standard data quality assurance framework for online studies. This study aims to develop and validate a new supervised online testing methodology, remote guided testing (RGT). A total of 85 healthy young adults were tested on 10 cognitive tasks assessing executive functioning (flexibility, memory, and inhibition) and learning. Tasks were administered either face-to-face in the laboratory (n=41) or online using remote guided testing (n=44) and delivered using identical web-based platforms (Cambridge Neuropsychological Test Automated Battery, Inquisit, and i-ABC). Data quality was assessed using detailed trial-level measures (missed trials, outlying and excluded responses, and response times) and overall task performance measures. The results indicated that, across all data quality and performance measures, RGT data was statistically-equivalent to in-person data collected in the lab (P>.40 for all comparisons). Moreover, RGT participants out-performed the lab group on measured verbal intelligence (P<.001), which could reflect test environment differences, including possible effects of mask-wearing on communication. These data suggest that the RGT methodology could help ameliorate concerns regarding online data quality—particularly for studies involving high-risk or rare cohorts—and offer an alternative for collecting high-quality human cognitive data without requiring in-person physical attendance.

CKG: Semantic City Planning Systems (SCPS): A Literature Review

Aurel von Richthofen, Pieter Herthogs, Markus Kraft, and Stephen Cairns, *Journal of Planning Literature*
DOI: 10.1177/08854122211068526

Abstract: This review focuses on recent research literature on the use of Semantic Web Technologies (SWT) in city planning. The review foregrounds representational, evaluative, projective, and synthetical meta-practices as constituent practices of city planning. We structure our review around these four meta-practices that we consider fundamental to those processes. We find that significant research exists in all four meta-practices. Linking across domains by combining various methods of semantic knowledge generation, processing, and management is necessary to bridge gaps between these meta-practices and will enable future Semantic City Planning Systems.

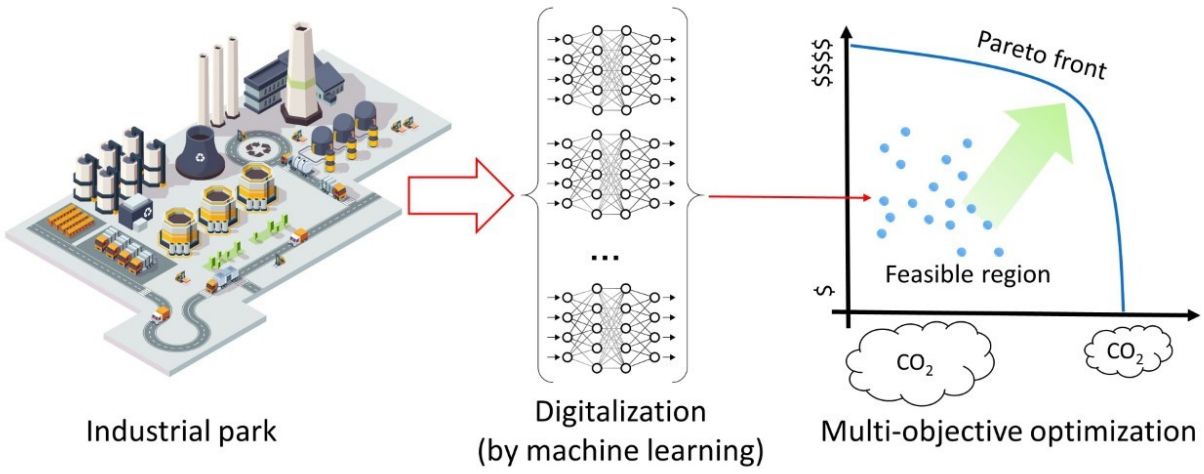


PIPS: Accelerating net zero from the perspective of optimizing a carbon capture and utilization system

Zhimian Hao, Magda Barecka, and Alexei Lapkin, *Energy & Environmental Science*

DOI: 10.1039/D1EE03923G

Abstract: Net zero requires an accelerated transition from fossil fuels to renewables. Carbon capture and utilization (CCU) can be an effective intermediate solution for the decarbonization of fossil fuels. However, many research works contain renewables in the design of CCU systems, which may mislead stakeholders regarding the hotspots of CCU systems. Herein, this work builds a CCU system with no renewables involved, and evaluates its greenhouse gas (GHG) emissions based on the life cycle assessment with a cradle-to-gate boundary. To pursue the best system performance, an optimization framework is established to digitalize and optimize the CCU system regarding GHG emissions reduction. The optimized CCU can reduce GHG emissions by 13% compared with the conventional process. Heating is identified as the most significant contributor to GHG emissions, accounting for 60%. Electrifying heating fully using low-carbon electricity can further reduce GHG emissions by 47%, but such extreme conditions will significantly sacrifice the economic benefit. By contrast, the multi-objective optimization can show how the decisions can affect the balance between GHG emissions and profit. Furthermore, this work discusses the dual effect of carbon pricing on the CCU system – raising the cost of raw materials and utilities, but also gaining credits when emissions are reduced in producing valued products.

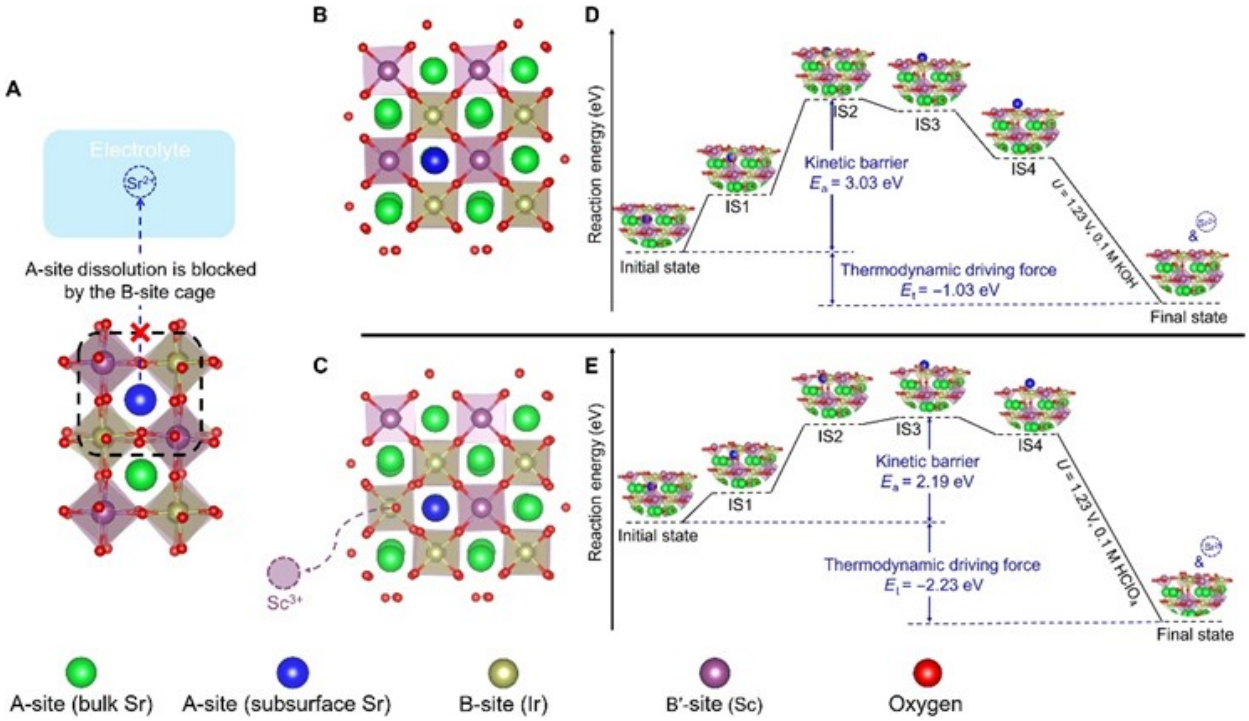


C4T Emerging Opportunities Fund: Lattice site–dependent metal leaching in perovskites toward a honeycomb-like water oxidation catalyst

Yubo Chen, Yuanmiao Sun, Maoyu Wang, Jingxian Wang, Haiyan Li, Shibo Xi, Chao Wei, Pinxian Xi, George Sterbinsky, and Zhichuan J. Xu, *Science Advances*

DOI: 10.1126/sciadv.abk1788

Abstract: Metal leaching during water oxidation has been typically observed in conjunction with surface reconstruction on perovskite oxide catalysts, but the role of metal leaching at each geometric site has not been distinguished. Here, we manipulate the occurrence and process of surface reconstruction in two model ABO3 perovskites, i.e., SrSc0.5Ir0.5O3 and SrCo0.5Ir0.5O3, which allow us to evaluate the structure and activity evolution step by step. The occurrence and order of leaching of Sr (A-site) and Sc/Co (B-site) were controlled by tailoring the thermodynamic stability of B-site. Sr leaching from A-site mainly generates more electrochemical surface area for the reaction, and additional leaching of Sc/Co from B-site triggers the formation of a honeycomb-like IrOxHy phase with a notable increase in intrinsic activity. A thorough surface reconstruction with dual-site metal leaching induces an activity improvement by approximately two orders of magnitude, which makes the reconstructed SrCo0.5Ir0.5O3 among the best for water oxidation in acid.



IRP 1

SUSTAINABLE REACTION ENGINEERING FOR CARBON NEUTRAL INDUSTRY

IRP 1 is focused on chemical technologies that allow rapid decarbonisation of 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

Professor ZENG Hua Chun
National University of Singapore

OVERVIEW

Phase 2 of IRP 1 is developing along three main directions: new structured nanomaterials for C1 feedstocks conversion and their scale up to industrially-relevant catalytic systems, development of new transformations for conversion of bio-waste streams into higher-value products, and engineering of catalytic processes for reduction of carbon emissions.

Recent advances in IRP 1 disclosed in the current report are in formalising the approach to developing circular chemicals use in the work of Dr Zhen Guo and PhD student Mr Adarsh Arun. A significant effort has been carried out in the theory of catalysis on developing the inverse design approaches and discovery of fundamental relationships governing activity of supported catalysts in the group of Prof Tej Choksi; this work is complementary to the continuing development of synthesis strategies for functional catalytic systems in the group of Prof Zeng Hua Chun.

Professor Alexei Lapkin, PI
University of Cambridge

Update on work package 1.1

Design of nano-structured catalysts

Dr LI Bowen (Research Engineer, NUS) has been focusing on the synthesis and application of supported metal nanoparticles. This has proven to be advantageous in many catalytic reactions, providing unique metal-support interaction to enhance catalyst reactivity, stability and product selectivity. Compared with supported catalysts, encapsulated catalysts could provide similar metal-support interaction with added features. The encapsulated morphology could provide spatial confinement effect, allowing synthesis of smaller metal nanoparticles and nanoclusters. In addition, confining metal particles within the porous channels of support materials could effectively reduce particle aggregation when subjected to harsh reaction conditions.

In the past few months under **Prof ZENG Hua Chun's (PI, NUS)** group, he has developed a new synthetic route for the encapsulation of metal nanoclusters within EMT zeolite (Figure 1.1a). The encapsulation was achieved via a step-wise approach. First, EMT support was synthesised from a mixture solution containing sodium hydroxide, sodium silicate and sodium aluminate, using water and alcohol mixture as a solvent. The as-prepared EMT has sodium ions trapped within its framework, which allows subsequent ion exchange with metal ions in solution (Figure 1.1b). The ion exchange process ensures deposition of metal within the microporous EMT channels. Further calcination in static air has yielded encapsulated metal oxide nanoclusters. Owning to the narrow channel diameter (~0.7 nm) of EMT, the produced metal nanoclusters have a diameter of ~0.7 nm, which is much smaller than conventional Pt nanoparticles. EMT with PtO nanocluster encapsulation was adopted for CO_2 hydrogenation reaction, demonstrating enhanced reactivity and CO selectivity. Pt nanoclusters have shown a TOF of 782 h-1, which is more than a 10-fold increase from Pt nanoparticles (64.6 h-1). The CO selectivity of this Pt nanocluster is ~99% at 400°C, which is also higher than the Pt nanoparticles (~93.3%).

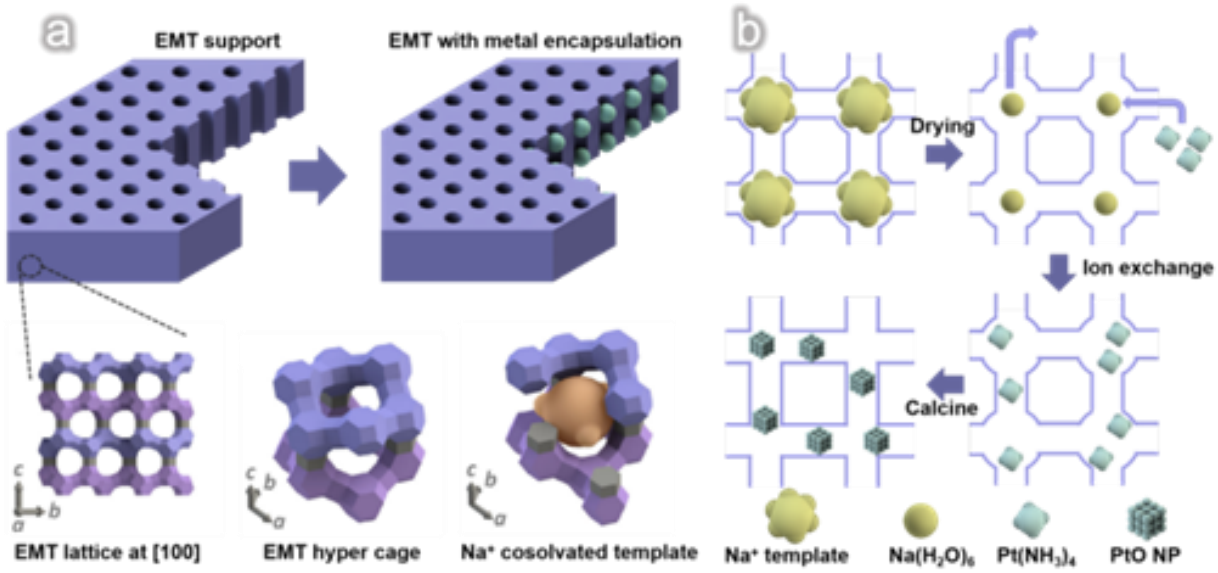


Figure 1.1: Schematic illustration of (a) metal encapsulated within EMT support and (b) synthesis route of encapsulated catalyst via ion exchange and calcination process.

Dr LI Bowen

Mr Alvin LIM Ming Hao (PhD student, NUS) and **Prof. ZENG Hua Chun (PI, NUS)** have transmuted Stöber silica nanospheres (~270 nm in diameter) into either ZnSiO (zinc-silicate) nanoflowers or MgSiO (magnesium-silicate) nanoflowers (c.a. 600 to 800 nm in diameter) through a facile one-pot hydrothermal process respectively (Figure 1.2a-c and Figure 1.3a-c). Unlike our previous works, which primarily uses a bottom-up approach, this work utilises a top-down approach, where silica nanospheres are etched as the sacrificial template. These 2D silicate nanosheets have a thickness approximately less than 10 m, with the EDX elemental mapping revealing homogenous distribution of the doped metals (Zn and Mg), oxygen and silicon throughout both zinc silicate and magnesium silicate structure (Figure 1.2d and 1.3d). While the BET surface area of the silica precursor is measured at 13.8 m2.g-1, the BET surface of Zn-silicate and Mg-silicate is evaluated at 185 and 519. Hence, the surface area is drastically increased over a factor of 10 and 35 respectively while maintaining as dispersed spherical nanoflowers. Current work will focus on functionalising zinc-silicate as catalyst material for methanol production via CO_2 hydrogenation.

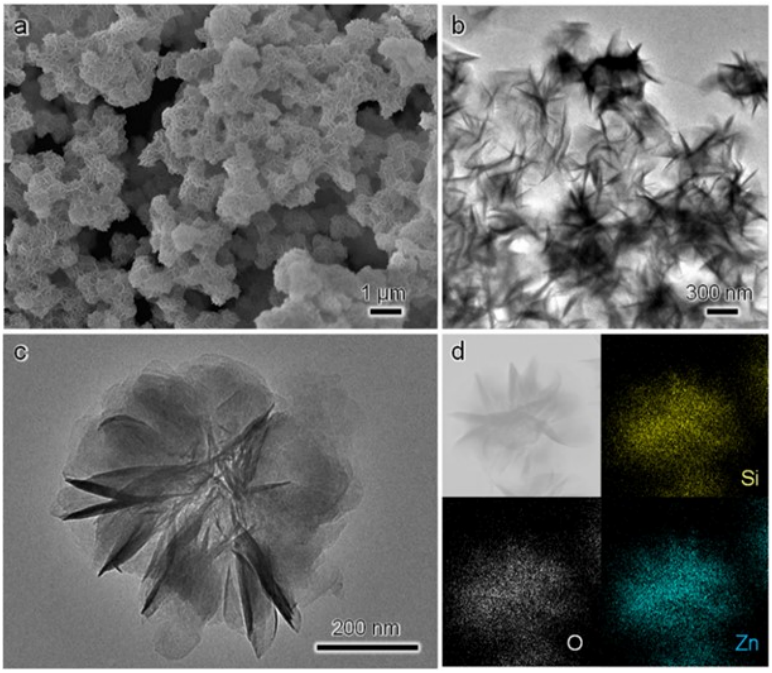


Figure 1.2 (a) SEM image, (b, c) TEM images, and (d) elemental mappings of zinc silicate (ZnSiO).

Mr Alvin LIM Ming Hao

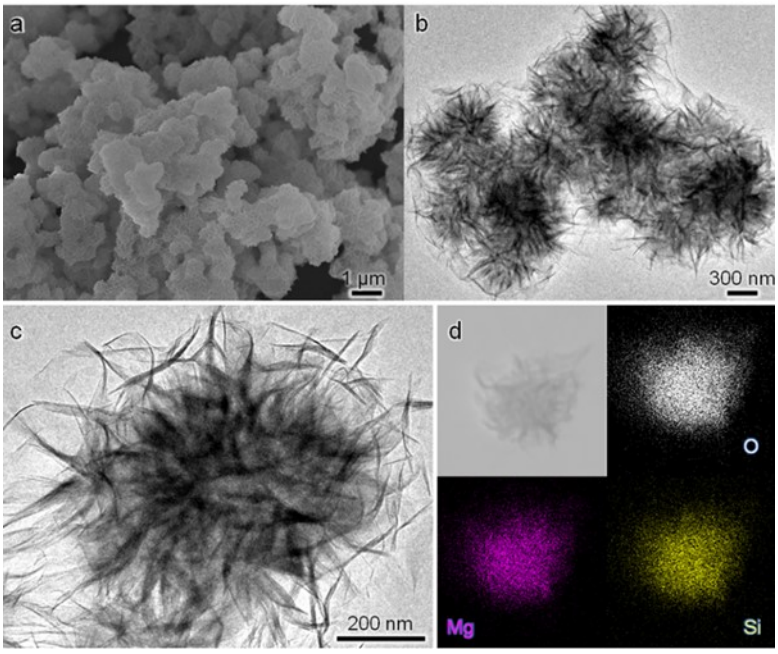


Figure 1.3 (a) SEM image, (b, c) TEM images, and (d) elemental mappings of magnesium silicate (MgSiO).

Mr Alvin LIM Ming Hao

Update on work package 1.2

Novel reactions and functional molecules

Guided by **Prof Alexei LAPKIN (PI, CAM)**, **Dr GUO Zhen (Research Fellow, CARES)** continues to work on three research projects:

1) Improving performance of a tool for chemical route searching. In this project, algorithms for searching long-range routes of complex molecules were implemented. The effectiveness of the method is validated by searching 12-steps synthetic routes of a complex drug which is used for treatment of lymphoma.

2) Working with **Mr Adarsh ARUN (PhD student, CARES)** on networks of bio-feedstocks for chemical productions. Identifying renewable feedstock is an indispensable element for sustainable reaction engineering. In this project, graph-based ontological database will be developed which covers key knowledge of bio-feedstocks from their geographical distributions to chemical conversions.

3) Collaborating with Dr Jana WEBER (University of Cambridge) on a paper regarding the role of digital chemistry in sustainable reaction routes. Combining analysis of big chemical data, energetic assessments and state-of-the-art decision-making, a methodological pipeline for automated reaction network optimisation will target sustainable chemical productions. These tools can guide the development of circular processes on the reaction pathway level. This work has been summarised in a recent paper accepted by *ACS Engineering Au*.

Next, Dr Guo will continue development of a tool to search for chemical routes by implementing new features and identifying new applications through collaboration with IRP members, as well as industrial partners.

Mr Adarsh ARUN (PhD student, CAM) is focusing on identifying sustainable routes from biowaste to chemicals using reaction networks and knowledge graphs. Previously, he submitted a paper entitled "Integration of biowaste into chemical reaction networks" outlining a case study of biowaste sources in Singapore, Malaysia and Indonesia, and an exergy analysis of an organosolv (organic solvent) pre-treatment process to yield cellulose, lignin and xylose feedstock from Oil Palm Empty Fruit Bunch (EFB). He is currently modifying the paper given reviewer feedback. He is also scaling up the workflow and assembling a knowledge graph containing information on countries, biomass sources, biowaste, pre-treatment processes, derivable feedstock, and value-added chemicals.

The other project he is working on involves data mining large chemical databases such as Reaxys to predict impurities and by-products in chemical reactions, which has the potential to aid early-stage process development. The 14-step workflow was successfully tested on three successful case studies, including prediction of impurities from Lersivirine synthesis, which has been performed in the CARES lab (PIPS). A manuscript has been completed and is ready for submission.

Ms Marsha ZAKIR's (Research Engineer, CARES) main interest lies in green electrocatalysis, specifically in the electrochemical reduction of greenhouse gas, carbon dioxide (CO_2R) into value-added chemicals (i.e. ethylene, ethanol etc.). Over the past 6 months, together with **Dr Mikhail KOVALEV (Senior Research Fellow, CARES)**, she developed a more cost-, time- and energy- efficient method to fabricate PTFE based gas diffusion electrodes (GDEs) for use in CO_2R. PTFE based GDEs are relatively new types of GDEs and currently the best performing GDE in the field in terms of long lifetime stability. For CO_2R GDEs to be used in an industrial setting, it is essential to possess long lifetime stability. In addition to fabrication methods, she is also looking to experiment with back pressures in the CO_2R system to extend the lifetime of the GDE. She, along with other researchers – **Dr Magda BARECKA (Research Fellow, CARES)** and **Dr Mikhail KOVALEV (Senior Research Fellow, CARES)** are also studying the reaction mechanism of C13 enrichment in CO_2R flow cell systems.

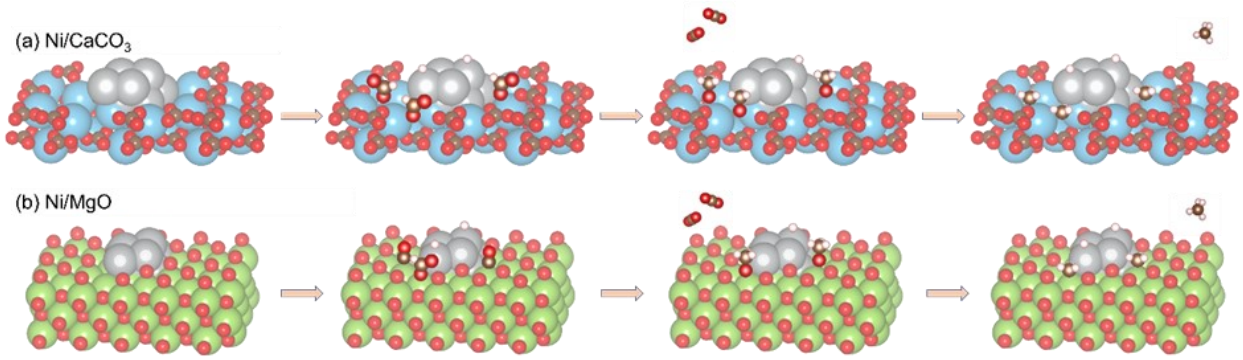


Figure 1.4: Schematic diagram showing the direct hydrogenation of (a) $MgCO_3$ and (b) $CaCO_3$ at the Ni/carbonate interface.

Ms Marsha ZAKIR

Ms KENCHA Satya (Research Engineer, CARES) is primarily focusing on refining the synthesis of zinc oxide nanostructures using the annular flow microreactor at kilogram batch sizes, optimising reactor conditions for process robustness. Quality control protocols are being developed in preparation for large scale synthesis trials.

A lower-cost, mobile version of the annular reactor was developed and is being tested. The housing has been 3D printed in a polypropylene carbon fibre composite (see Figure 1.5).

She plans to continue her research on ZnO nanoparticles synthesis and characterisation, and establish quality control procedures for ZnO nanoparticles synthesis and antibacterial activity testing.

Figure 1.5: 1kg scale ZnO synthesis using annual flow microreactor

Ms KENCHA Satya

Update on work package 1.3

Novel reactors and process technology

Mr FAN Qianwenhao (PhD student, NTU) has been working on the structural modification of Fe -based materials, which are widely utilised as chemical looping oxygen carriers because of their low price, high mechanical strength and environmentally friendly nature. However, the sintering problem restrains its further improvement on redox reactivity and stability. Recently, he developed a yolk–shell structured Fe_2O_3@Y_2O_3 oxygen carrier, with a thin, porous Y_2O_3 shell surrounding a nano-sized Fe_2O_3 core. The synthesis procedure consists of three steps including coating and etching (Figure 1.6a), and the morphology of the resulting products was confirmed by TEM (Figure 1.6b-e). The performance of the oxygen carrier was preliminarily tested by thermogravimetric analysis (TGA) at 650 °C. In each cycle the sample was reduced in 5% H_2 and re-oxidised in air with N_2 purge separating the two phases.

As shown in Figure 1.6f, the Fe_2O_3@Y_2O_3 exhibited an unchanged oxygen carrying capacity of 4 wt% during 100 consecutive redox cycles, without any distinguishable structural damage (Figure 1.6f top inset). The satisfactory sintering resistance of this proposed structure demonstrates the exploitation of transition metal oxides-based nanoreactors as a powerful tool to improve the cycling stability of oxygen carriers. He has also started to apply this nanostructure in other chemical looping reactions and explore various core/shell material combinations.

Dr WONG Roong Jien (Research Fellow, NTU) has been working on photothermal catalytic conversion of CO_2 to methanol and other hydrocarbon chemical feedstock. His current research focuses on using Cu and Zn catalysts. Over the past six months, most of the work has revolved around setting up the reactor system, including commissioning a new gas chromatograph,

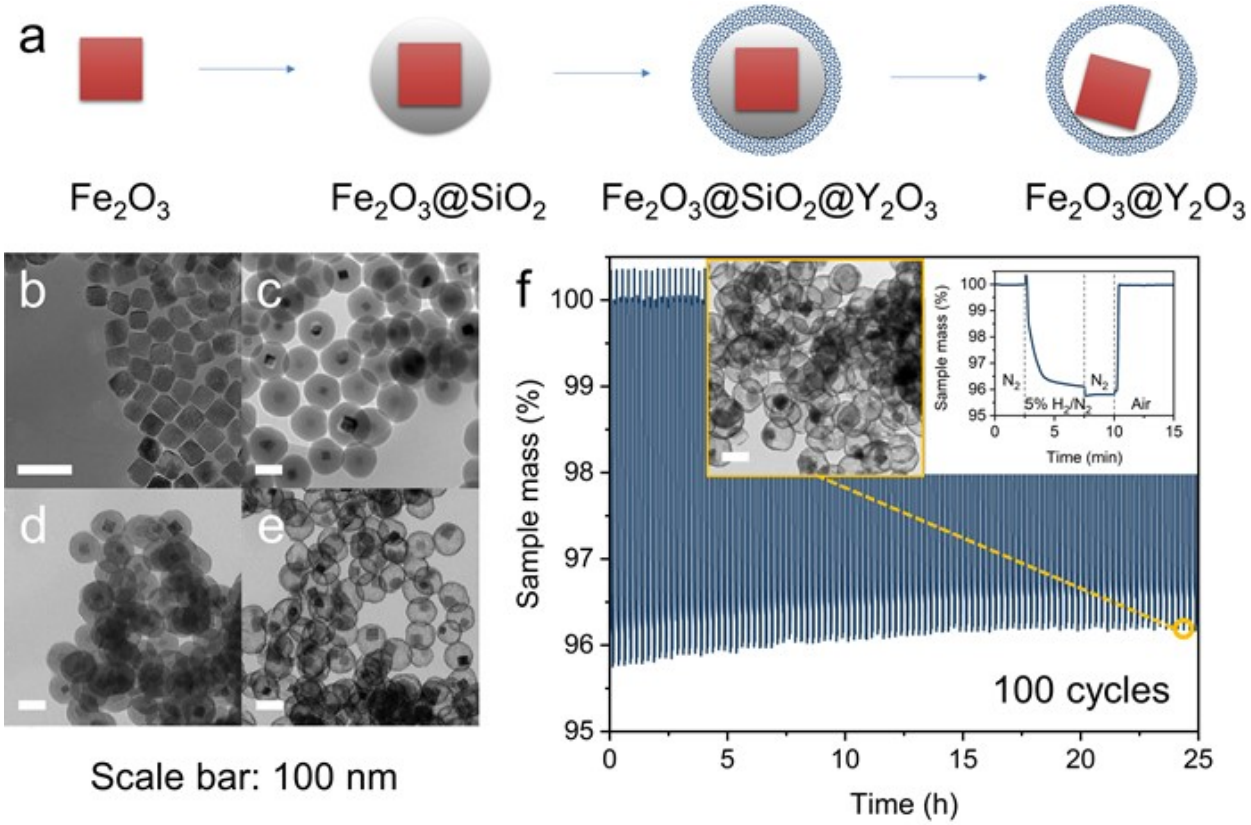


Figure 1.6: Design and performance of Fe_2O_3@Y_2O_3 oxygen carriers for chemical looping combustion.

Mr FAN Qianwenhao

troubleshooting reactor system, calibration, analysis method development, and testing catalyst performance. The reaction involves the use of a high-power Xenon lamp as the light source, which was previously found to boost catalyst performance, promote selectivity, and reduce temperature requirement. He was also training three other students on a related project. He is also involved in multiple grant applications and internal/external collaborations, which resulted in several high impact publications.

Dr TAN Hui Ling's (Research Fellow, NTU) main research interest lies in the development of (photo)catalysts for generation of renewable energy and pollutant abatement. Recently, she has been focusing on the utilisation of Fourier-transform infrared spectroscopy (FTIR) to probe the surface chemistry of numerous catalysts (organic and inorganic materials) with the reactants. The main project that she has been working on is the identification of the adsorption structures of formic acid on TiB_2 and TiB_2-supported Pd catalysts. The strong metal-support interaction (SMSI) between TiB_2 and Pd was found to promote the catalytic activity for formic acid dehydrogenation. Using in-situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) technique, she investigated the temperature and temporal effects of formic acid adsorption on the surfaces of TiB_2 and Pd/TiB_2 catalysts. She has found that formic acid dissociates into formate species on both catalyst surfaces, primarily in monodentate configuration (refer to Figure 1.7). The results would help to provide understanding of the reaction pathways of formic acid dehydrogenation on TiB_2-based catalysts.

Mr Syed SAQLINE (PhD student, NTU) is currently working on the synthesis and evaluation of two new materials – $Ba_3Fe_2O_6$ and $Ba_5Fe_2O_8$, which serve a dual purpose as both oxygen carriers exhibiting chemical looping oxygen uncoupling properties and CO_2 sorbent for reversible CO_2 capture and release. The materials are prepared using the modified Pechini sol-gel method and characterised to determine the phase structure and morphology. The CO_2 uptake capacity of $Ba_3Fe_2O_6$ and $Ba_5Fe_2O_8$ remained unchanged after 20 cycles of sorption-desorption (shown in Figure 1.8). The materials exhibit excellent stability compared to the standard CaO based sorbents where activity deterioration is a major problem. The evolution of the phase compositions of the two barium ferrites during sorption are to be studied by in-situ XRD at high temperature in reactive gas environments.

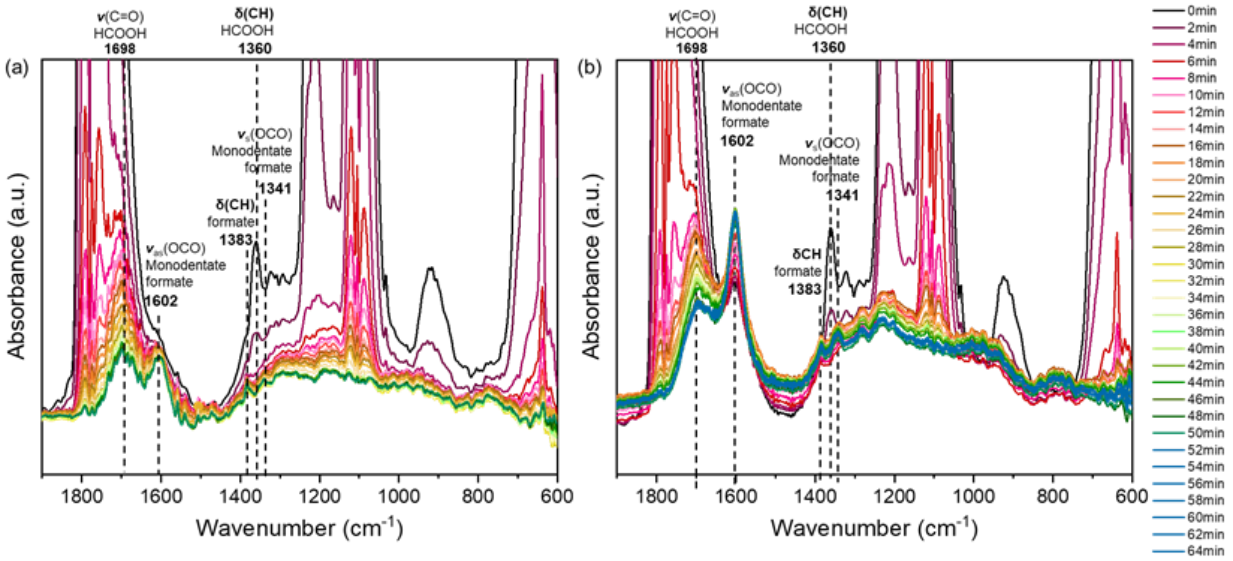


Figure 1.7: In-situ DRIFTS spectra of the time-evolution of HCOOH dissociation into formate species on the surface of (a) TiB_2 and (b) Pd/TiB_2 at 150 °C. All spectra are background corrected using the spectrum of the respective catalysts.

Dr TAN Hui Ling

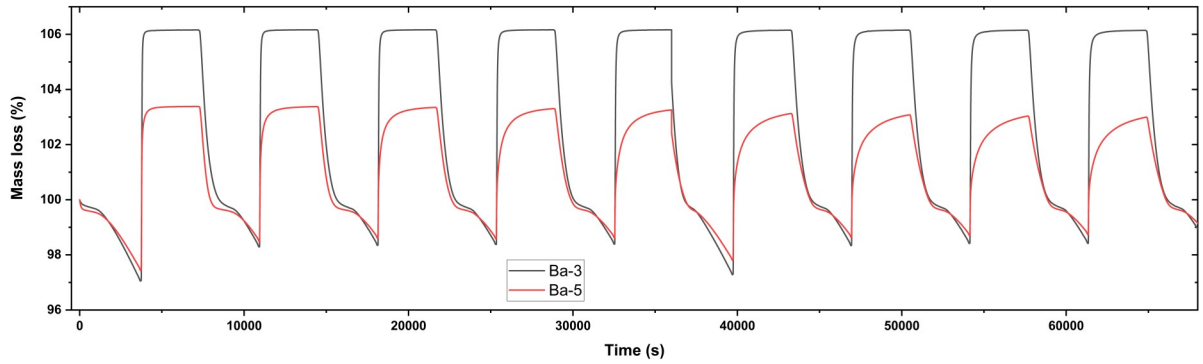


Figure 1.8: Pressure swing between pure CO_2 and N_2 at 900 °C

Mr Syed SAQLINE

Ms Xianyue WU's (Doctoral student, NTU) main research interest lies in the study of CO_2 capture and utilisation. Currently, she is working on an in -situ two-step CO_2 capture and methanation process using Ni-supported-on-alkaline earth metal carbonate dual-function materials. It was discovered that CO_2 conversion and CH_4 selectivity are improved with increasing $CaCO_3/MgCO_3$ ratio, which is attributed to enhanced surface basicity and metal-support interactions. By operating at moderate temperatures, the two-step CO_2 capture -hydrogenation proceeds by allowing direct hydrogenation on carbonates, hence CH_4 production is achieved. She proposed different reaction pathways on $Ni/MgCO_3$ and $Ni/CaCO_3$ interphases and suggested a correlation between the performance of conventional one-step CO_2 methanation and two-step CO_2 capture-hydrogenation, which could be a useful approach to study CO_2 hydrogenation performance of dual -function materials in the future.

Asst Prof Tej CHOKSI's (co-PI, NUS) group is funded by the Emerging Opportunities Fund 08. This grant aims to advance first principles methods to design supported metal catalysts for CO_2 valorisation. In relation to this grant, the group has made the following progress:

1. Established a computational framework to predict the catalytic descriptors (e.g. the binding energy of CO*) at every surface atom of a supported nanoparticle. This model can be generalised across 2D and 3D carbides, nitrides, oxides, and sulphides. The fundamental studies involved in developing this model addressed a long-standing question in the catalysis community related to structure-sensitivity of catalytic reactions. We show that support effects strongly influence structure sensitivity with more negatively charged metal active sites being less structure sensitive.
2. We are in the process of developing a computational framework to determine the equilibrium morphology of a generic supported nanoparticle. A key input to this framework is the adhesion energy between the metal and the support. In the last 6 months, we conceptualised simple linear models that correlate this adhesion energy with basic chemical properties of elements constituting the supported metal nanoparticle. By predicting the adhesion energy on-the-fly, we can build atomistic models of supported nanoparticles that will, in turn, enhance the accuracy of first principles based microkinetic studies.
3. The group has five publications currently in advanced stages of preparation for submission.

Additional collaborative work pursued with other CARES investigators are:

The group with **Asst Prof Paul LIU (PI, NTU)** are unravelling how the strong metal support phenomena (SMSI), ubiquitous to supported metal particles, influences reaction rates. To this end, they created a bespoke microkinetic model for formic acid dehydrogenation on a series of metal/support interfaces. This microkinetic model will be used to understand stability-reactivity

trade-offs engendered by SMSI phenomena.

The group with **Prof Alexei LAPKIN (PI, CAM)** are developing an inverse design approach to identify bimetallic systems that are resistant to coking during the dry reforming of methane. In the last 6 months, they have formalised the plan of action and begun first principles studies on 30+ Ni-bimetallic systems. These first principles studies will be used to build linear scaling relations that will enable efficient interpolation across the space of materials being screened.

The group with **Prof WANG Xin (PI, NTU)** are designing single site catalysts on carbon supports that enable the direct synthesis of H_2O_2 through oxygen electro-reduction. To that end, they used first principles density functional theory to rationalise why sulphur modified Ni sites increase the selectivity to H_2O_2 production. This manuscript is currently in preparation.

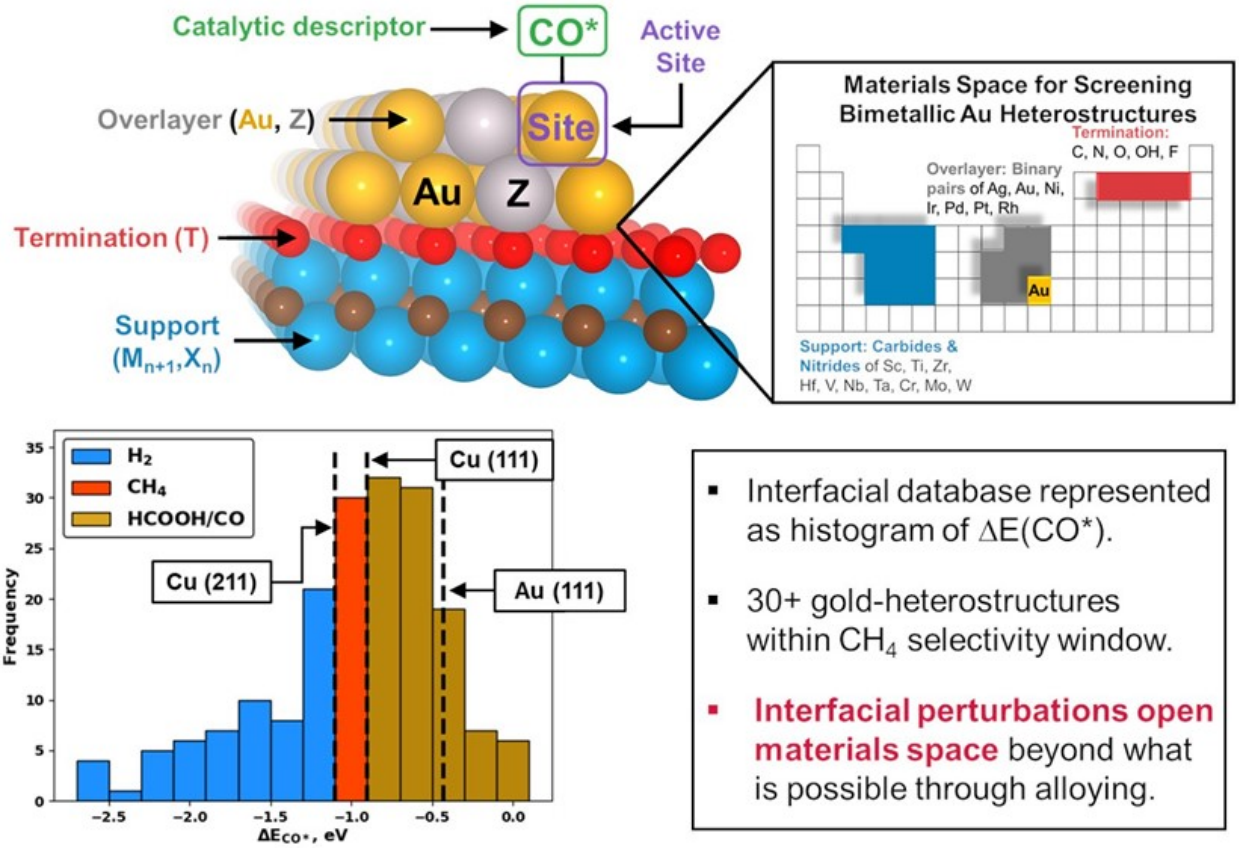


Figure 1.9: Tej Choksi's group developed a high-throughput screening strategy to identify gold/support heterostructures that are selective towards CH_4. The electronic interactions between the gold atoms and the support lead to several materials entering the selectivity window for CH_4, a window ordinarily restricted to only monometallic copper and its alloys.

Asst Prof Tej CHOKSI

Dr Mikhail KOVALEV's (Senior Research Fellow, CARES) research interests focuses in the area of gas diffusion electrodes preparation (GDE) and analytical studies of its performance. The complicated GDE structure comprises of many layers that were optimised for large sizes over 100 cm^2 which has increased from previously reported sizes of 16 cm^2. Large electrodes tested in a flow cell with working size of 10x10 cm^2 showed similar efficiency to smaller cells of 1x1 cm^2 and 2x2 cm^2. Analytical studies of reasons for GDE failure revealed that the formation of some polymerisable intermediates can significantly reduce hydrophobicity. Identification of this failure mechanism for Cu-GDEs has important consequences for their application to industrial-scale CO_2 reduction. First, while the use of strongly basic electrolytes has ben shown to increase FEs

to useful products such as ethylene, their use may also accelerate the polymerisation of minor products, reducing the useful lifetime of the system via the mechanism described here. Secondly, it points out the importance of selectivity; it would be advantageous to avoid to the degree possible, the formation of reactive products such as aldehydes, although this may be difficult as they are believed to be intermediates to ethylene. Finally, it suggests that long-term operation of Cu-GDEs at industrially viable current densities in strong bases may require either maintenance or regeneration to mitigate the effects of surface hydrophilisation by PA or other species.

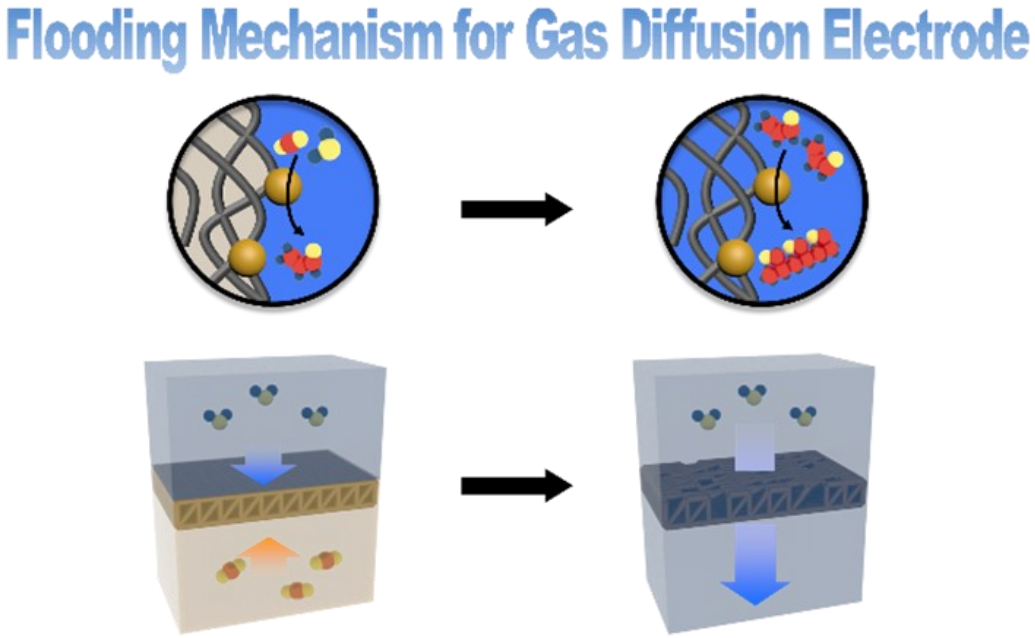
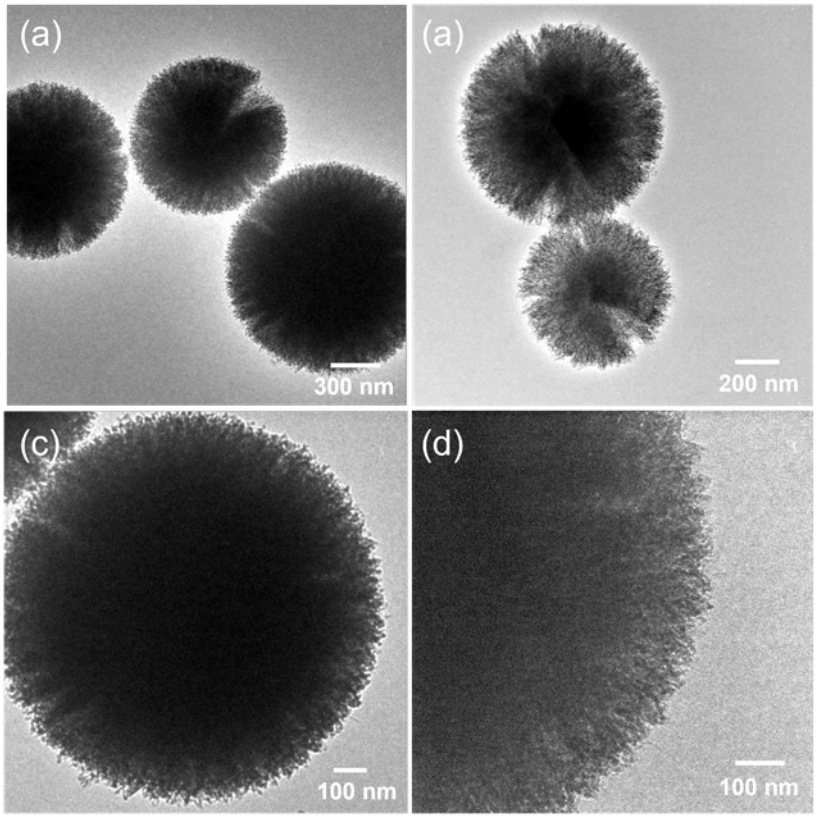


Figure 1.10: Diagram showing flooding mechanism for gas diffusion electrodes (GDE)

Dr Mikhail KOVALEV

Dr ZHOU Shenghui (Research Fellow, NUS) and **Prof ZENG Hua Chun (PI, NUS)** developed a trimetal (Co, Fe and Zn) atoms confined in N-doped carbon catalyst for CO_2 hydrogenation via pyrolysis of Co, Fe doped amorphous ZIF-90. First, the amorphous ZIF-90 precursor with a dandelion-like morphology composed of numerous radially distributed nanorods, was obtained using a surfactant assisted method. Then, after precise controlling of exchange of Co^{2+}, Fe^{3+} cations with Zn^{2+} in ZIF-90, the Co, Fe doped ZIF-90 (CoFe-ZIF-90) could be prepared. Next, the CoFe -doped ZIF-90 precursor was transformed to CoFeZn/NC catalyst via a heat-treatment in an Ar atmosphere for 1 h. The HRTEM images (Figure 1.11a-d) showed that CoFeZn/NC catalysts keep the dandelion-like morphology after pyrolysis process. The absence of visible metal nanoparticles indicate that the doped transition metals are highly dispersed. According to our ICP results presented in Figure 1.11e, the contents of Co, Fe and Zn in the CoFeZn/NC catalysts were 1 wt%, 0.22 wt% and 7.46 wt%, respectively. This dandelion-like CoFeZn/NC catalyst was used for CO_2 hydrogenation reaction. The result show that CoFeZn/NC has high catalytic activity (TOF = 21.32 $mol_{Co}/mol_{CO2}/h$) and CO selectivity (92.4%) at mild reaction temperature.



(e) Catalyst	Co	Fe	Zn
CoFeZn/NC	1.0	0.22	7.46

Figure 1.11: (a-d) Representative TEM images of dandelion-like CoFeZn/NC catalyst. (e) ICP results of Co, Fe and Zn contents in CoFeZn/NC catalyst.

Dr ZHOU Shenghui

Dr Nicholas JOSE (Research Fellow, CARES) has been working on a number of different projects over the previous six months:

Scale-up platform: A scale-up platform for advanced materials utilising a "numbering-up" approach with passive regulation, which was previously simulated, was built in Cambridge. Sensors were installed to enable measurement of individual reactor flowrates. A full user interface was developed for digital operation and automated experiments. The device was tested on three test reactions at low flowrates, and performed within specification; however, a number of issues were discovered that need to be improved upon before transitioning to the synthesis of materials at higher flowrates, pressures and temperatures. This device has the capability to scale nanomaterial synthesis up to 160 kg/day.

Simulations: Simulations on the annular flow reactor, which were performed in a master's project, have had successful preliminary results, with close agreement to measured reactor parameters like micromixing speed and pressure drop. These results are being further refined and are being drafted for publication.

Automation: A coding framework for rapid automation of laboratory equipment has been devised and is currently being tested for automating reaction equipment. This framework, Flab (standing for Fast, Flexible and Fun) is designed to be experimentalist-friendly with a modular architecture, fast implementation of device drivers and a simple interface. After a number of successful case studies, the platform has been improved upon, and is now published on Pypi, and a more robust user interface has been built for student use. New capabilities to allow remote use without screen sharing software and the implementation of machine learning algorithms are now being developed.

Scientific output

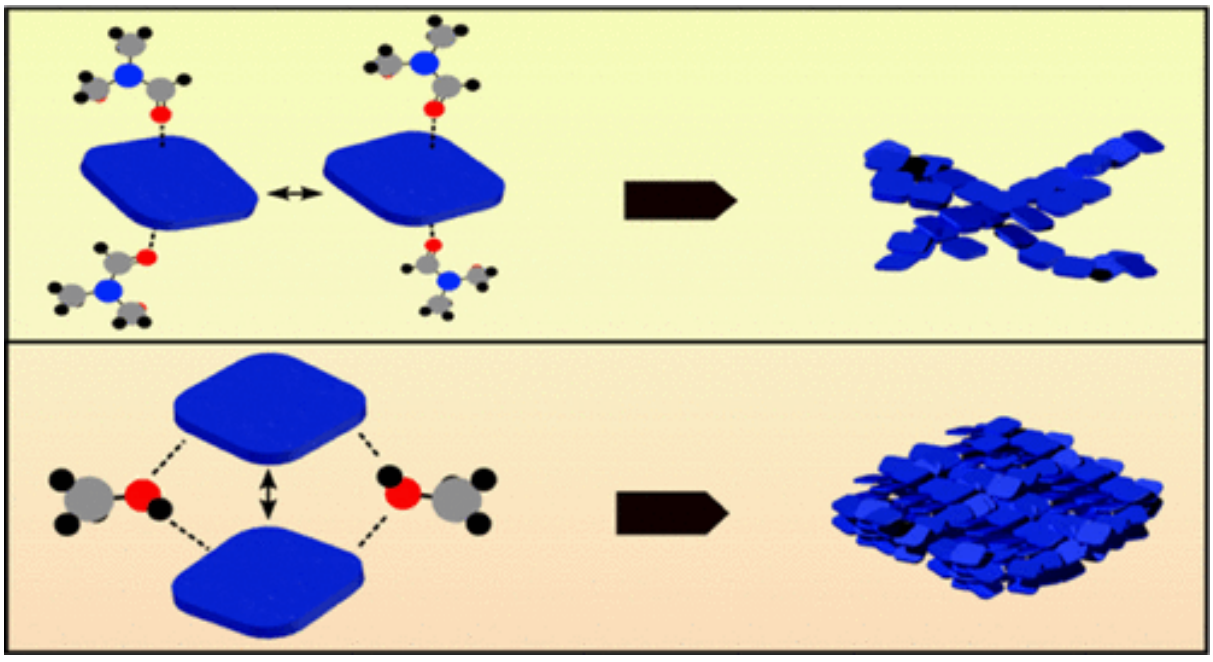
The following are the CREATE-acknowledged publications generated by IRP 1 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Assembly of Two-Dimensional Metal Organic Framework Superstructures via Solvent-Mediated Oriented Attachment

Nicholas Jose, Jithin Varghese, Samir Mushrif, Hua Chen Zeng, and Alexei Lapkin, *Journal of Physical Chemistry*

DOI: 10.1021/acs.jpcc.1c06699

Abstract: Due to their high anisotropy and tunable chemical composition, two-dimensional metal organic frameworks (2D MOFs) have great potential as building blocks for next-generation materials in a diverse range of applications—from electrochemical catalysis to membrane separation. However, the controllable synthesis is complicated by the environment–surface interactions that arise from the high anisotropy, thinness, and functionally diverse surfaces of 2D MOFs. Liquid cell transmission electron microscopy (LCTEM) offers a unique opportunity to study these interactions in situ. In this work, we analyzed the effects of different solvent environments on the structure and aggregation dynamics of copper benzene dicarboxylic acid (CuBDC) nanosheets, which were synthesized using a high shear annular microreactor. LCTEM revealed that 2D MOF nanosheets undergo oriented attachment and that the rate and direction of oriented attachment is controlled by solvent–surface interactions. We investigated the nature of these solvent interactions using density functional theory calculations, which suggest that the binding energy of solvents to different MOF surfaces is likely responsible for this behavior. The CuBDC nanosheets were then applied as adsorbents in organic solvents, in which we showed how solvent-mediated oriented attachment could significantly affect adsorption properties.



Revamping SiO_2 Spheres by Core–Shell Porosity Endowment to Construct a Mazelike Nanoreactor for Enhanced Catalysis in CO_2 Hydrogenation to Methanol

Mohammadreza Kosari, Uzma Anjum, Shibo Xi, Alvin M. H. Lim, Abdul Majeed Seayad, Emmanuel A. J. Raj, Sergey M. Kozlov, Armando Borgna, and Hua Chun Zeng, *Advanced Functional Materials*

DOI: 10.1002/adfm.202102896

Abstract:: Beyond the catalytic activity of nanocatalysts, the support with architectural design and explicit boundary could also promote the overall performance through improving the diffusion process, highlighting additional support for the morphology-dependent activity. To delineate this, herein, a novel mazelike-reactor framework, namely multi-voids mesoporous silica sphere ($MVmSiO_2$), is carved through a top-down approach by endowing core-shell porosity premade Stöber SiO_2 spheres. The precisely-engineered $MVmSiO_2$ with peripheral one-dimensional pores in the shell and interconnecting compartmented voids in the core region is simulated to prove combined hierarchical and structural superiority over its analogous counterparts. Supported with CuZn-based alloys, mazelike $MVmSiO_2$ nanoreactor experimentally demonstrated its expected workability in model gas-phase CO_2 hydrogenation reaction where enhanced CO_2 activity, good methanol yield, and more importantly, a prolonged stable performance are realized. While tuning the nanoreactor composition besides morphology optimization could further increase the catalytic performance, it is accentuated that the morphological architecture of support further boosts the reaction performance apart from comprehensive compositional optimization. In addition to the found morphological restraints and size-confinement effects imposed by $MVmSiO_2$, active sites of catalysts are also investigated by exploring the size difference of the confined CuZn alloy nanoparticles in CO_2 hydrogenation employing both in-situ experimental characterizations and density functional theory calculations.

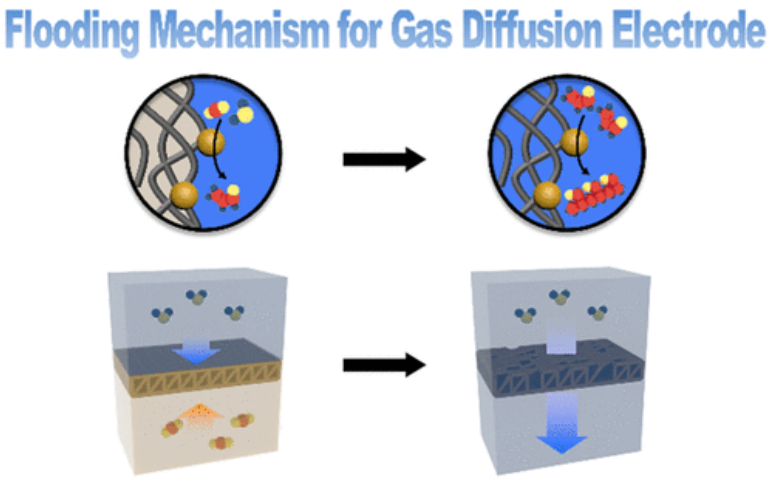
Minor Product Polymerization Causes Failure of High-Current CO_2-to-Ethylene Electrolyzers

Mikhail Kovalev, Hangjuan Ren, Marsha Zakir Muhamad, Joel Ager, and Alexei Lapkin,

ACS Energy Letters

DOI: 10.1021/acsenergylett.1c02450

Abstract: Flooding of gas diffusion electrodes (GDEs) used in electrochemical conversion of CO_2 to ethylene is caused by polymerization of minor products. The polymer so created reduces the hydrophobicity of the GDE, leading initially to a reduction in the ethylene yield and finally to complete failure.

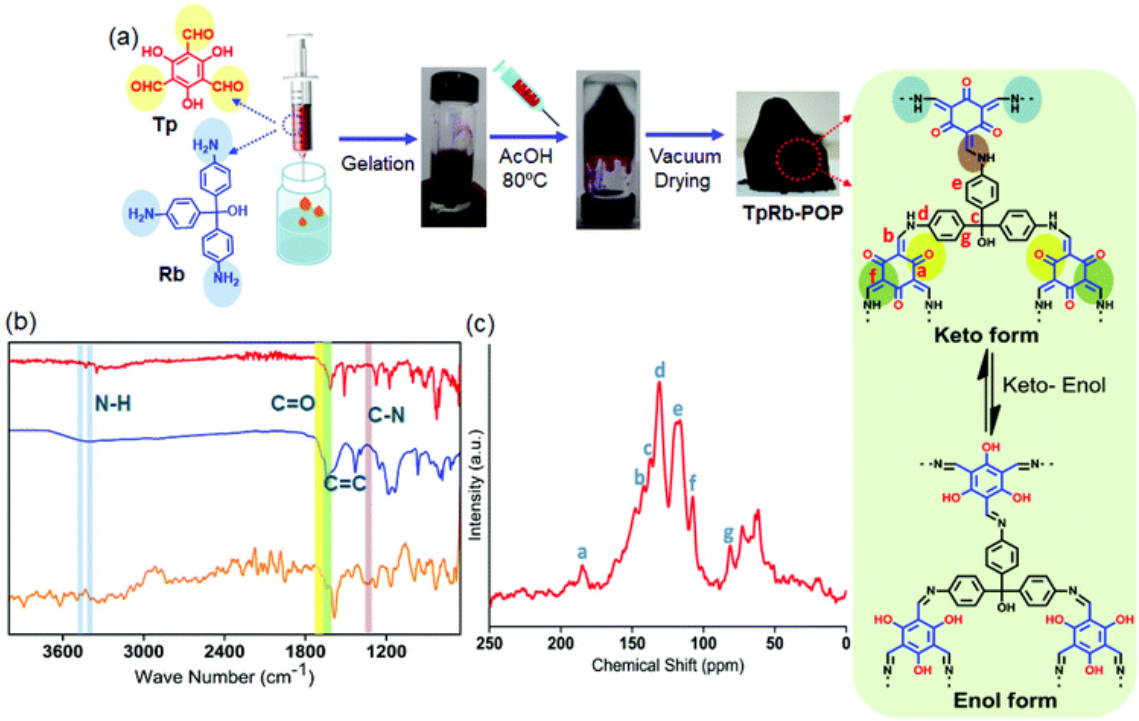


Organogel-assisted porous organic polymer embedding Cu NPs for selectivity control in the semi hydrogenation of alkynes

Ratul Paul, Subhash Chandra Shit, Arunima Singh, Roong Jien Wong, Duy Quang Dao, Boby Joseph, Wen Liu, Saswata Bhattacharya, and John Mondal, *Nanoscale*

DOI: 10.1039/D1NR07255B

Abstract: Heteroatom-rich porous-organic-polymers (POPs) comprising highly cross-linked robust skeletons with high physical and thermal stability, high surface area, and tunable pore size distribution have garnered significant research interest owing to their versatile functionalities in a wide range of applications. Here, we report a newly developed organogel-assisted porous-organic-polymer (POP) supported Cu catalyst (Cu@TpRb-POP). The organogel was synthesized via a temperature induced gelation strategy, employing Schiff-base coupling between 2,4,6 -triformylphloroglucinol aldehyde (Tp) and pararosaniline base (Rb). The gel is subsequently transformed to hierarchical porous organic structures without the use of any additive, thereby offering advantageous features including extremely low density, high surface area, a highly cross-linked framework, and a heteroatom-enriched backbone of the polymer. During the semi-hydrogenation of terminal and internal alkynes, the Cu@TpRb-POP-B catalyst with Cu embedded in the TpRb-POP structure consistently demonstrated improved selectivity towards alkenes compared to Cu@TpRb-POP-A, which contains Cu NPs exposed at the exterior surfaces of the POP support. Additionally, Cu@TpRb-POP-B showed higher stability and reusability than Cu@TpRb-POP-A. The superior performance of the Cu@TpRb-POP-B catalyst is attributed to the steric hindrance effect, which controls the product selectivity, as well as the synergistic interaction between the heteroatom-rich POP framework and the embedded Cu NPs. Both the effects are corroborated by experimental characterization of the catalysts and density functional theory (DFT) calculations.

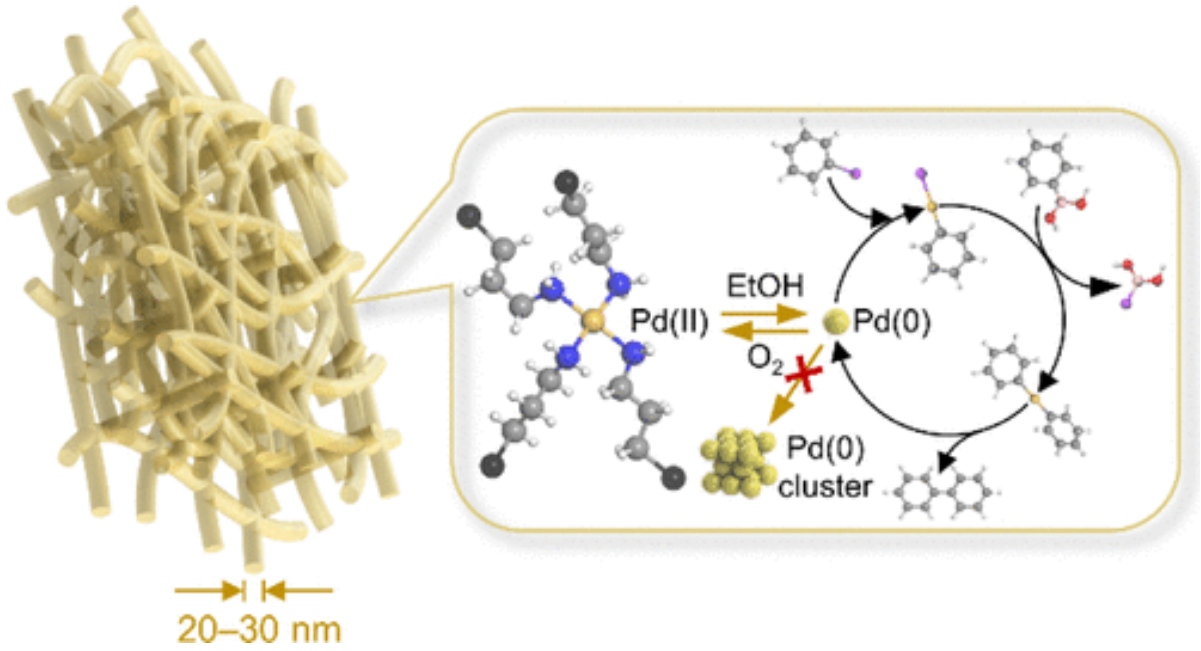


Nanowire Networks of Metal–Organosilicates as Reversible Pd(II) Reservoirs for Suzuki Coupling Reactions

Yu Shao and Hua Chun Zeng, *ACS Applied Nano Materials*

DOI: 10.1021/acsanm.1c02311

Abstract: Formation of metallic palladium nanoclusters is an issue that hampers effective utilization of this precious metal in Suzuki–Miyaura and other cross-coupling reactions. In this regard, reversibility of shuttling between oxidative-state precatalysts and metallic-state acting catalysts is considered as a key for the design of Pd-based nanocatalysts. Herein, three-dimensional (3D) copper–organosilicate (Cu–OS) nanowire networks derived from 3-aminopropyl trimethoxysilane precursors have been demonstrated as an effective, reversible Pd(II) reservoir for Suzuki coupling reactions. In particular, the Pd ion-exchanged 3D nanowire networks exhibit excellent reactivity, stability, and recyclability, with no detectable formation of palladium nanoclusters and no perceptible loss of catalytic activity throughout 10 reaction cycles. A reversible Pd(II)–Pd(0)–Pd(II) shuttling between the solid-phase reservoir and liquid-phase coupling reaction was recognized through our extensive mechanistic investigations and material characterizations. High-throughput studies suggest that besides the decent recyclability, outstanding catalytic performance was due to the structural and compositional merits of the 3D nanowire networks. The scale of the overall macroscopic framework is in the micrometer range, which facilitates facile catalyst recovery. Meanwhile, the nanometer-scale 1D constituents offer high openness and accessibility for effective Pd shuttling. Chemically, the relatively weak alkylamine ligands circumvent the over-coordination issue commonly encountered by strong ligands and effectively prevent the formation of Pd nanoclusters. Compared with a number of state-of-the-art Pd-based catalysts, our 3D nanowire networks manifest excellent performance and recyclability simultaneously.

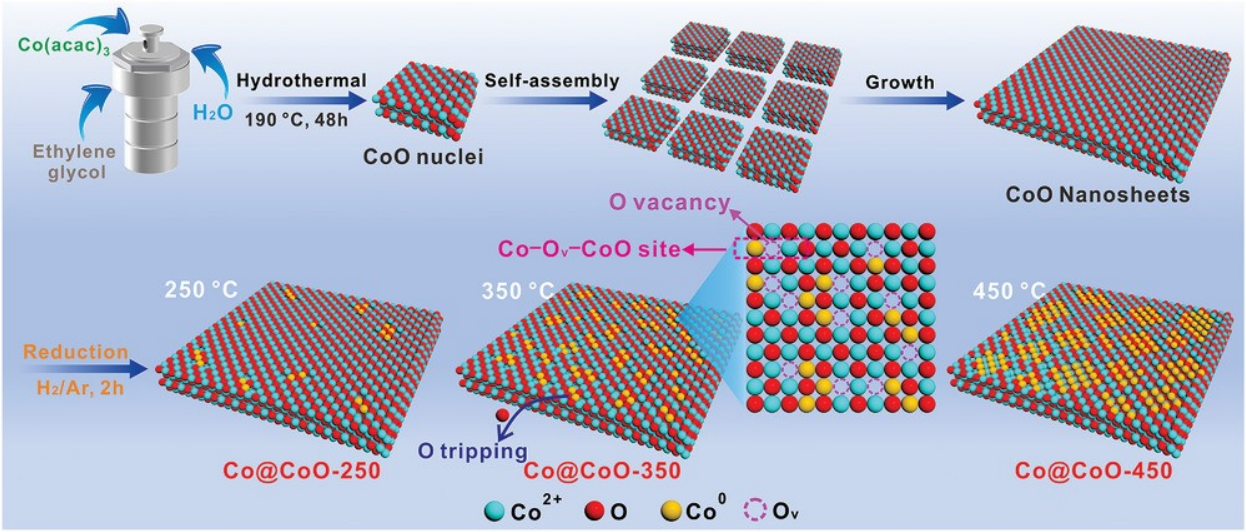


Elucidating the Strain–Vacancy–Activity Relationship on Structurally Deformed Co@CoO Nanosheets for Aqueous Phase Reforming of Formaldehyde

Kaicheng Qian, Yong Yan, Shibo Xi, Tong Wei, Yihu Dai, Xiaoqing Yan, Hisayoshi Kobayashi, Sheng Wang, Wen Liu, Renhong Li, *Small*

DOI: 10.1002/smll.202102970

Abstract: Lattice strain modulation and vacancy engineering are both effective approaches to control the catalytic properties of heterogeneous catalysts. Here, Co@CoO heterointerface catalysts are prepared via the controlled reduction of CoO nanosheets. The experimental quantifications of lattice strain and oxygen vacancy concentration on CoO, as well as the charge transfer across the Co–CoO interface are all linearly correlated to the catalytic activity toward the aqueous phase reforming of formaldehyde to produce hydrogen. Mechanistic investigations by spectroscopic measurements and density functional theory calculations elucidate the bifunctional nature of the oxygen-vacancy-rich Co–CoO interfaces, where the Co and the CoO sites are responsible for C-H bond cleavage and O□H activation, respectively. Optimal catalytic activity is achieved by the sample reduced at 350 °C, Co@CoO-350 which exhibits the maximum concentration of Co–CoO interfaces, the maximum concentration of oxygen vacancies, a lattice strain of 5.2% in CoO, and the highest aqueous phase formaldehyde reforming turnover frequency of 50.4 h−1 at room temperature. This work provides not only new insights into the strain–vacancy–activity relationship at bifunctional catalytic interfaces, but also a facile synthetic approach to prepare heterostructures with highly tunable catalytic activities.

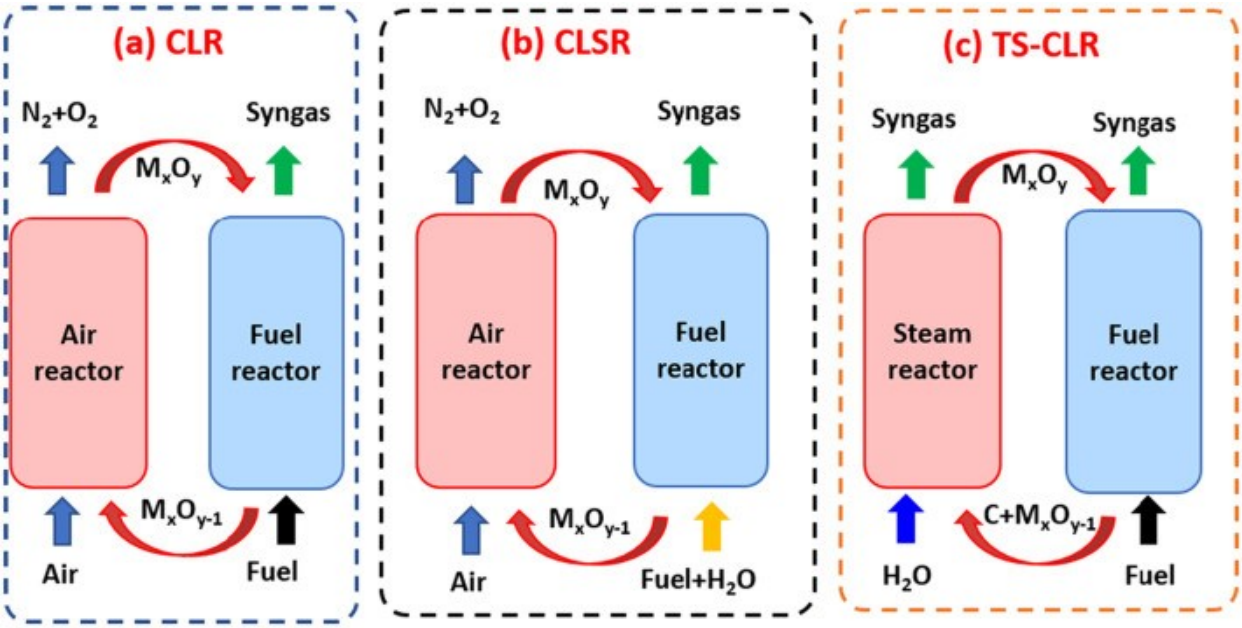


Optimisation of syngas production from a novel two-step chemical looping reforming process using Fe-dolomite as oxygen carriers

Tingting Xu, Xun Wang, Bo Xiao, Haibo Zhao, Wen Liu, *Fuel Processing Technology*

DOI: 10.1016/j.fuproc.2022.107169

Abstract: The production of syngas from hydrogen carbon feedstocks such as natural gas and biomass is of high importance to the chemical industry. In conventional chemical looping steam reforming (CLSR), the composition of the syngas produced is limited by the chemical equilibrium of the water-gas-shift reaction. In this study, we demonstrate that a two-step chemical looping reforming (TS-CLR) process is capable of alleviating the equilibrium limit to produce syngas of higher CO and H_2 contents. For example, the total mole fraction of H_2 and CO in the syngas produced from the conventional CLSR of toluene at 900 °C is limited to below 89.4 vol% (dry basis), whereas TS-CLR could produce syngas with >94 vol% of CO and H_2 under the same conditions. The TS-CLR process is best carried out in a bed of Fe-dolomite oxygen carriers with a Ca:Fe ratio of 1:1 (denoted as C1F1). Compared to the pure Ca2Fe2O5 and Fe2O3/Al2O3 oxygen carriers, the C1F1 affords improvements in syngas yield, carbon conversion and syngas purity. The superior performance of C1F1 is attributed to the promotion of the lattice oxygen activities of Ca2Fe2O5 by MgO, as well as its excellent phase reversibility over redox cycles.

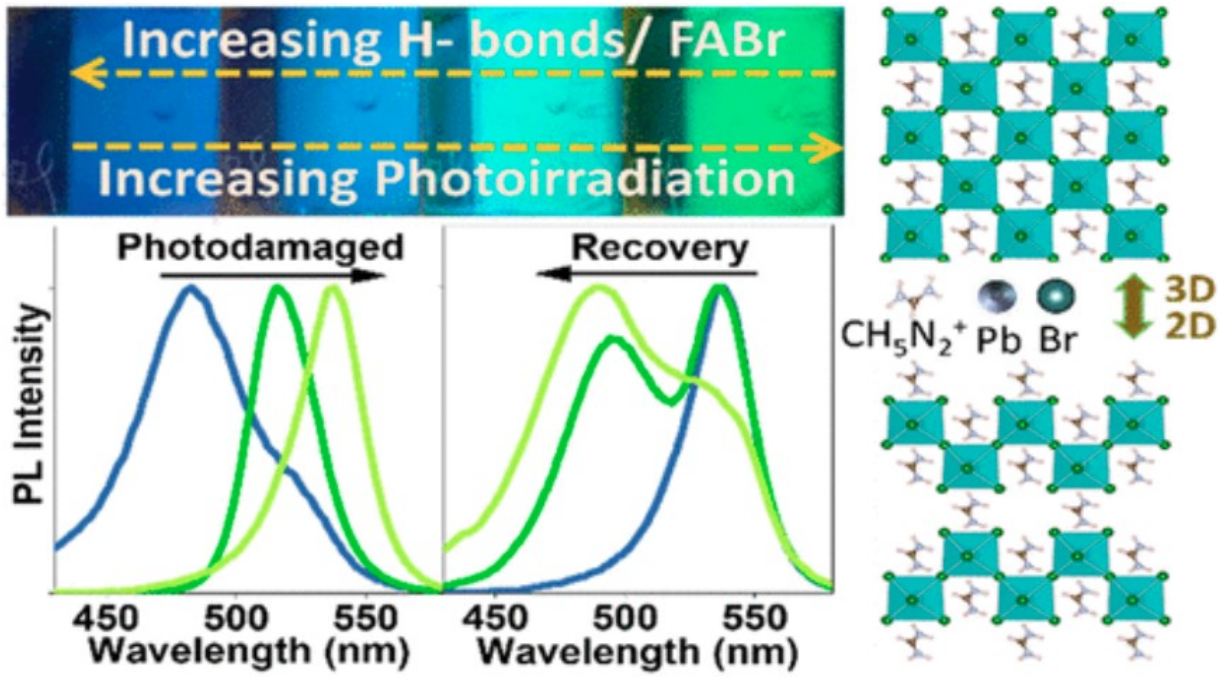


Reversible Photochromism in ⟨110⟩ Oriented Layered Halide Perovskite

Anil Kanwat, Biplab Ghosh, Si En Ng, Prem J. S. Rana, Yulia Lekina, Thomas J. N. Hooper, Natalia Yantara, Mikhail Kovalev, Bhumika Chaudhary, Priyanka Kajal, Benny Febriansyah, Qi Ying Tan, Maciej Klein, Ze Xiang Shen, Joel W. Ager, Subodh G. Mhaisalkar, and Nripan Mathews, *ACS Nano*

DOI: 10.1021/acsnano.1c10098

Abstract: Extending halide perovskites' optoelectronic properties to stimuli-responsive chromism enables switchable optoelectronics, information display, and smart window applications. Here, we demonstrate a band gap tunability (chromism) via crystal structure transformation from three-dimensional FAPbBr3 to a ⟨110⟩ oriented FAn+2PbnBr3n+2 structure using a monohalide/cation composition (FA/Pb) tuning. Furthermore, we illustrate reversible photochromism in halide perovskite by modulating the intermediate n phase in the FAn+2PbnBr3n+2 structure, enabling greater control of the optical band gap and luminescence of a ⟨110⟩ oriented monohalide/cation perovskite. Proton transfer reaction-mass spectroscopy carried out to precisely quantify the decomposition product reveals that the organic solvent in the film is a key contributor to the structural transformation and, therefore, the chromism in the ⟨110⟩ structure. These intermediate n phases ($2 \leq n \leq \infty$) stabilize in metastable states in the FAn+2PbnBr3n+2 system, which is accessible via strain or optical or thermal input. The structure reversibility in the ⟨110⟩ perovskite allowed us to demonstrate a class of photochromic sensors capable of self-adaptation to lighting.



Other activities and achievements

Asst. Prof Paul LIU (PI. NTU) gave a presentation (virtual) at AIChE Annual meeting 2021 titled: Strong Metal-Support Interaction for 2D Materials: Application in Noble Metal/TiB2 and Their Remarkable Catalytic Performance for Formic Acid Dehydrogenation, on 16 November 2021.

Asst. Prof Tej CHOKSI's (co-PI, NTU) team gave a presentation (virtual) at three conferences. Two were presented at the AIChE Annual Meeting in Boston in November 2021, titled "Elucidating How Nanoparticle Stability Metrics Depend on the Choice of Exchange Correlation Functionals Using Analytical Frameworks" and "Tailoring Structure Sensitivity of Metal Nanoparticles on 2D and 3D Supports by Controlling Electrostatic Interactions at the Metal-Support Interface". One presentation was delivered in December 2021 at the Young Electrochemists: Recent Advances in Theoretical Electrochemistry at the University of Barcelona titled: "Enhancing the Selectivity of Oxygen and CO_2 Reduction Electrocatalysts by Tailoring Chemical Environments Beyond the Binding Site".

Prof ZENG Hua Chun (PI, NUS) has a journal article in press for *ACS Catalysis* titled "Single Solid Precursor-Derived Three-Dimensional Nanowire Networks of CuZn-Silicate for CO_2 Hydrogenation to Methanol".

Ms KENCHA Satya (Research Engineer, CARES) has been engaging with Dow Chemical and Grafoid Inc in Singapore for the industrial use of nanostructured zinc oxides in antimicrobial applications. Her current work focuses on validation of formulation efficacy against *E.coli* models, in qualitative and quantitative assays.

Dr Nicholas JOSE (Research Fellow, CARES) has completed successful trials with Dow Chemical, showing that antimicrobial zinc oxides that were previously synthesised in the AMPLE project, performed as good as conventional antimicrobials in pavement coatings, but with much less toxicity and environmental impact. These results are being drafted into a report.

His team has also been accepted as a part of the Wolfson College Living Labs to demonstrate their zinc oxide coatings in a college setting. In this project, they are collaborating with Crown Paints, a large paint producer in the UK, to produce indoor paint formulations.

He also founded a company called Accelerated Materials Ltd., a spin-off to commercialise the innovations made in reactor technology and machine learning for nanomaterials, which won first place in the Cambridge Enterprise Chris Abell Postdoc Business Plan Competition, held in November 2021. The prize was 20,000GBP and a 1-year membership at Cambridge's Ideaspace.

A short film entitled "Small Solutions for Big Problems" was created with artists in the UK as part of the University of Cambridge's Creative Encounters. The objectives of this film were to attract the general public to the research mission in IRP1 (i.e. using nanomaterials for sustainability) and to also cast nanotechnology in a positive light. It was screened at the ESRC Festival of Social Sciences and the recent Cambridge Festival, and can be seen here: https://www.youtube.com/watch?v=HZiXsjoi5Es. The film features an original song and handmade animations.

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:

Dr Adrian FISHER
University of Cambridge

Professor WANG Xin
Nanyang Technological University

Professor LEE Jim Yang
National University of Singapore

OVERVIEW

The IRP 2 research team have focused on development of novel electrocatalytic routes for the development of low-carbon, clean synthesis methods in the areas of hydrogen, formate and a range of speciality chemicals. As with previous studies these have combined experimental and computational strategies to allow translation of the new electrocatalytic processes to be employed in novel electrosynthetic reactors.

Dr Dai Chencheng and Dr Sun Libo have continued their work in the area of microfluidic devices fabricated in the IRP 2 clean room facilities, alongside exploring new catalytic processes. Electrocatalytic oxidation of methanol has been explored leading to new electro-oxidation routes for methanol to formate. This approach has employed iron-substituted lanthanum cobaltite ($LaCo1-xFexO3$) with Fe/Co ratios identified as providing substantial influence in both activity and selectivity. On detailed examination the higher affinity of Fe and Co to the two reactants: CH_3OH and $OH-$, respectively was identified as a key aspect of electrocatalytic performance.

The work of Ms Freyja Dagbjartsdóttir, who is sponsored by our industrial collaborator Syngenta, and Prof Adrian Fisher in Cambridge has targeted new numerical approaches and models for the intelligent design of the electrosynthesis plants located in the IRP 2 laboratories. The complexities of designing dynamic electrosynthetic devices with the array of competing electrocatalytic processes and adaptive/temporal changes make it difficult to develop first-principle models to aid in the study of the electron path and mechanistic complexity of redox reaction. In this reporting period in Cambridge with Prof Adrian Fisher we have been exploring the application of a time series analysis and long short-term memory (LSTM) network approach to tackle rapid design and online interpretation of the reactor i/V characteristics. In this work, a Seasonal and Trend Decomposition route is adopted using locally estimated scatterplot smoothing or LOESS (STL) to decompose the current density profile of the i/V characteristics of a electrochemical signal. A Long Short-Term Memory (LSTM) network is then used to predict the one-step-ahead current density using lagged values of the output.

Ms Dagbjartsdóttir's work has been exploring the application of electrochemical impedance spectroscopy in the analysis of non-Newtonian fluids. The relationship between the electrochemical impedance signal and non-Newtonian flow is poorly understood and the effects of viscosity variation, and the influence on current density characteristics is critical to the performance of an electrochemical reactor. This work also connects to the design of novel membrane structures at NUS with the work of Dr Liu Jianbo.

IRP 2 Singapore-based start-up company Datum ElectroniX which was launched by Dr Kamal Elouarzaki and Prof Adrian Fisher, has progressed with a range of new industrial collaborations underway.

IRP 2 outreach activities have continued during COVID-19, with a focus on online courses. We have contributed to the Cambridge Science Festival in collaboration with Cambridge Zero and also an activity in Kenya as part of an ongoing collaboration through Cambridge Africa.

Dr Adrian Fisher, PI
University of Cambridge

Update on work package 2.1

Advanced electrode architectures

Dr DAI Chencheng (Research Fellow, NTU) has been studying the electro-oxidation of methanol to formate, catalysed by iron-substituted lanthanum cobaltite ($LaCo_{1-x}Fe_xO_3$). The Fe/Co ratio in the oxides greatly influences the activity and selectivity. This effect is attributed to the higher affinity of Fe and Co to the two reactants: CH_3OH and OH^-, respectively. Because a balance between these affinities is favoured, $LaCo_{0.5}Fe_{0.5}O_3$ shows the highest formate production rate, at 24.5 mmol h^{-1} g_{oxide}^{-1}, and a relatively high Faradaic efficiency of 44.4% in a series of ($LaCo_{1-x}Fe_xO_3$) samples (x = 0.00, 0.25, 0.50, 0.75, 1.00) at 1.6 V versus a reversible hydrogen electrode.

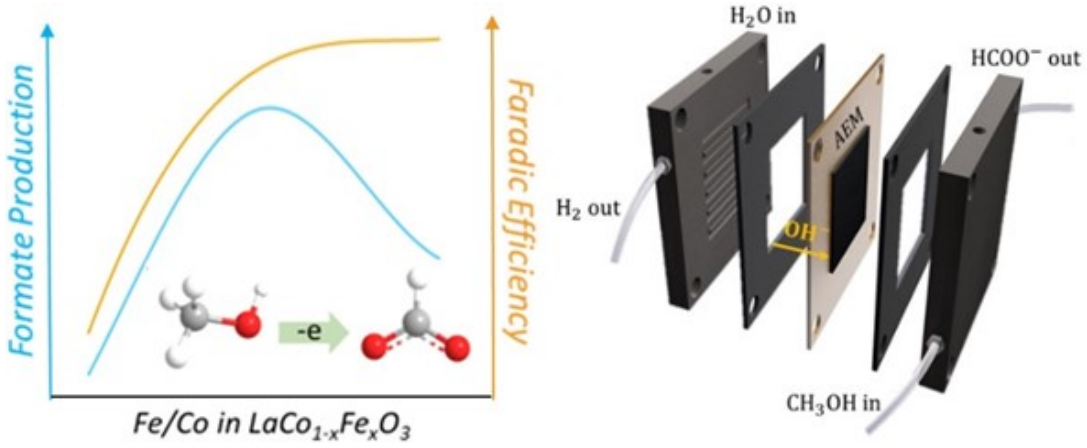


Figure 2.1: Methanol electro-oxidation to formate on iron-substituted lanthanum cobaltite perovskite oxides in a membrane electrolyte assembly electrolyser.

Other works that have been carried out, include the electro-oxidation of glycerol on a series of $ZnFe_xCo_{2-x}O_4$ (x = 0, 0.4, 1.0, 1.4, and 2.0) spinel oxides. Seven types of value-added C1–C3 products including formate, glycolate, lactate, and glycerate can be obtained by this approach. The selectivity and Faraday efficiency toward these products can be tuned by adjusting the Fe/Co ratio and other experimental parameters, such as the applied potential, glycerol concentration, and electrolyte pH. With more Fe, the selectivity toward C1 product gradually increases from 61.62 to 74.69%, while the molar percentage of C3 products significantly decreases from 20.75 to 6.73%. A selectivity of 47.80% with a Faraday efficiency (FE) of 37.25% for C2/C3 products can be obtained by the $ZnCo_2O_4$ catalyst.

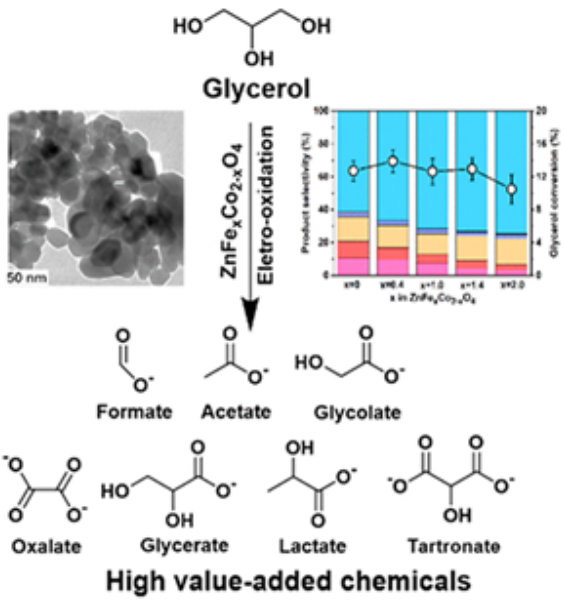


Figure 2.2: Electro-Oxidation of Glycerol to High-Value-Added C1–C3 Products by Iron-Substituted Spinel Zinc Cobalt Oxides.

Dr DAI Chencheng

Ms Freyja Björk DAGBJARTSDÓTTIR's (PhD student, CAM) research interests lie in investigating novel electrochemical systems where a complex relationship exists between chemistry and mass transport. The aim is to make mathematical descriptions of electrochemical systems that can be used to investigate, design and monitor these systems.

Ms Dagbjartsdóttir's recent focus has been on electrochemical impedance spectroscopy in non-Newtonian fluids. The relationship between the electrochemical impedance signal and non-Newtonian flow is poorly understood, but the impedance signals carry information on the physical parameters of the electrolyte. Extracting this information from the signals could be useful in a range of use cases, such as high-throughput screening of materials and on-line/in-line process monitoring. She uses a microfluidic channel electrode setup, and starting with a reversible redox couple in an electrolyte with power law fluid behaviour, she aims to demonstrate that this extraction of information can be performed, and that various parameters of this system can be decoupled using one or few measurements.

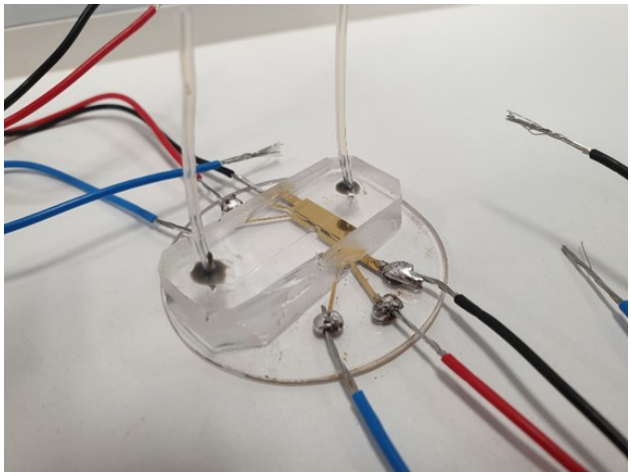


Figure 2.3: A microchannel electrode device fabricated in the CARES lab. *Ms Freyja DAGBJARTSDÓTTIR*

Mr SHANG Chuning (Non-C4T PhD student, NUS) worked together with **Dr LIU Jianbo (Research Fellow, NUS)** on a project focusing on electrode-assisted membrane anti-fouling strategies. Specifically, electric voltage was applied on the membrane cell to generate an electric field through the membrane. The salt rejections were measured first. Then, an unsaturated $CaSO_4$ solution was applied to measure the membrane's anti-scaling performance.

Based on the salt rejection results, several conclusions were made: (1) High negative voltage leads to the generation of Fe ions to the permeate; (2) Frequency of alternating voltage plays a negligible role to membrane permeability and rejection; (3) Alternating current does not change the membrane transport properties with high feed concentration. Results from scaling tests suggest that voltage may improve the membrane anti-scaling performance.

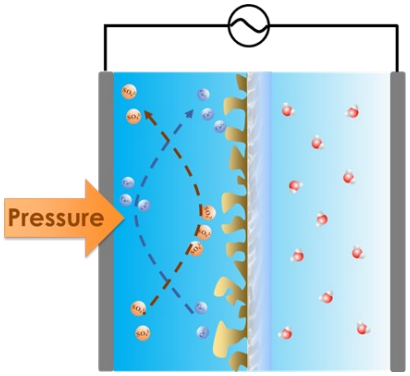


Figure 2.4: An illustration of the electric voltage integrated membrane system for fouling resistance.

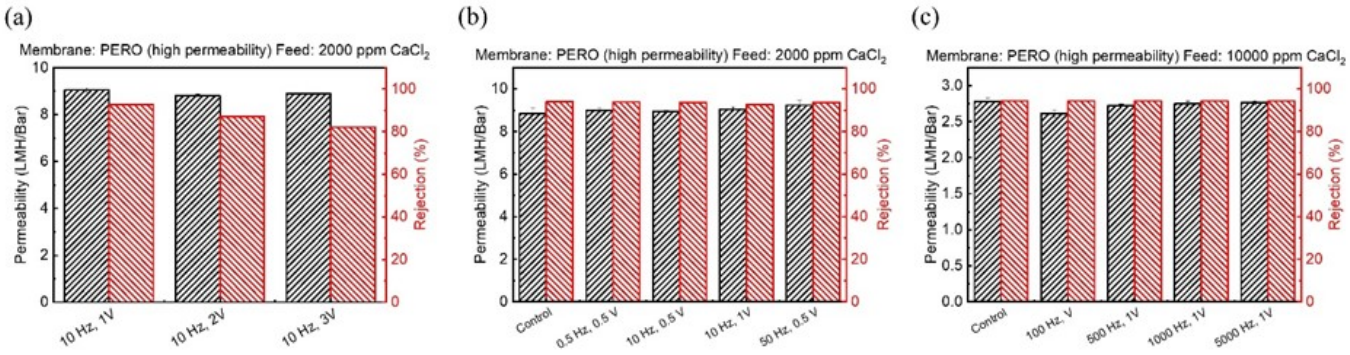


Figure 2.5. The permeability and rejection of salts under applied voltage. *Mr SHANG Chuning*

Update on work package 2.2

Co-generation and electrolytic synthesis reactor engineering

Dr SUN Libo (Research Fellow, NTU) reports that ligands play a critical role in electrocatalytic CO_2 reduction reaction (CO_2RR) based on heterogeneous molecular catalysts. Previous research on heterogeneous molecular electrocatalysis mainly deal with N4 ligands with pyrrole as subunits (porphyrin, phthalocyanine, etc.), while ligands constructed from pyridine subunits remain uncommon. Herein, we focused on the development of new N4 cobalt complexes based on pyridine subunits. After anchoring onto carbon nanotubes, they can exhibit CO_2RR activity at a low overpotential of 140 mV, and high activity from -0.30 to -0.60 V vs. RHE with selectivity of above 98%. Excellent performance at large current densities can also be observed in a flow cell. From DFT calculations, pyridine-based cobalt complex on carbon substrate can lower the barrier for formation of COOH* and CO* than counterpart pyrrole-based ones. Further, the semimetal behaviour by optimised d-orbitals may facilitate charge transfer and increase the activity. In-situ attenuated total reflectance-Fourier transform infrared spectroscopy proves that such electrocatalysts exhibit CO production at lower overpotential and moderate CO adsorption ability over a wide potential range.

He currently has two journal articles in submission titled "Cobalt Quaterpyridine Complexes for Highly Efficient Heterogeneous CO_2 Reduction in Aqueous Media" and "Heterogeneous multiatom cluster catalysts for efficient electrocatalysis".

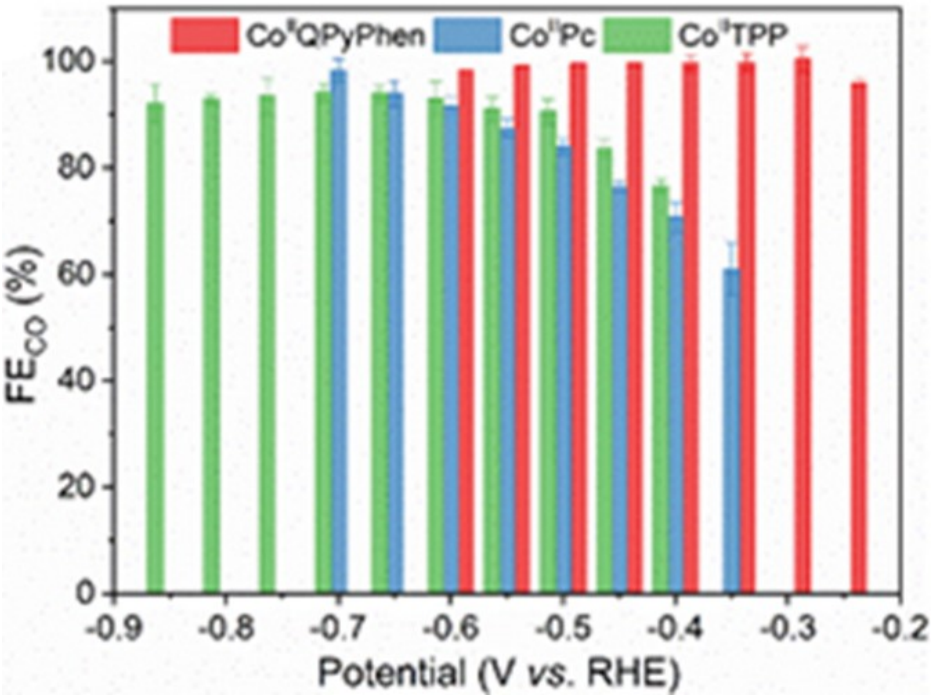


Figure 2.6: The Faradaic efficiency comparison of these electrocatalysts.

Dr SUN Libo

Update on work package 2.3

Micro-variable pressure and temperature electrosynthesis plant

Time series decomposition has been used by the Cambridge research group to explore and unravel the characteristics of biological fuel cells. In this reporting period we have been developing this approach to a more broad range of electrocatalytic processes and ultimately towards reactor design. In a time series of electrolysis i/V measurements current density profiles can be decomposed to reveal underlying patterns in the data, namely trend, seasonal and remainder components. This is a useful first step in developing forecasting models as the underlying patterns can inform the modelling process. The current density profiles were decomposed by the seasonal and trend decomposition using locally estimated scatterplot smoothing or LOESS (STL) method Python's statsmodel module was used to implement STL. The three components are related in an additive manner as shown below:

$$y(t) = T(t) + S(t) + R(t)$$

$$y(t) = T(t) \times S(t) \times R(t) \equiv \log[y(t)] = \log[T(t)] + \log[S(t)] + \log[R(t)]$$

Here where y(t) is the photocurrent profile, T(t) is the trend component, S(t) is the seasonal component, and R(t) is the remainder component at time step t. The multiplicative model is more appropriate when the variation in the seasonal component is seen to be proportional with the level of the time series. The two main parameters to define for STL decomposition are the length of the trend and seasonal smoothers. The length of the seasonal smoother (odd integer) is the number of consecutive periods used in estimating each value of the seasonal component. As its value increases, the seasonal component becomes smoother. The trend smoother (odd integer) is the number of consecutive observations used in estimating the trend component. The formula 1.5 × period length/(1 − 1.5/seasonal smoother) was used to automatically set the trend smoother as suggested in the original implementation of STL.

In future reporting periods we will explore specific electrochemical process and examine the ability of the approach to be employed for electrosynthesis reactor design.

Scientific output

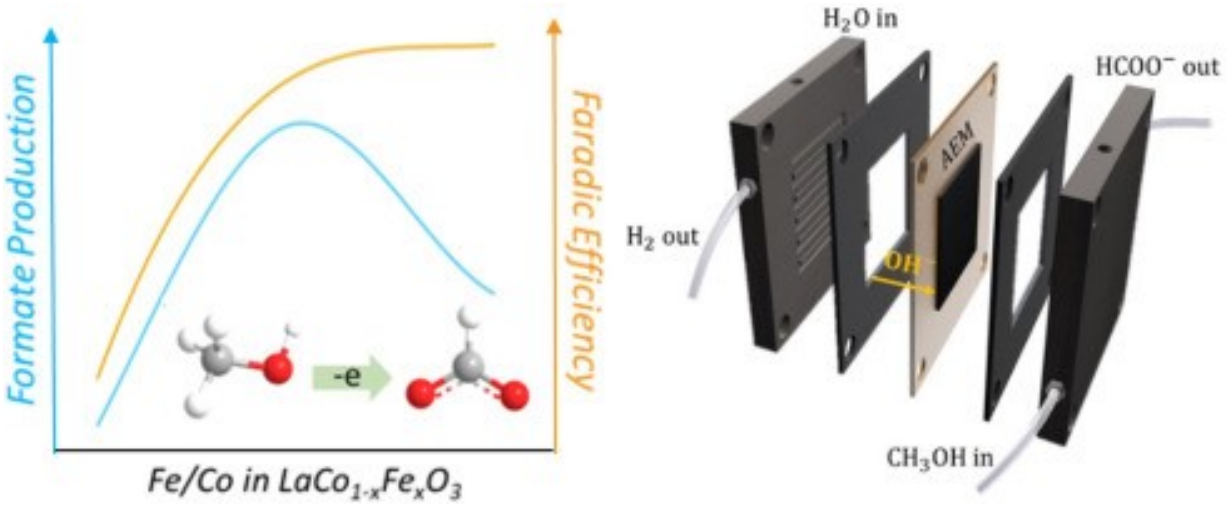
The following are the CREATE-acknowledged publications generated by IRP 2 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Methanol electro-oxidation to formate on iron-substituted lanthanum cobaltite perovskite oxides

Fanxu Meng, Chencheng Dai, Zheng Liu, Songzhu Luo, Jingjie Ge, Yan Duan, Gao Chen, Chao Wei, Riccardo Ruixi Chen, Jiarui Wang, Daniel Mandler, and Zhichuan J. Xu, *eScience*

DOI: 10.1016/j.esci.2022.02.001

Abstract: Electrochemically producing formate by oxidizing methanol is a promising way to add value to methanol. Noble metal-based electrocatalysts, which have been extensively studied for the methanol oxidation reaction, can catalyze the complete oxidation of methanol to carbon dioxide, but not the mild oxidation to formate. As a result, exploring efficient and earth-abundant electrocatalysts for formate production from methanol is of interest. Herein, we present the electro-oxidation of methanol to formate, catalyzed by iron-substituted lanthanum cobaltite (LaCo1−xFexO3). The Fe/Co ratio in the oxides greatly influences the activity and selectivity. This effect is attributed to the higher affinity of Fe and Co to the two reactants: CH3OH and OH−, respectively. Because a balance between these affinities is favored, LaCo0.5Fe0.5O3 shows the highest formate production rate, at 24.5 mmol h−1 goxide−1, and a relatively high Faradaic efficiency of 44.4% in a series of (LaCo1−xFexO3) samples (x = 0.00, 0.25, 0.50, 0.75, 1.00) at 1.6 V versus a reversible hydrogen electrode.



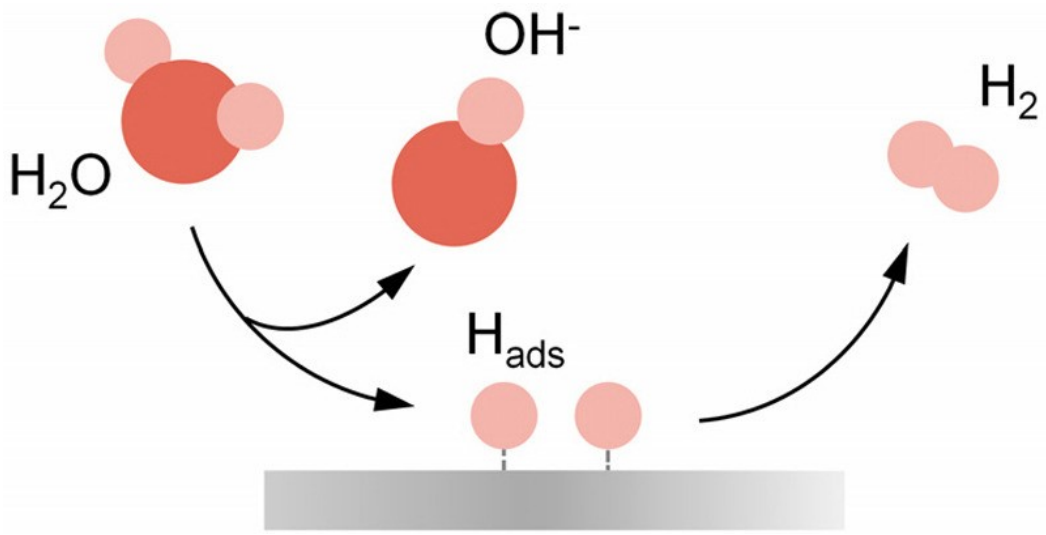
Methanol electro-oxidation to formate on iron-substituted lanthanum cobaltite perovskite oxides in a membrane electrolyte assembly electrolyzer.

The possible implications of magnetic field effect on understanding the reactant of water splitting

Chao Wei, and Zhichuan J. Xu, *Chinese Journal of Catalysis*

DOI: 10.1016/S1872-2067(21)63821-4

Abstract: Electrochemical water splitting consists of two elementary reactions i.e., hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Developing robust HER and OER technologies necessitates a molecular picture of reaction mechanism, yet the reactants for water splitting reactions are unfortunately not fully understood. Here we utilize magnetic field to understand proton transport in HER, and hydroxide ion transport in OER, to discuss the possible implications on understanding the reactants for HER and OER. Magnetic field is a known tool for changing the movement of charged species like ions, e.g. the magnetic-field-improved Cu2+ transportation near the electrode in Cu electrodeposition. However, applying a magnetic field does not affect the HER or OER rate across various pH, which challenges the traditional opinion that charged species (i.e. proton and hydroxide ion) act as the reactant. This anomalous response of HER and OER to magnetic field, and the fact that the transport of proton and hydroxide ion follow Grotthuss mechanism, collectively indicate water may act as the universal reactant for HER and OER across various pH. With the aid of magnetic field, this work serves as an understanding of water might be the reactant in HER and OER, and possibly in other electrocatalysis reactions involving protonation and deprotonation step. A model that simply focuses on the charged species but overlooking the complexity of the whole electrolyte phase where water is the dominant species, may not reasonably reflect the electrochemistry of HER and OER in aqueous electrolyte.



The observation that magnetic field does not affect hydrogen or oxygen evolution reaction, and the knowledge of Grotthuss mechanism, collectively suggest the reactant for these two reactions is H_2O, possibly not H+ or OH–.

Other activities and achievements

Prof Adrian FISHER (PI, CAM) presented an overview of the prospects of hydrogen technologies contributing to low carbon manufacturing at the Futures We Want Model United Nations symposium in Dubai in March 2022.

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

Over the last few months, we have been working both experimentally and computationally on the electrochemical CO_2 reduction reaction (eCO_2RR) that allows turning carbon dioxide into value-added chemicals. In the lab, we have coated commercially available gas diffusion layers with copper oxide nanoparticles in order to produce gas diffusion electrodes that function as the cathode in the eCO_2RR. We have accomplished this using a flame synthesis rig previously developed in our lab, in which the flame is stabilised on a rotating metal plate. The gas diffusion layers are mounted on the rotating surface for intermittent exposure to the flame, thereby limiting the damage due to the high temperature of the flame whilst still achieving good deposition rates in order to produce copper oxide nanostructured film coatings.

On the computational side, we have assembled a micro-kinetic model for the eCO_2RR by collecting intermediates and pathways from a number of sources in the literature, as well as density functional theory calculations. We then calibrated the mechanism against experimentally measured Faradaic efficiencies, also reported in the literature. Simulations with the calibrated mechanism surprisingly suggest that the dominant pathway is not the one that is commonly assumed.

In other developments, we have continued our investigations into how soot particles in flames are beginning to form. Previous work has shown that charge plays an important role in this, and we are now able to inject charges from a non-thermal plasma into coflow diffusion flames, thus enabling us to study various aspects of soot formation as a function of ion concentration.

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

TAN Yong Ren (PhD student, CAM) is currently investigating a charge injection system from a non-thermal plasma to study the impact of charge on soot formation. The base flame is an atmospheric-pressure helium-diluted laminar coflow diffusion ethylene flame, generated using a modified Yale Steady Flame burner. Non-thermal plasma was injected into the fuel tube of the burner at different ion concentrations. The ion concentration was controlled by altering the high voltage (HV) frequency at 22-25 kHz. Laser-induced incandescence (LII) measurements of the flame with and without the charge injection was carried out to determine the soot volume fraction of the flame. As shown in Figure 3.1, with the increase in HV frequency, the ion concentration injected into the burner decreases. As a general trend, the decrease in HV frequency (*i.e.* increase in the ion concentration) decreases the soot volume fraction as compared to the ethylene flames without charge injection. The degree of the decrease also changes with the helium dilution of the ethylene flame. The ethylene flame that has the most dilution of helium (32% C_2H_4) showed the highest drop in soot volume fraction at the same HV frequency. It is then followed by 40% and 60% ethylene flames.

Dr ZONG Yichen (Research Fellow, CARES-NUS) has been leading the experimental research on future fuels for low emission energy utilisation. The research activities are conducted under the collaboration between NUS and Cambridge researchers. Experimental research continues in the last six months as the COVID situation improves in Singapore. This set of experiments aims to reveal the effect of additives on jet fuel blends with new sampling methods. A research paper based on the experiments has been published in *Fuel* which systematically investigates the particulate formation process of diesel/jet fuel blends in a diesel engine. A relevant report has been made at the International Conference on Applied Energy addressing the butanol additive. Moreover, Dr Zong is also working on engine simulation with CMCL engineers and air quality monitoring with the collaboration of JPS team and environmental scientists.

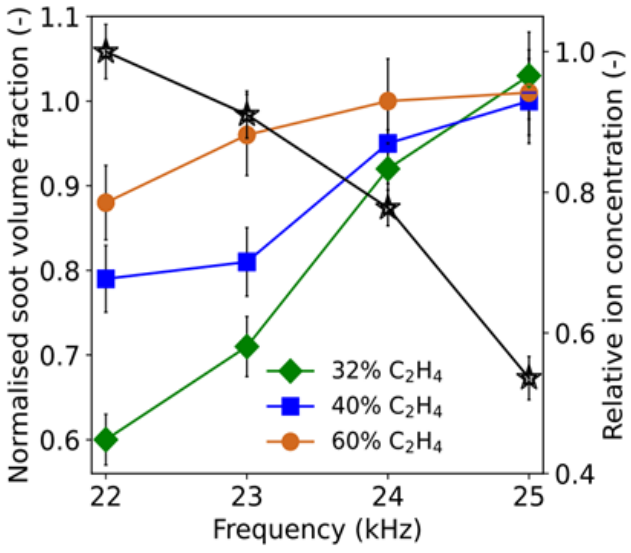


Figure 3.1: Left axis: Normalised maximum soot volume fraction versus HV frequency for the He-diluted 32%, 40% and 60% ethylene flames. The normalisation is based on the maximum soot volume fraction observed in each flames without charge injection. The error bars show the standard error for each of the measurements. The lines are drawn to guide the eye. Right axis: Relative ion concentration of the charge injection.

Mr TAN Yong Ren

Update on work package 3.2

Refinery, fuel and engine of the future — modelling

Chemical mechanisms, PAH chemistry, after-treatment

Dr Laura PASCAZIO's (Research Fellow, CARES) main research interest lies in the study of combustion-generated carbonaceous nanoparticle (also known as soot) formation using computational methods. The understanding of soot inception mechanism remains one of the most debated topics in the combustion scientific community.

Recently, Dr Pascazio submitted a paper on the development of a knowledge-graph based framework for the automated parameterisation of reactive force fields derived from relaxed potential energy surface (PES) scans. Jointly with **Dr Angiras MENON (PDRA, CAM)** and CMCL, an ontological representation for Potential Energy Surface scans, OntoPESScan, has been developed that allows for the semantic enrichment of quantum chemical calculations within the World Avatar project (theworldavatar.com). Following this, she developed a software agent able to perform PES scans results retrieval and reactive force field calibration tasks.

Currently, her aim is to use OntoPESScan and the force field fitting agent to calibrate a reactive force field able to describe the bond formation between two π-radical sites. In one of her previous publications, she showed that these compounds bond strongly enough for stability at flame temperature. The obtained force field will allow the use of reactive molecular dynamics to simulate the clustering of these compounds at flame temperature.

She currently has a journal article under review in the Journal of *Chemical Information and Modeling* titled "OntoPESScan: An Ontology for the Exploration of Potential Energy Surfaces".

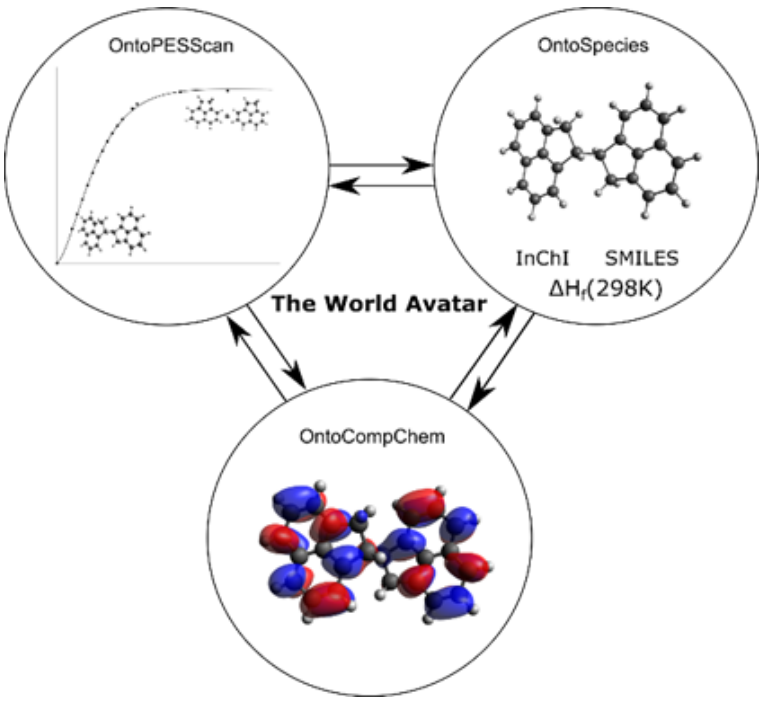


Figure 3.2: OntoPESScan ontology, linked to OntoSpecies and OntoCompChem, is developed in the World Avatar framework to extend the chemistry domain.

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 SHENG Yuan (Research Fellow, NTU) has developed a method of coating commercial gas diffusion layers (GDLs) with films of CuO_x nanoparticles as they are being synthesised in $C_2H_4/O_2/Ar$ and $H_2/O_2/N_2$ flames (Figure 3.3). The GDLs were mounted on a rotating metal plate for intermittent exposure to the flame, and by tuning the rotating speed of the plate, thermal damage to the GDLs was minimised without compromising the deposition rate of the CuO_x films. A method of strengthening the films post-synthesis has been developed and optimised for the resulting gas diffusion electrodes (GDEs) to serve as the cathode in the eCO_2RR. Moreover, Dr Sheng has designed and built an electrochemical flow cell with narrow inter-electrode spacing to reduce iR loss during operation. Using the abovementioned GDEs and flow cell, he has achieved stable eCO_2RR performance for 2 h with the cell running at 300 mA/cm² and a low cell voltage of 2.8 V (Figure 3.4). Current densities of up to 900 mA/cm² have also been demonstrated with the Faradaic efficiency toward C_2H_4 reaching 50%.

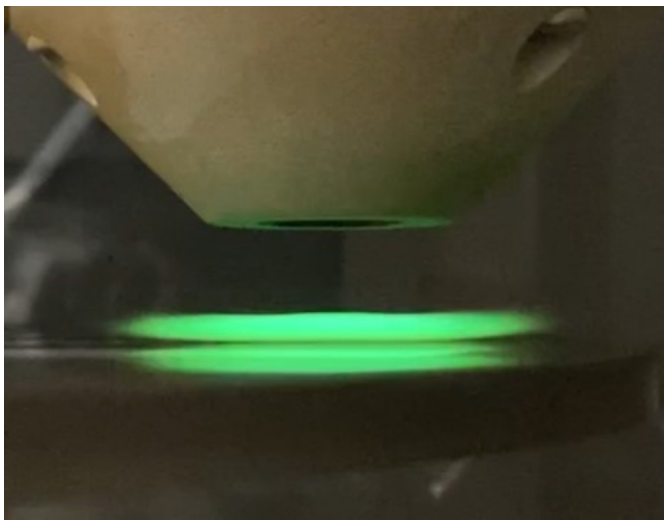


Figure 3.3: A particle-laden $H_2/O_2/N_2$ flame during the deposition of CuO_x films.

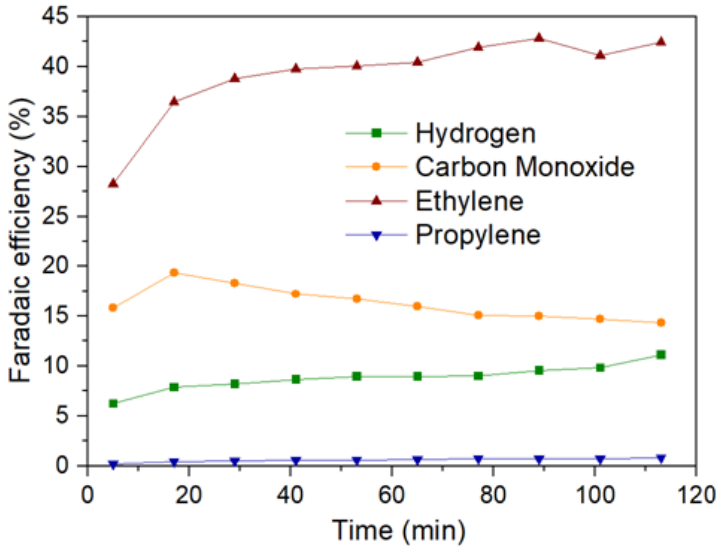


Figure 3.4: The selectivity toward major gaseous products of eCO_2RR on a flame-made CuO_x GDE, measured in galvanostatic mode at 300 mA/cm². Electrolyte: 3.5 M KOH.

Dr SHENG Yuan

Update on work package 3.4

Better, cheaper, cleaner nanostructures — modelling

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

Dr Manoel MANUPUTTY (Research Fellow, NTU) has recently completed a manuscript on the "Effects of particle collection in a premixed stagnation flame synthesis with a rotating substrate", currently submitted for publication. The paper investigates the effect of particle collection mechanisms on the oxygen vacancies and crystallinity of titanium dioxide nanoparticles produced in the flame synthesis reactor. He has also finished a set of preliminary experiments to investigate the catalytic activity of Pt-TiO_2 nanoparticles with iron, sulphur, and boron doping for dehydrogenation reaction of perhydro dibenzyl toluene (H18DBT). The dehydrogenation reaction is an important part of the use of liquid organic hydrocarbon (LOHC) as a hydrogen storage material. The results show promising activity for Pt-TiO_2 with a small amount of sulphur doping while iron and boron doping are found to be detrimental. Further experimental characterisations, including elemental and surface analysis, are now being planned to further understand the structure-performance relationship of the flame-made catalysts.

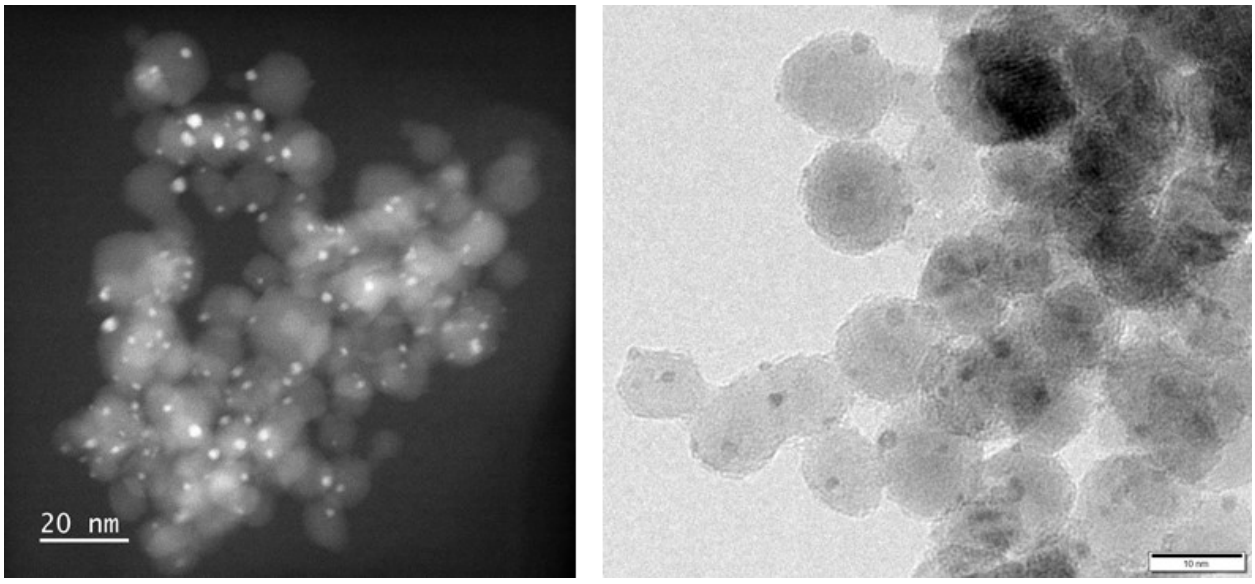


Figure 3.5: TEM images (left: dark field, right: bright field) of Pt-decorated TiO_2 nanoparticles prepared from the one-step flame synthesis.

Dr Manoel MANUPUTTY

Mr Simon RIHM (PhD student, CARES) finished his work on kinetic modelling of the CO_2 Reduction Reaction (CO_2RR) by utilising data from first-principles calculations as well as measurement data of H-cell reactor setups. He used a CO_2RR mechanism towards a multitude of different products that was established within a prior literature review by compiling hypothesised reaction paths and intermediates from many different sources. The developed micro-kinetic model (MKM) was then fed with results of Density Functional Theory (DFT) calculations and calibrated towards experimentally measured Faradaic efficiencies. For a first fully-functioning elementary-step model, he focused on single-facet Cu(100) as a widely studied catalyst surface with good availability of data across the literature.

The calibrated model was found to offer some interesting insights into the reaction mechanism: Most interestingly, it finds a dimerisation step via *CHO intermediate as far more likely than the more commonly hypothesised *CO intermediate. Moreover, it shows how coupling or other limiting steps are not necessarily related to large surface coverages as the catalyst is easily poisoned via reaction paths with one or more steps severely slowed down.

These findings support the novel approach to micro-kinetic modelling that solely relies on already published DFT data of different sources for a large reaction network and uses intrinsic uncertainties as variation intervals for subsequent calibration. This opens up potential application to and combination with other catalyst surfaces as automation of the modelling process.

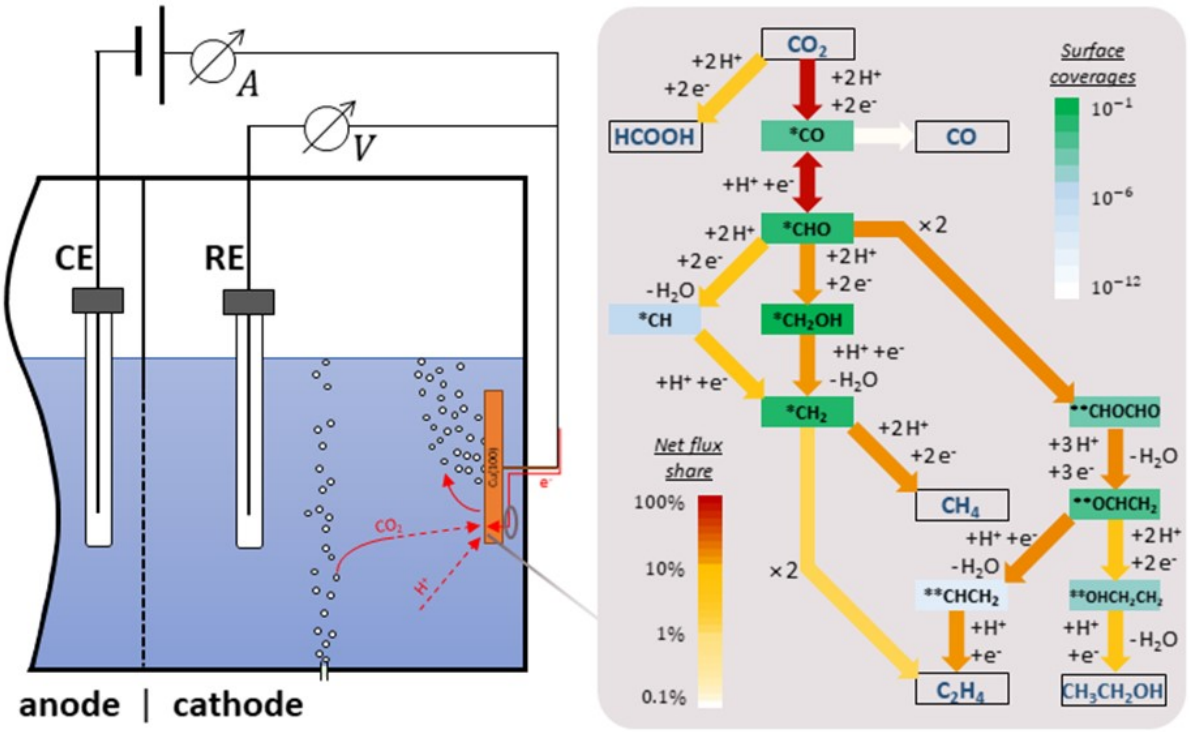


Figure 3.6: Micro-kinetic modelling of electrocatalytic CO_2 reduction, showing a common reactor setup on the left and a simplified reaction flux diagram on the right.

Mr Simon RIHM

Scientific output

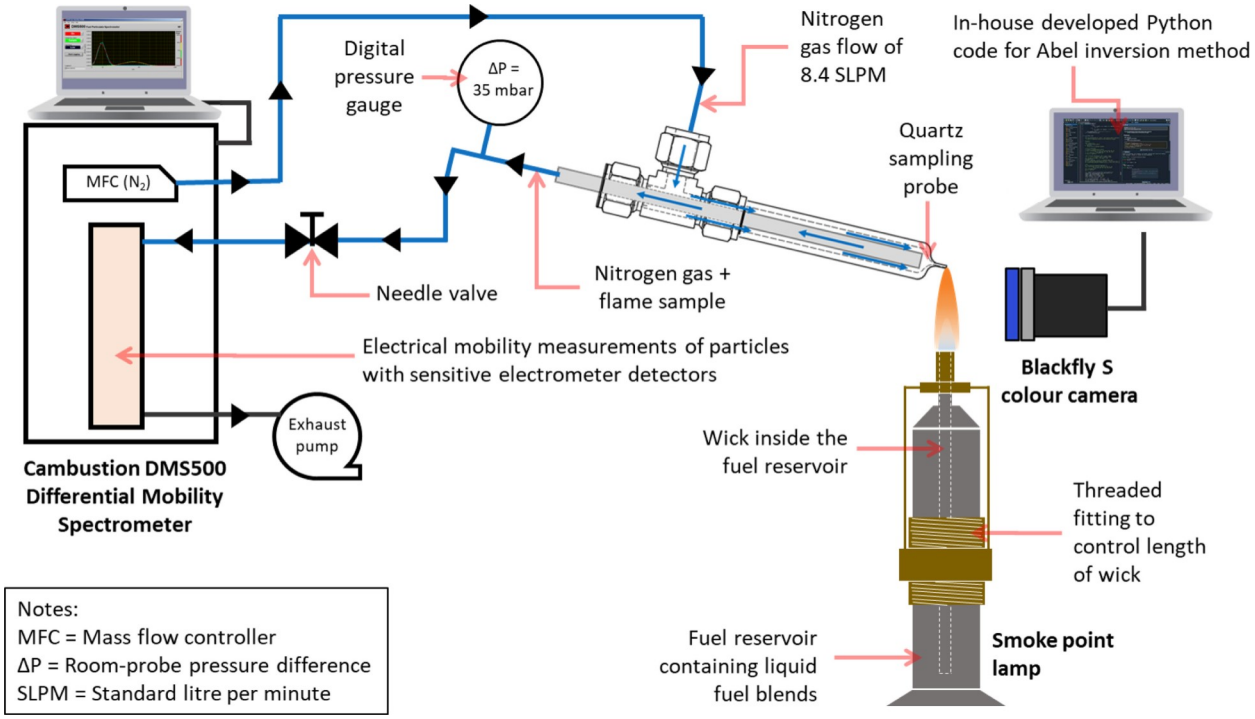
The following are the CREATE-acknowledged publications generated by IRP 3 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

How do the oxygenated functional groups in ether, carbonate and alcohol affect soot formation in Jet A2 diffusion flames?

Yong Ren Tan, Maurin Salamanca, Jethro Akroyd, and Markus Kraft, *Combustion and Flame*

DOI: 10.1016/j.combustflame.2021.111849

Abstract: Four oxygenated fuels: ethanol (EtOH), dimethyl carbonate (DMC), dimethoxymethane (DMM) and polyoxymethylene dimethyl ether (PODE3) were blended with Jet A2 to investigate the sooting behaviour of the fuel mixtures. The smoke point was measured using wick-fed laminar diffusion flames as per the ASTM D1322 standard. The oxygen extended sooting index (OESI) was calculated to determine the sooting tendency of each mixture. Colour-ratio pyrometry and differential mobility spectrometry were used to measure the soot volume fraction (fv) and particle size distribution (PSD). The addition of oxygenated fuels caused a strong reduction in sooting tendency (i.e. OESI) at low blend strengths (5%) and a weaker linear reduction at higher blend strengths (10% and 20%). Each mixture showed a similar reduction at a given mole fraction of oxygenated fuel. The OESI broadly correlated with the soot volume fraction and particle size measurements. Increasing blend strengths resulted in smaller particles at the tip of the flame. The average particle size at the tip was influenced by the oxygen content but not the molecular structure of the oxygenated fuels, whereas the soot volume fraction in the wings was influenced by both the molecular structure of the oxygenated fuels and the oxygen/carbon ratio of the mixture. For the first time, fv and PSD have been reported for flames produced using Jet A2 blends in an ASTM D1322 lamp. The ability to relate data gathered using the ASTM D1322 standard for the sooting behaviour of different mixtures is going to be increasingly important as the aviation industry seeks to switch to sustainable fuels.



Schematic of the experimental set-up

Other activities and achievements

Dr ZONG Yichen's (Research Fellow, CARES-NUS) had a paper titled "Evaluating the effect of n-butanol additive in a common-rail diesel engine" accepted at the International Conference on Applied Energy 2021 which ran from November 29 to December 2 in Bangkok, Thailand. Other authors on the paper were Mr Qiren ZHU, Assoc Prof Wenming YANG, and Prof Markus KRAFT.

Mr Simon RIHM (PhD student, CARES) has been invited to give an oral presentation at the 39th International Symposium on Combustion in Vancouver in July 2022.

The work carried out in IRP3 to find alternative fuels for cleaner combustion could reduce air pollution in Singapore and around the world.

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 activities for better energy efficiency, lower pollution, and decarbonisation in the marine sector is gathering pace and importance worldwide. This IRP addresses these significant problems by a series of connected work packages, including fundamental studies on particulate emissions from marine engines burning fossil or alternative fuels, waste heat utilisation methods such as the use or Organic Rankine Cycles and the associated turbomachinery, high-efficiency heat exchangers, and estimates and measurements of pollutant dispersion from ships and its reception in port and urban areas.

During the reporting period, two of the Tasks were not active due to shortage of personnel. The engine modelling work continued with more conditions studied by numerical simulation, revealing that the trends of pollutant are captured well by the model. The CARES emissions measurement drone has been developed further with some new sensors and the dataset from last year's field trip have been written up for a journal paper. This activity is vital for understanding the pollutant-carrying plume structure close to ships, which is important information for modelling pollutant dispersion in ports and coastal areas.

Professor Epaminondas Mastorakos, PI
University of Cambridge

Update on work package 4.1

Engine combustion — best fuel, best operating condition

Dr Ramesh KOLLURU (Research Fellow, CARES) joined CARES on 1st April 2022 and will be using numerical work to investigate turbulent flows related to dispersion and mixing of pollutants in the atmosphere arising from marine traffic around Singapore. He will also be looking into developing CFD models for the mixing processes in the development of reacting flows that deal with the transformation of pollutants.

Dr Shrey TRIVEDI (Research Associate, CAM) took a career break for most of this reporting period. The limited time spent was utilised to discuss the implementation of a newer CMC code for the next set of results on soot and NOx emissions from the ETH-LAV heavy-duty diesel engine. There were also discussions about using constant volume engine in future simulations, which is a more convenient tool for validation purposes.

Update on work package 4.2

Closed power cycles—selection and analysis

Update on work package 4.3

High-efficiency heat exchanger

There are no updates for work packages 4.2 and 4.3 in this report due to recruitment difficulties over the past few months.

Update on work package 4.4

Process system model for the J-Park Simulator

Dr Ghulam MAJAL (Software Developer, CARES) in close collaboration with **Mr Wilson ANG (Software Developer, CARES)** has developed a weather station agent called CARESWeatherStationAgent. The purpose of this agent is to collect weather data from a sensor near the CARES lab. The sensor data is stored in a website called Weather Underground and the agent retrieves the data using an API. A UML diagram of the various JAVA classes of the agent is shown below. The weather readings include information such as temperature, humidity, precipitation, pressure, and wind speed. The sensor's weather readings can independently optimise the internal environment of the lab to ensure consistent experiments. The agent is a part of a larger project associated with the Digital Chemistry Lab. Other collaborators in this project are **Mr Simon RIHM (PhD Student, CARES)** and **Mr Hou Yee QUEK (Research Associate, CARES)**.

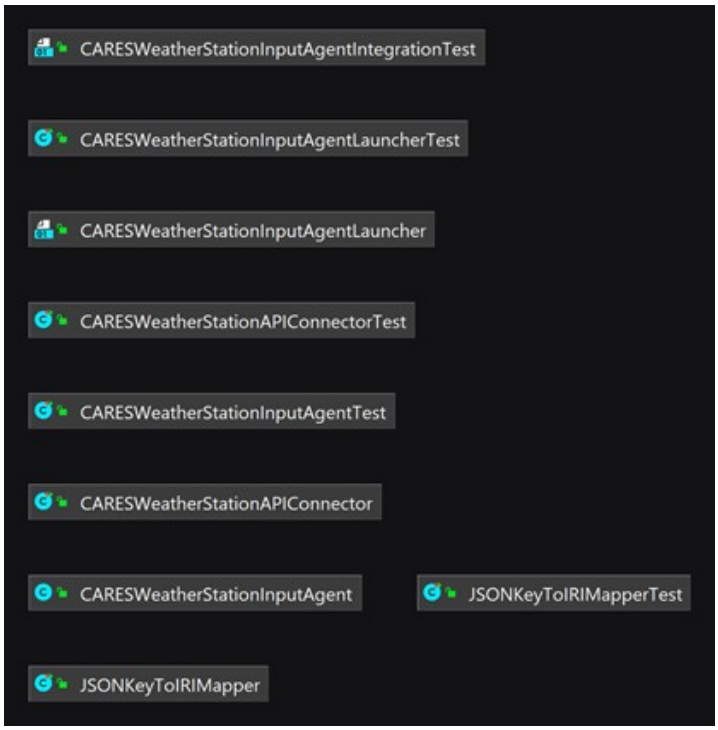


Figure 4.2: UML diagram of the various JAVA classes of CARESWeather-StationAgent

Dr Ghulam MAJAL

Dr Savvas GKANTONAS (University of Cambridge)**, Dr Molly HAUGEN (CARES Visiting Scientist, CAM), Prof. Epaminondas MASTORAKOS (PI, CAM), and Dr Adam BOIES (Co-I, CAM)** conducted a study at the Port of Rafina, Greece in September 2021 measuring particle number (PN), lung deposited surface area (LDSA), and black carbon (BC) in both the port and using an unmanned aerial vehicle (UAV) for at-sea measurements. They were supported by work from Mr Rohit PATHANIA and Ms Ingrid EL HELOU in Cambridge for the design and optimisation of the drone-based sensors.

The campaign resulted in land-based measurements showing that LDSA averages, which are influenced by both the soot and nucleation mode of particles, deviate more significantly as an emission plume progresses downwind compared to BC concentrations, which are dominated by the soot mode of particles. The ground and UAV-based particle measurements (shown in Figure 4.1) had similar results with PN, which are dominated by nucleation mode particles, and LDSA being more sensitive to position within the maritime plume than BC particles, specifically in port environments. The point measurements during

this campaign were used to evaluate a novel approach that can be considered an improvement over current "Box" models typically used to evaluate chemical transformations within a plume. The approach is based on Conditional Moment Closure theory and the Incompletely Stirred Reactor Network (ISRN) modelling framework that can account for the various non-homogeneities and turbulence-chemistry interaction effects that might be present in the near field of a plume but usually neglected. Although incorporating more physical phenomena, the approach is computationally very efficient as it decouples the evolution of reacting scalars from the atmospheric dispersion problem that can be based on a simple Gaussian model (typically used for chimney plume problems) or Computational Fluid Dynamics. The ISRN framework was employed here to estimate the effects of simultaneous coagulation, mixing, and dilution downwind from the emission sources. Together the ISRN estimates, UAV, and land-based results show that the atmospheric particle characteristics are evolving downwind of maritime emissions sources, thus the particle metric measured, and location of sampling could have lasting impacts in political and ecological decisions, especially in port environments.

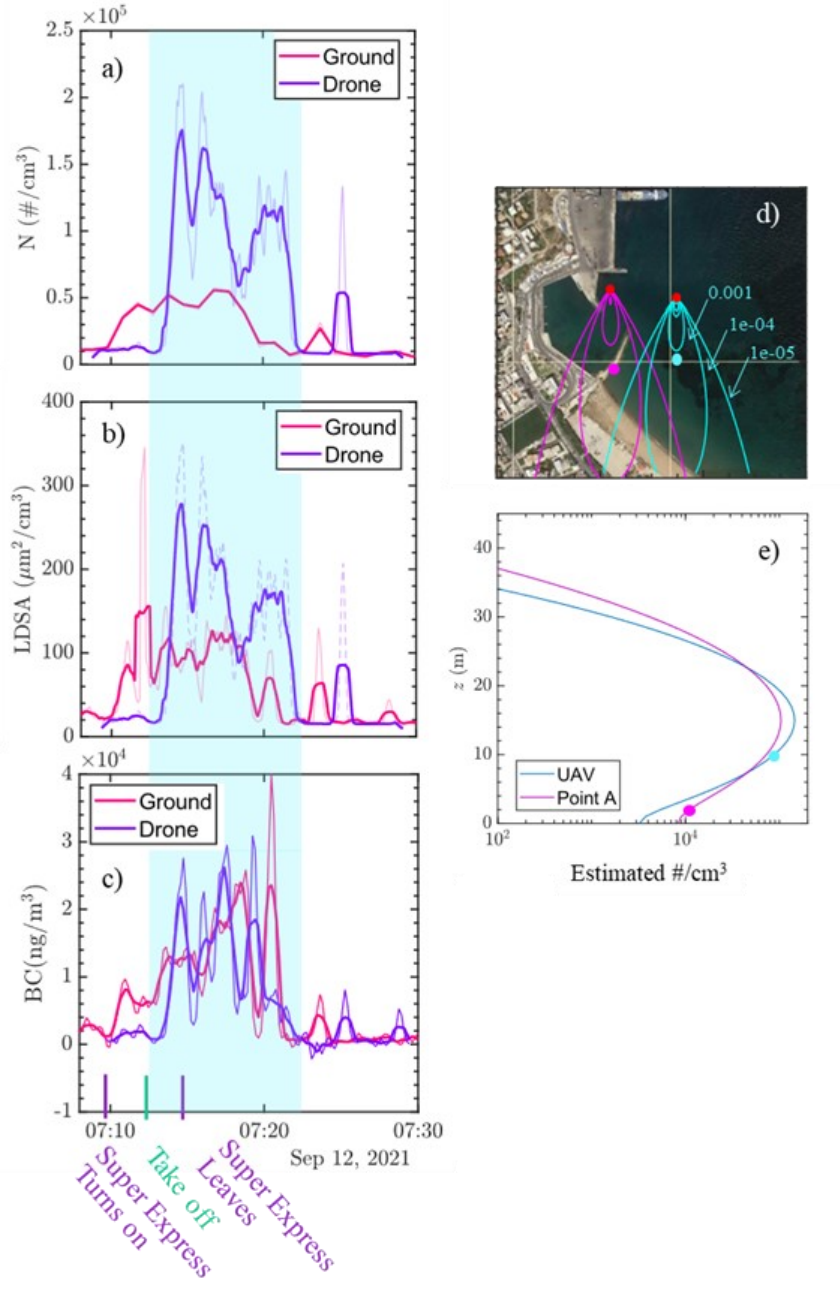


Figure 4.1: a) PN, b) LDSA, and c) BC results are shown for ground (pink) and drone (purple) measurements. Fig d) shows the ISRN estimates for a normalised plume dispersion and e) shows an example of a vertical, non-normalised PN dispersion with the corresponding locations indicated.

Dr Savvas GKANTONAS, Dr Molly HAUGEN, and Dr Adam BOIES

Scientific output

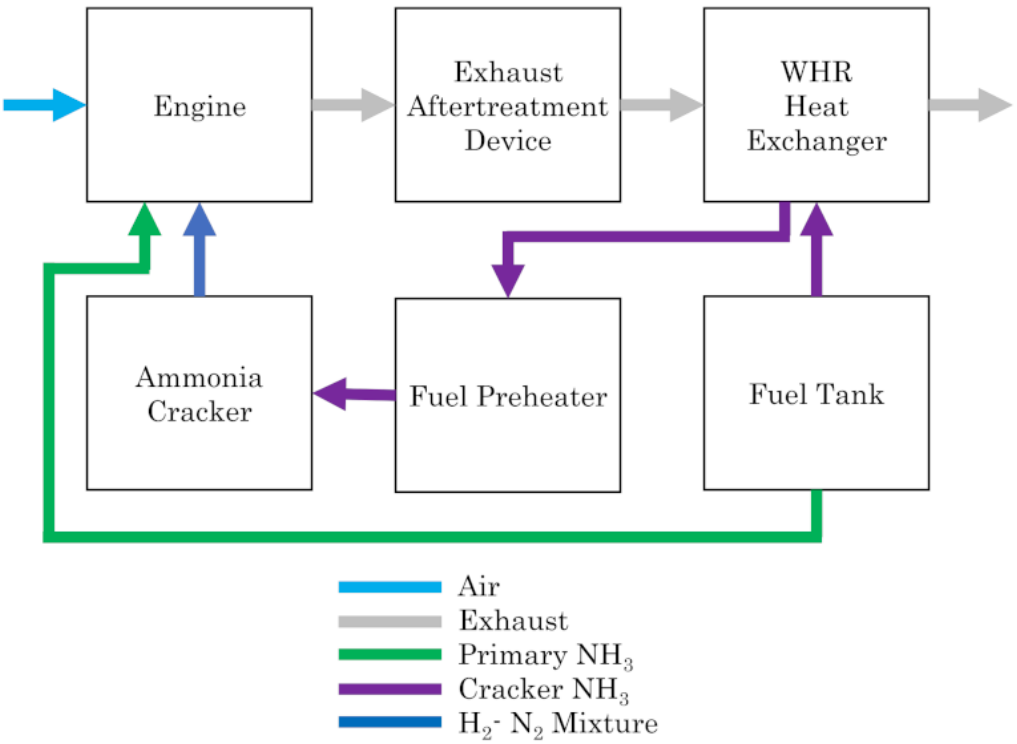
The following are the CREATE-acknowledged publications generated by IRP 4 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Analysing the Performance of Ammonia Powertrains in the Marine Environment

Thomas Buckley Imhoff, Savvas Gkantonas, and Epaminondas Mastorakos, *Energies*

DOI: 10.3390/en14217447

Abstract: This study develops system-level models of ammonia-fuelled powertrains that reflect the characteristics of four oceangoing vessels to evaluate the efficacy of ammonia as an alternative fuel in the marine environment. Relying on thermodynamics, heat transfer, and chemical engineering, the models adequately capture the behaviour of internal combustion engines, gas turbines, fuel processing equipment, and exhaust aftertreatment components. The performance of each vessel is evaluated by comparing its maximum range and cargo capacity to a conventional vessel. Results indicate that per unit output power, ammonia-fuelled internal combustion engines are more efficient, require less catalytic material, and have lower auxiliary power requirements than ammonia gas turbines. Most merchant vessels are strong candidates for ammonia fuelling if the operators can overcome capacity losses between 4% and 9%, assuming that the updated vessels retain the same range as a conventional vessel. The study also establishes that naval vessels are less likely to adopt ammonia powertrains without significant redesigns. Ammonia as an alternative fuel in the marine sector is a compelling option if the detailed component design continues to show that the concept is practically feasible. The present data and models can help in such feasibility studies for a range of vessels and propulsion technologies.



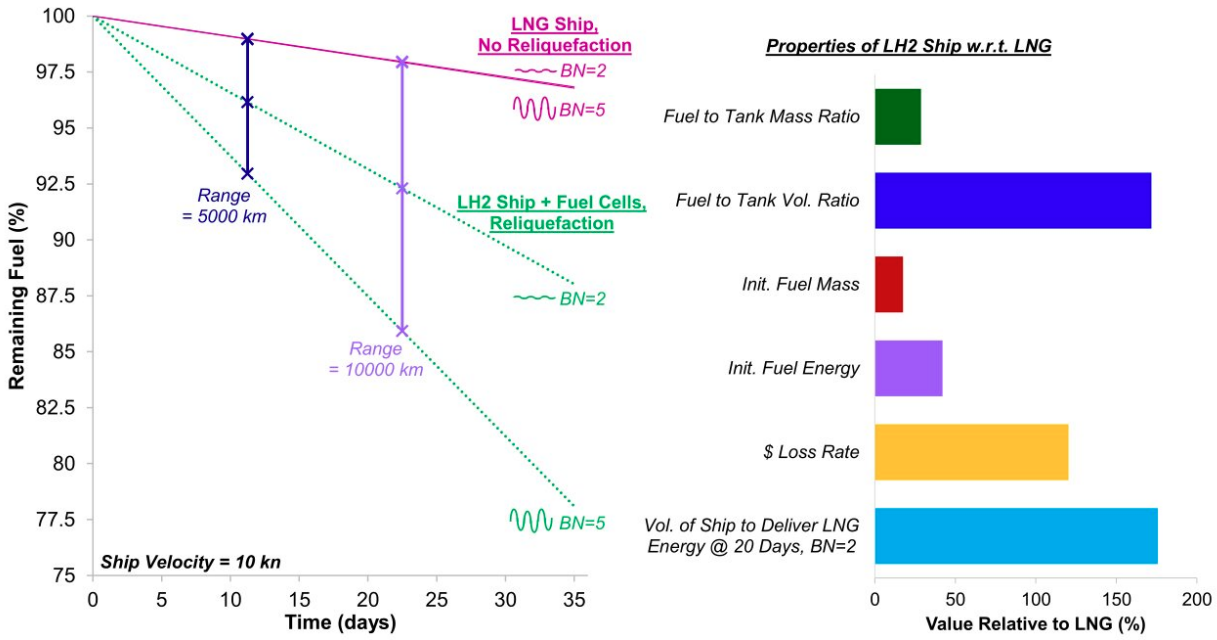
The layout of the proposed ammonia powertrain.

Modelling of Boil-Off and Sloshing Relevant to Future Liquid Hydrogen Carriers

Jessie R. Smith, Savvas Gkantonas, and Epaminondas Mastorakos, *Energies*

DOI: 10.3390/en15062046

Abstract: This study presents an approach for estimating fuel boil-off behaviour in cryogenic energy carrier ships, such as future liquid hydrogen (LH2) carriers. By relying on thermodynamic modelling and empirical formulas for ship motion and propulsion, the approach can be used to investigate boil-off as a function of tank properties, weather conditions, and operating velocities during a laden voyage. The model is first calibrated against data from a liquefied natural gas (LNG) carrier and is consequently used to investigate various design configurations of an LH2 ship. Results indicate that an LH2 ship with the same tank volume and glass wool insulation thickness as a conventional LNG carrier stores 40% of the fuel energy and is characterised by a boil-off rate nine times higher and twice as sensitive to sloshing. Adding a reliquefaction unit can reduce the LH2 fuel depletion rate by at least 38.7% but can increase its variability regarding velocity and weather conditions. In calm weather, LH2 boil-off rates can only meet LNG carrier standards by utilising at least 6.6 times the insulation thickness. By adopting fuel cell propulsion in an LH2 ship, a 1.1% increase in fuel delivery is expected. An LH2 ship with fuel cells and reliquefaction is required to be at least 1.7 times larger than an existing LNG carrier to deliver the same energy. Further comparison of alternative scenarios indicates that LH2 carriers necessitate significant redesigns if LNG carrier standards are desired. The present approach can assist future feasibility studies featuring other vessels and propulsion technologies, and can be seen as an extendable framework that can predict boil-off in real-time.



Other activities and achievements

Dr Molly HAUGEN (CARES Visiting Scientist, CAM) presented an oral presentation of their study at the Port of Rafina titled "In-use Particle Measurements of Maritime Emissions in Rafina, Greece" at the 32nd Coordinating Research Council Workshop in San Diego, California on 15th March 2022. The conference was not funded by CARES.

Prof Epaminondas MASTORAKOS (PI, CAM) presented an oral presentation of his and Dr Savvas GKANTONAS' (University of Cambridge) work titled "Effects of micromixing in the near-field evolution of a chemically reactive plume behind a ship" at the 13th International ERCOFTAC Symposium in Rhodes, Greece on 15th - 17th September 2021.

Ms Jessie SMITH (Non-C4T PhD student, University of Cambridge), as part of her PhD work on decarbonisation of aviation and shipping with hydrogen supervised by **Prof Epaminondas MASTORAKOS (PI, CAM)**, published the paper "Modelling of boil-off and sloshing relevant to future liquid hydrogen carriers".

A Memorandum of Understanding was signed with **DeepSea Technologies**, a company developing AI tools for the shipping sector, with the aim of discussing how physics-based models developed by CARES and UCAM can be implemented in the practical tools offered by DeepSea to their clients.

A meeting with **Maran Tankers Management** took place where all shipping-related projects in IRP4 were presented and discussed. They received good feedback and there was agreement such sessions will continue. In addition, there was agreement that an internship in Athens at the company's Headquarters would be considered if an appropriate student was found.

Discussions with the **Global Centre of Maritime Decarbonisation** in Singapore have started.

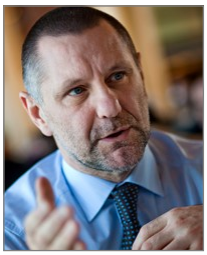
The work carried out in IRP 4 could help us better understand the effects of the shipping industry on air quality in Singapore.

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.

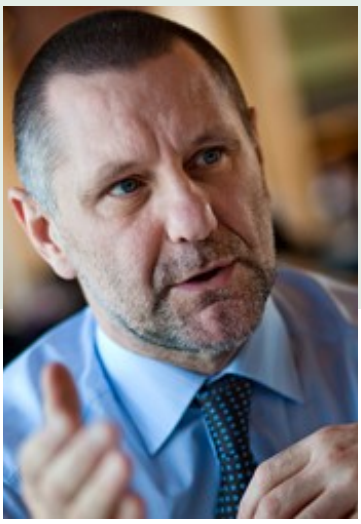
IRP BB Principal Investigators:



Professor Steve EVANS
University of Cambridge

Professor S. VISWANATHAN
Nanyang Technological University

Assoc Professor Kenneth HUANG Guang-Lih
National University of Singapore



OVERVIEW

In the last six months, the members of IRP BB have been working on existing and starting new projects related to our work packages.

In the research on business model innovations related to solar energy adoption, they are working on revising the manuscript for submission by introducing a hybrid pricing mechanism to the third-party ownership models. The survey study fieldwork and analysis were concluded, and the paper was submitted to the journal, *Environment and Behaviour*. A new research project on how the booming of venture capital influences the pollution behaviour of chemical and energy-intensive firms in the context of China is being analysed. They will be aiming to submit it to a management journal when the manuscripts are finalised. At last, they will be continuing working on the decarbonisation road-mapping activity and collaborations with other IRPs for potential commercialisation evaluations.

Professor Steve Evans, PI
University of Cambridge

Update on work package BB.1

Business model innovation potentials

Following up on the work by the previous research fellow, **Dr Lemy MARTIN (Research Fellow, CARES-NTU)** has continued to work on business model innovations for adopting sustainable innovations and technologies.

The focus is on solar energy adoption through different business models, from direct ownership, wherein customers buy, use, and maintain the panels; to third-party ownership models, wherein firms own and maintain the panels installed on the customer's property. Under a leasing or power purchasing agreement contract, customers buy electricity from the firm. A model is generated using a game-theoretic approach to understand the interaction between the firm and a representative customer and shows the conditions under which each business model may be preferred, as mentioned in previous reports. It is now generalised to multiple heterogeneous customers, generating additional insights. In particular, it has been found that solar firms gain more profit from offering a mixture of third-party ownership models instead of sticking to a single one. It has also been extended to allow for feed-in tariff structures and shows that the results continue to hold. Currently, they are looking at generalising the third-party ownership models by introducing a hybrid pricing mechanism that utilises both leasing and PPA structures to strengthen the paper manuscript for submission.

In addition, they are exploring the transformation strategies for the ecosystem business model towards digitalisation and sustainability. They are currently reviewing the literature on the ecosystem, transformation strategy, and change management. They will collect more data from industry practice and design the framework accordingly.

Update on work package BB.2

Policy formulation, customer and industry perceptions

The survey study was concluded, and the paper was submitted to the journal, *Environment and Behaviour*. The study's main contributions include cross-sectoral similarities and differences related to behaviours towards clean technology adoption. Another theoretical contribution from the survey study is a new adapted Belief-Action-Outcome framework to delineate the different parameters and possible correlations related to clean technology adoption.

The adapted framework in Figure 5.1 below includes the Beliefs (and attitudes) of senior management and the pressures on organisations that define their attitudes towards the environment and clean technology adoption. The actions include the direct and indirect measurable actions in terms of reporting (of actions) and green certifications and the frequency and amount of clean technology-related adoptions. As the outcomes are not yet tangible, they have introduced the concept of expected outcomes (which are second-order beliefs constructs). The fulfilment of such outcomes will strengthen the belief in adopting clean technology.

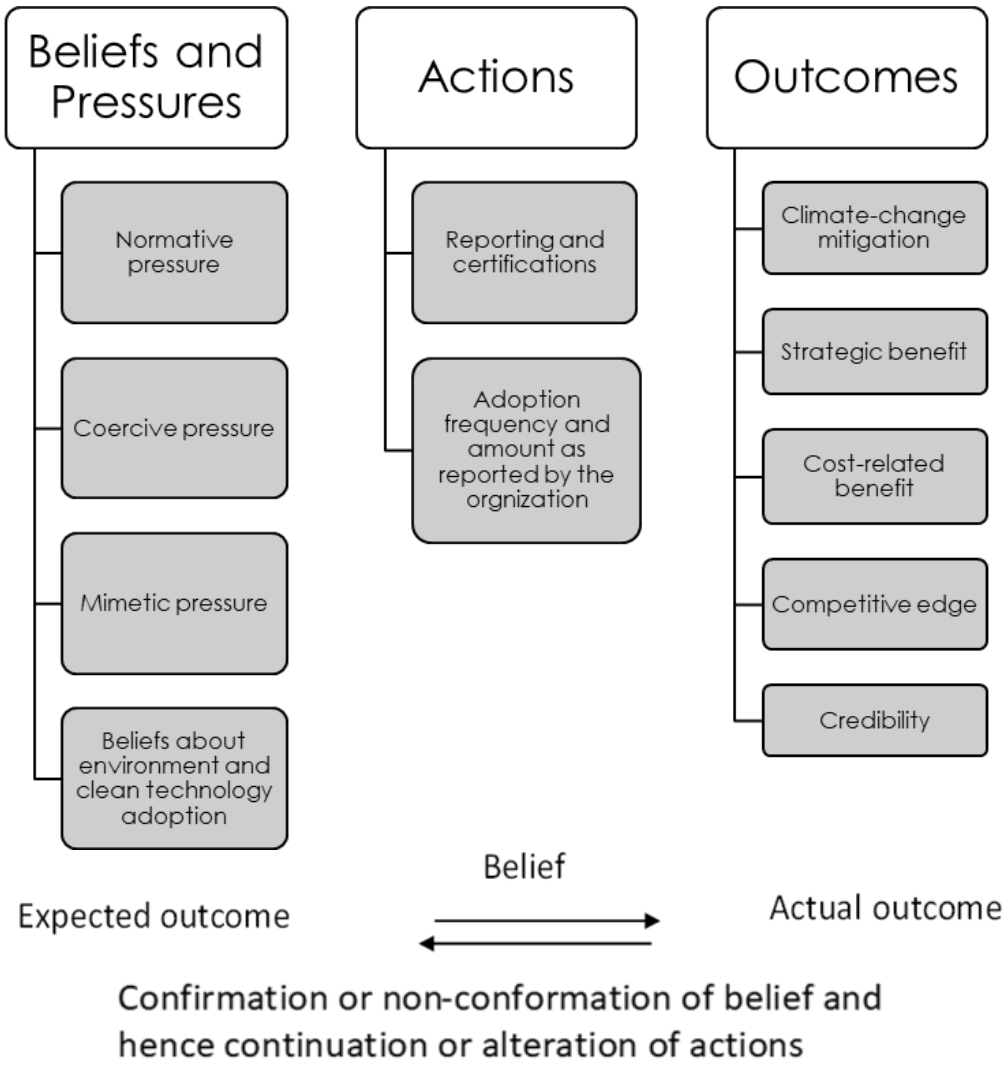


Figure 5.1: The Relationship between Beliefs, Actions, and Outcomes

Update on work package BB.3

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

The new research fellow **Dr Michelle FAN Xiaomin (Research Fellow, NUS)** is working with **Prof Kenneth HUANG (PI, NUS)** to analyse how VC investment influences the pollution behaviour of firms in the chemical and energy-intensive sectors in China. A comparison could be drawn with Singapore firms in the future. The manuscript is 70% ready and will be submitted to a top management journal before July 2022.

China has witnessed rapid economic development but has also been accompanied by severe environmental issues during the recent decades. As a critical driver of economic output and a source of pollution; firms, especially those in the chemical and energy-intensive sectors, face challenging trade-offs between making a profit, achieving growth, and reducing pollution emissions. Based on the dominant coalition theory, they investigate how firms in the chemical and energy-intensive industries, which are a critical source of pollution, will respond to the policy driving the venture capital boom in China, and moderate policy effects. They choose two critical air and water pollution sources for pollution emission: sulphur dioxide (SO_2) and chemical oxygen demand (COD) emissions.

Using proprietary data sources from the Annual Tax Survey, CVSource, and Environment Survey and Reporting, they prepared a detailed overview of these firms in the chemical and energy-intensive industries, including basic information for analysis, financial indicators, and environmental performance. Focusing on the 2009 top-down policy directive to boost VC investment in the Chinese market, they adopt a difference-in-differences methodology with firm fixed effects based on matched samples using propensity score matching to estimate the impact on environmental performance of invested firms. Specifically, they identify the VC-active firms (treatment group) and VC-inactive firms (control group) to capture the difference in pollution, and identify

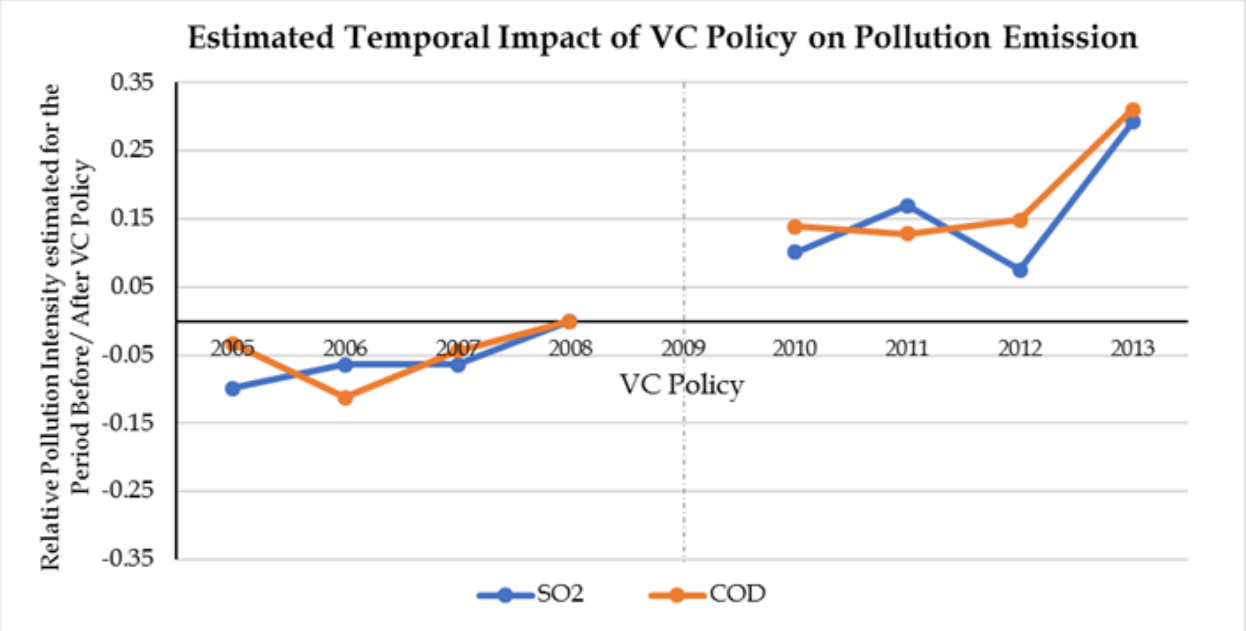


Figure 5.2: Estimated temporal impact of VC policy on pollution emission. This illustrates the estimated temporal impact of VC policy shock on the pollution emission for each year preceding and following the shock. Before the policy shock, there were no clear pre-trends that satisfied the parallel trend assumption for the difference-in-differences approach. They observe a significant positive effect on the pollution intensity for both SO_2 and COD.

firm performance between these two groups before and after the VC boom.

They found that the VC boom resulting from the 2009 policy shock increased the SO_2 and COD emission intensities for VC-active firms relative to VC-inactive ones. Furthermore, they find that VCs with prior investment experience in chemical and energy-related industries would mitigate the policy effects on pollution emissions. Provincial environmental protection officers would mitigate the policy effects at the provincial level.

Update on work package BB.4

Future roadmap for industrial decarbonisation, including international comparisons

For WP3, IRP-BB continues to work closely with the technology IRPs, including meetings with emerging (and potential) spinouts from IRP1, IRP2 and IRP3.

They have started modelling the hydrogen production process through a waste-to-energy route and aim to perform a Life Cycle Analysis to compare it to different hydrogen production routes. This information will be useful to understand the decarbonisation options and put it in perspective to local decarbonisation road-mapping activity. Prof Steve Evans spent a month in Singapore, attending the Singapore Business Federation Summit and meeting with various organisations – SBF, American Chamber of Commerce, EcoLabs, 3DP@NTU, SimTech, ISCE2, etc., as part of preparing for wider sector level future road-mapping.

Emerging Opportunities Fund

The team also worked closely with C4T Emerging Opportunities Fund 06 (Carbon reduction strategies of top chemical companies) , see page 145 for further updates.

Other activities and achievements

Dr. Abhiruchi GADGIL (Research Fellow, NTU), is a mentor for EB Impact's Sustainability Exchange. Sustainability Exchange is a mentorship initiative first launched in 2020 by EB Impact. The first leg of this mentorship program has concluded and the team she is mentoring has submitted their proposal. They have been invited for a pitching session in front of investors such as OCBC and Meta for their idea on 29 May 2022.

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

Assoc Professor Raymond LAU Wai Man
Nanyang Technological University

Professor Iftekhar KARIMI
National University of Singapore

OVERVIEW

Over the past six months, the J-Park Simulator (JPS) has progressed on several fronts with regard to developing new capabilities for enhancing the existing JPS architecture and developing new functionalities to demonstrate its multi-domain capabilities, and to augment its degree of autonomy and connectivity to the physical world. For instance, we have been working on containerising code. The advantage of containerisation is that the code and all dependencies are isolated from the host system. This allows for very easy and rapid deployment. Furthermore, we have tested and implemented cloud platform-based solutions to complement the existing hardware being used. The cloud offers highly flexible storage and computing options for hosting our triplestores and agents. This will support the needs of our growing knowledge graph.

In addition, we have collected and instantiated building data in the knowledge graph for Singapore. The building data are obtained from a public data source. The collected data were visually checked for accuracy and completeness, before being instantiated in the knowledge graph. The data contained approximately 13,755 residential and commercial buildings in CityGML Level of Detail 3 (LOD3).

We have also proposed and integrated a new algorithm for unsupervised instance matching based on heuristics and statistics called 'AutoCal', into an automated instance matching framework. The performance of AutoCal was evaluated with six different settings for instance matching: two new settings with power plant instances exhibiting a mixture of properties with short string, numerical and missing values, as well as four settings from domains that are frequently used in the literature (containing a large portion of text). AutoCal achieves results competitive to recently proposed unsupervised instance matchers from the field of Machine Learning and is specifically well-suited for use in an automated environment.

Moreover, we have improved the existing power flow (PF) analysis agent by introducing a newly created algorithm that can automatically handle model divergent problems by analysing the generated Jacobian matrices, thereby providing a robust calculation regardless of model complexity. The new algorithm identifies the 'weakest' bus node that results in the model diverging and applies a novel bus-type switching strategy to the identified bus node to alter its bus type. A new round of simulation with the updated bus node configuration will then be triggered and the entire process will be repeated until the model converges or until the model reaches termination condition.

Professor Markus Kraft, PI
University of Cambridge

Update on work package JPS.1

Big data — sensors and data modelling

As part of an attempt to digitalise and automate the CARES Laboratory, **Dr Ghulam MAJAL (Software Developer, CARES)**, **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, **Mr Wilson ANG (Software Developer, CARES)** and **Mr Simon RIHM (PhD student, CAM)** have made progress in several areas including the development of a smart meter prototype and the installation of a weather station. For instance, Mr Ang in close collaboration with Mr Chadzynski, has been working on a smart meter prototype that can measure the electricity consumption (current, voltage, active power, active energy and power factor) of a fridge in the CARES Laboratory, and the temperature and humidity of the surroundings. To prevent the prototype from overheating, the internal operating temperature of the smart meter is also being measured and a cooling fan has been integrated into the prototype. The smart meter prototype transmits electricity consumption, temperature, and humidity measurement data to a third-party platform called 'ThingsBoard'; and cooling fan switch status data to a webserver called 'ESPHome'. Mr Ang also created a 'ThingsBoard' agent and an 'ESPHome Update' agent to periodically retrieve measurement and cooling fan switch status data from the ThingsBoard platform and ESPHome webserver respectively.

The agents convert the measurement or switch status data into a time-series format and store it in the knowledge graph. In addition, he created an 'ESPHome' agent to periodically query the knowledge graph for the smart meter's most recent internal operating temperature and cooling fan switch status. When the internal operating temperature of the smart meter exceeds the specified threshold value, the ESPHome agent will send a POST request to the ESPHome webserver to turn on the cooling fan switch (if the switch is in an off position) and vice versa when the internal operating temperature of the smart meter falls below the specified threshold value.

Dr Majal in close collaboration with Mr Ang has developed a 'CARESWeatherStation' agent to

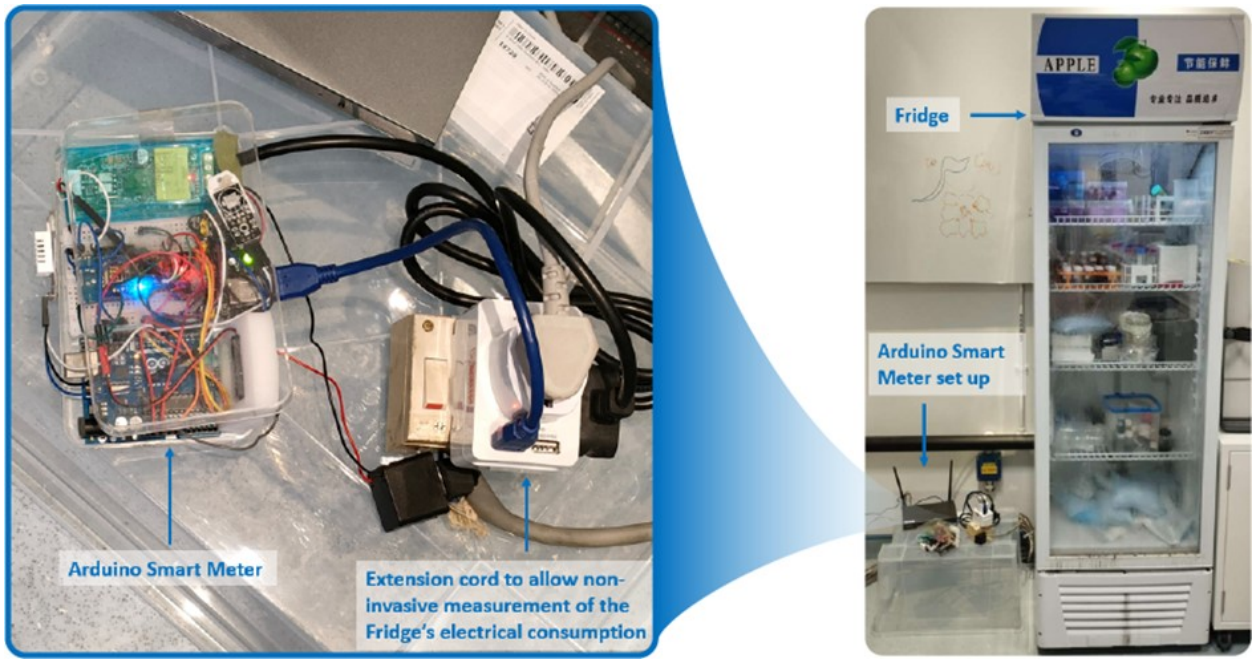


Figure 6.1: Smart meter prototype to measure the electricity consumption of a fridge in the CARES Laboratory, and the temperature and humidity of the surroundings.

periodically retrieve weather measurement data (temperature, humidity, precipitation, pressure, and wind speed) from a weather station located in the CREATE Tower. The weather station transmits measurement data to a webserver called 'Weather Underground' and the data is retrieved periodically by the CARESWeatherStation agent using an Application Programming Interface (API).

After a thorough review of the work done to date, Mr Rihm prioritised potential use cases such as asset management based on their effort and impact towards developing a digital twin of the CARES laboratory. He is currently working on extending ontologies to allow for multi-level and multi-aspect representations of the CARES Lab, as well as the assets and activities occurring within the Lab.

Figure 6.2: Weather station located in the CREATE Tower.

Update on work package JPS.2

Surrogate models, superstructure and architecture development

Dr Jethro AKROYD (Senior Research Fellow, CARES), **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, **Dr Feroz FARAZI (Research Associate, CAM)**, **Dr Casper LINDBERG (Research Fellow, CARES)** and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)** have continued to drive forward the overall JPS architecture. For instance, Dr Lindberg together with Dr Mosbach, have been improving the development workflow and infrastructure of The World Avatar (TWA) project. A more streamlined workflow is needed to support the rapid development and deployment of software, and to coordinate a larger, geographically distributed development team. This was achieved by switching to a new Git version control-based development workflow called GitHub Flow. GitHub Flow offers a lightweight workflow that is geared towards the continuous deployment of software while maintaining standards for testing and code review.

Dr Lindberg is also involved in containerising TWA code using Docker software. The advantage of containerisation is that the code and all dependencies are isolated from the host system and will run consistently on any Docker equipped infrastructure. This allows for very easy and rapid deployment. Furthermore, he tested and implemented cloud platform-based solutions to complement the existing hardware used by TWA. The cloud offers highly flexible storage and computing options for hosting triplestores and agents. Lightweight virtual machines equipped with Docker software run containerised code and can be scaled up and down as needed. This will support the needs of the growing knowledge graph. More recently, Dr Lindberg and Dr Mosbach have started working on agent routing. This will equip agents with methods to locate other agents in the knowledge graph in a more consistent and straightforward manner.

Mr Chadzynski is heavily involved in training, supporting and providing guidance, especially to new members of the team concerning documentation, questions on software design, agent development and non-functional requirements such as performance and scalability. **Ms Srishti GANGULY (Project Engineer, CARES)** is involved in the testing, deployment, and maintenance of various projects in TWA.

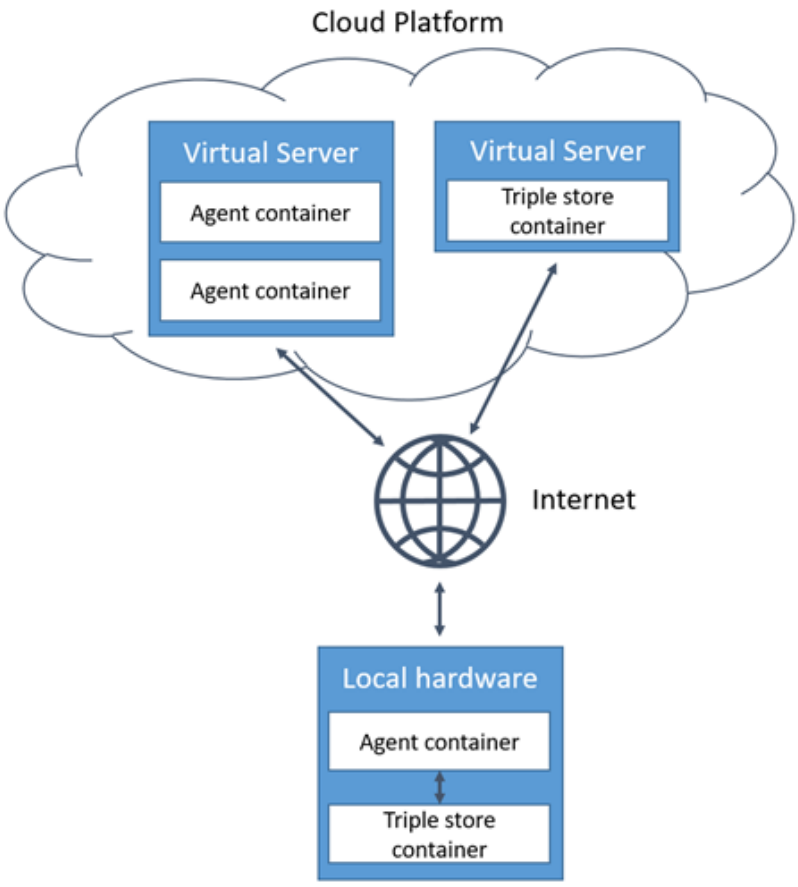


Figure 6.3: Schematic diagram of decentralised architecture for TWA.

Update on work package JPS.3

Implementation

Dr Jethro AKROYD (Senior Research Fellow, CARES), **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)** and **Dr Feroz FARAZI (Research Associate, CAM)** have been working to formalise a dynamic knowledge graph approach for digital twins to perform 'what-if' scenario analysis for the energy system.

Solving the energy challenge will involve the widespread deployment of renewable technologies including, solar photovoltaics, wind turbines, and bioenergy. Deploying these technologies has significant implications for land use and cannot be considered in isolation from the impact on food production and biodiversity. The knowledge graph-based digital twin is an effort to use The World Avatar (TWA) to create a semantic digital twin of real-world entities that share data and answer complex queries. The aim of this work is to provide a comprehensive live distributed platform to support the optimal use, planning and development of infrastructure; for example, by supporting the decarbonisation of the energy landscape. Work to date has therefore focused on the electric power system, the gas grid, and land use, all of which are critical to the future of the energy landscape. UK is used in the first instance to develop the proof of concept as data for the UK is readily and publicly available. This work can easily be extended and applied to other regions where data is available, in particular Singapore.

Dr Akroyd, Dr Mosbach, Dr Farazi, Ms Sophie HALL and Mr Toby LATCHAM (Both non-C4T students, University of Cambridge) have developed web data query tools to extract wind and solar energy generation and consumption data available on the Web. Relevant ontologies such as Wind Turbine, Weather Property, Solar Panels, and Electricity Consumption were also created. For instance, the Wind Turbine ontology consists of classes including Turbine, Dimension, Property, and its more specific classes such as Cut-in-Speed, Cut-off-Speed, Rated Power, Rated Speed and Survival Speed. The Weather Property ontol-

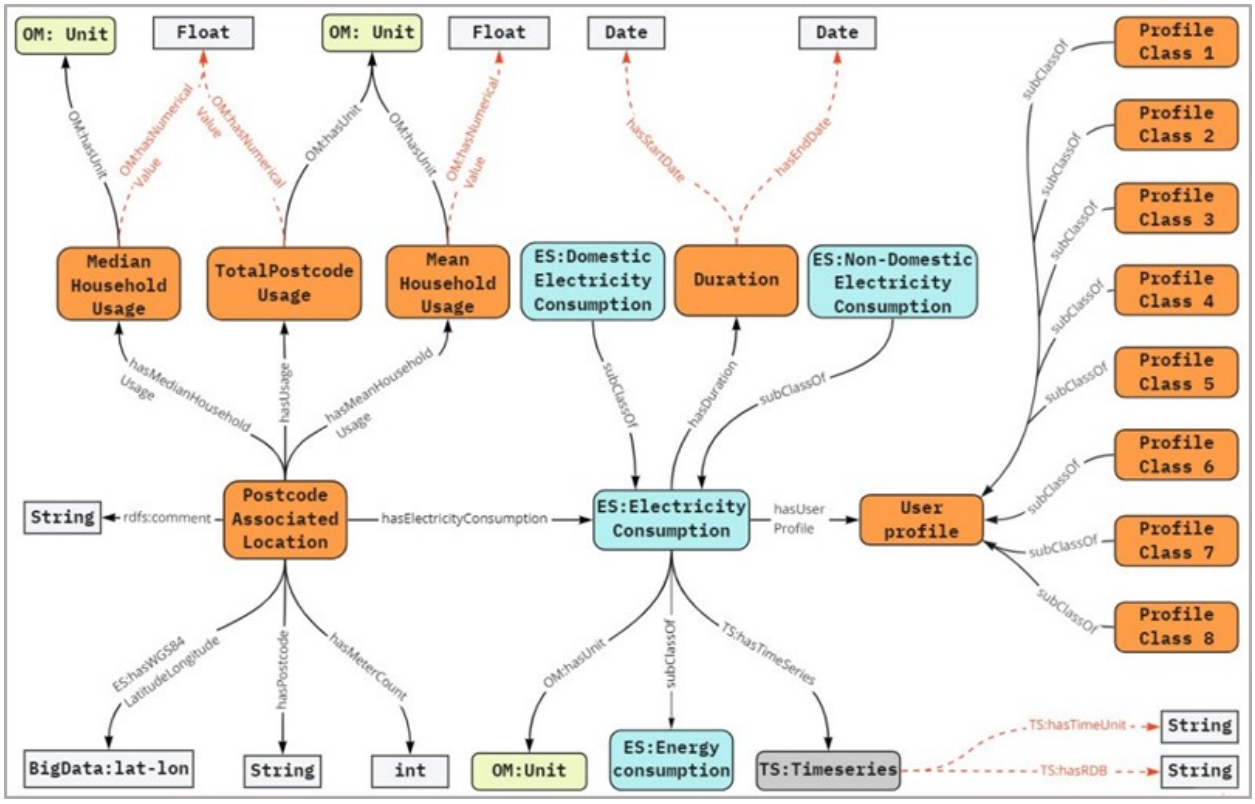


Figure 6.4: Ontology for representing electricity consumption associated with a postcode.

ogy comprises classes including Wind Speed, Wind Direction, Mean Wind Speed, Mean Wind Direction, Maximum Wind Gust Speed and Maximum Wind Gust Direction. Data such as Solar Radiation, Wind Speed, and Electricity Consumption have been represented as time series in the knowledge graph using the time series client by means of a link to a relational database storing the data.

Dr Akroyd, Dr Mosbach, Dr Farazi and Mr Chufeng XIAO (Non-C4T PhD student, University of Cambridge) have designed the first version of an ontology for describing forest data in the UK. This ontology will eventually be extended to represent forest data in the entire world. The ontology currently consists of classes including Administrative Division, Forest, Forest Cover, and Woodland. The Woodland class has more specific sub-classes, including Coniferous, Broad-leaved, Shrub Land, Young Trees, and Low-Density Woodland. Furthermore, they have developed a SPARQL Endpoint using Ontop, a system that exposes the content of relational databases as knowledge graphs by translating SPARQL queries expressed over the knowledge graphs into SQL queries executed by the relational data sources. This enables users to apply spatial functions by defining an Ontop Ontology-Based Data Access (OBDA) mapping while querying crop map data of England.

Mr Markus HOFMEISTER (PhD student, CAM) has been investigating the applicability of TWA to build a Universal Digital Twin for broad smart city contexts. In particular, he has focussed on assessing the impact of potential flood scenarios across different domains to foster their interoperability. Although many digital twins have been previously proposed to improve decision making in smart cities, most of these suggestions do not leverage the connected nature of data arising from different sources. Data usually remains fragmented, and analyses mainly focus on isolated fields. By contrast, this work is centred around Findable, Accessible, Interoperable, and

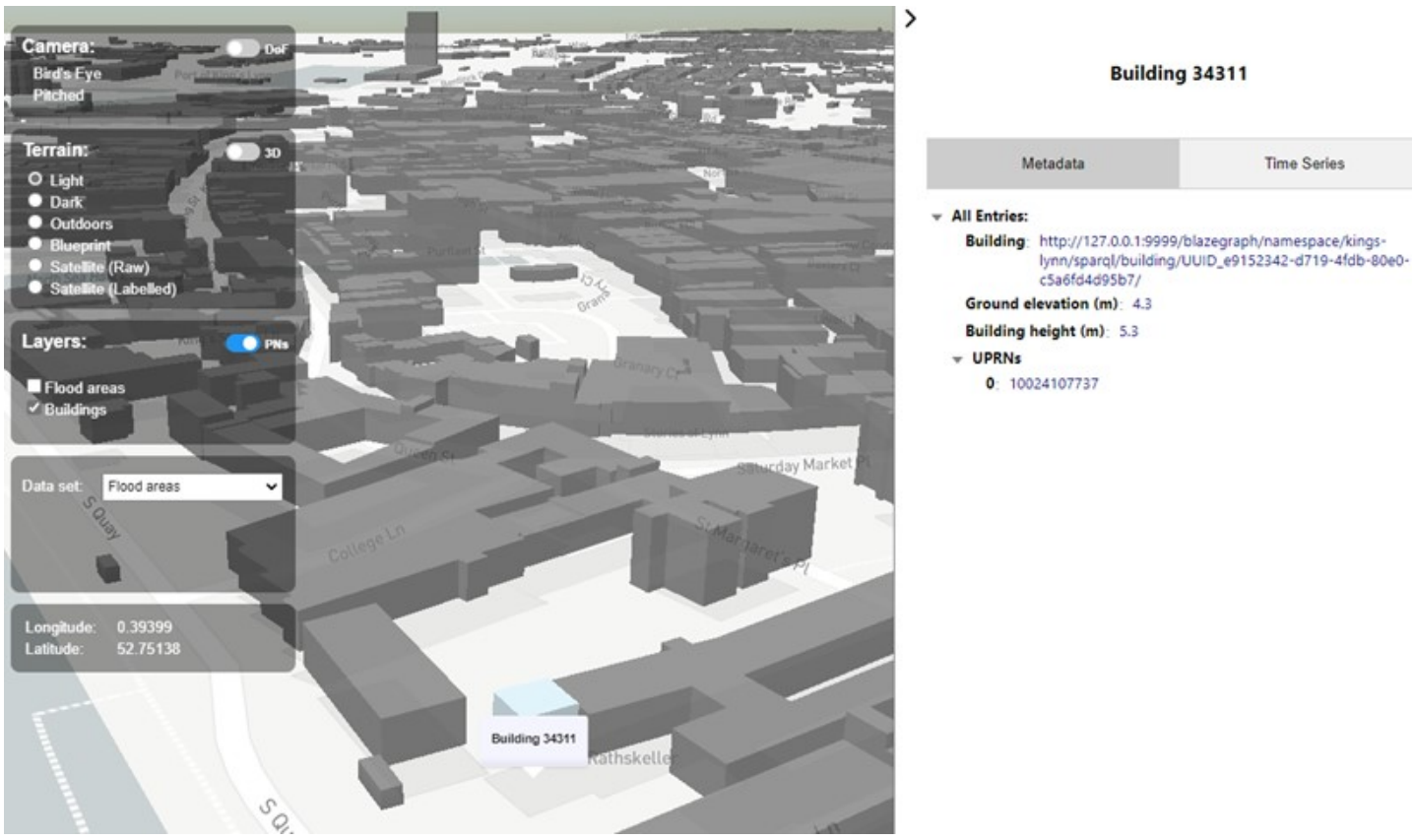


Figure 6.5: Visualisation of instantiated King's Lynn building data in the knowledge graph as a basis for evaluation of potential flood damage.

Reusable (FAIR) data principles, and combines multiple publicly available data streams into an ever-evolving, unified data asset, that is accessible for humans, autonomous software agents, and artificial intelligence. It combines geo-spatial city data, such as information about the built environment and land use; with building metadata, such as usage, and near real-time environmental observation data, as well as transient information such as river water levels and flood warnings.

Mr Hofmeister has developed three new ontologies to extend the knowledge graph and to enable cross-domain assessments between prior isolated data sources. He is in the process of developing computational agents to incorporate multiple publicly available data streams into the knowledge graph via Application Programming Interfaces (APIs). In the future, he will develop more agents that act on the knowledge graph to estimate the impact of potential flooding events, for example, with regards to the number of affected people and property value at risk.

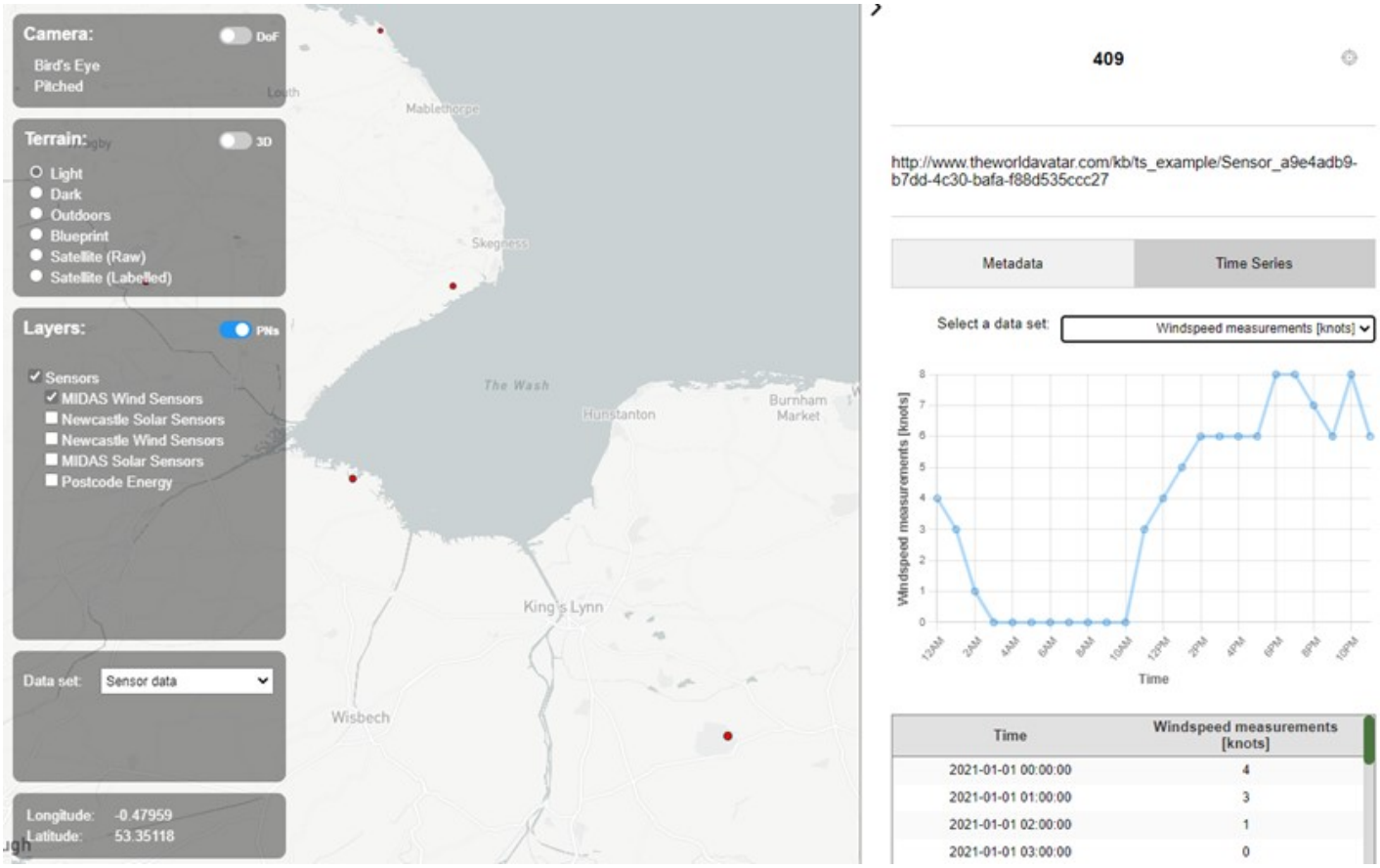


Figure 6.6: Visualisation of near real-time environmental observation data.

Ms Wanni XIE (Non-C4T PhD student, University of Cambridge) has continued to work on the development of the knowledge graph-based digital twin of the UK and its data-agent integrated ecosystem framework. In particular, she has focused on improving the power flow (PF) analysis agent by introducing a newly created algorithm that can automatically handle model divergent problems, thereby providing a robust calculation regardless of model complexity. The PF agent performs a numerical analysis of the flow of electric power in a power system. Through analysing the Jacobian matrix generated from the first iteration of Newton's method, the new algorithm identifies the 'weakest' bus node that results in the model diverging. A novel bus-type switching strategy is then applied to the identified bus node to alter its bus type from PQ to PV. A new round of simulation with the updated bus node configuration will then be triggered and the entire process will be repeated until the model converges or until the model reaches termination condition.

Ms Xie also utilised the derived information framework to annotate the knowledge graph. The derived information framework helps to manage and track data flow while running a simulation and to identify relationships and dependencies between a variant of model entities.

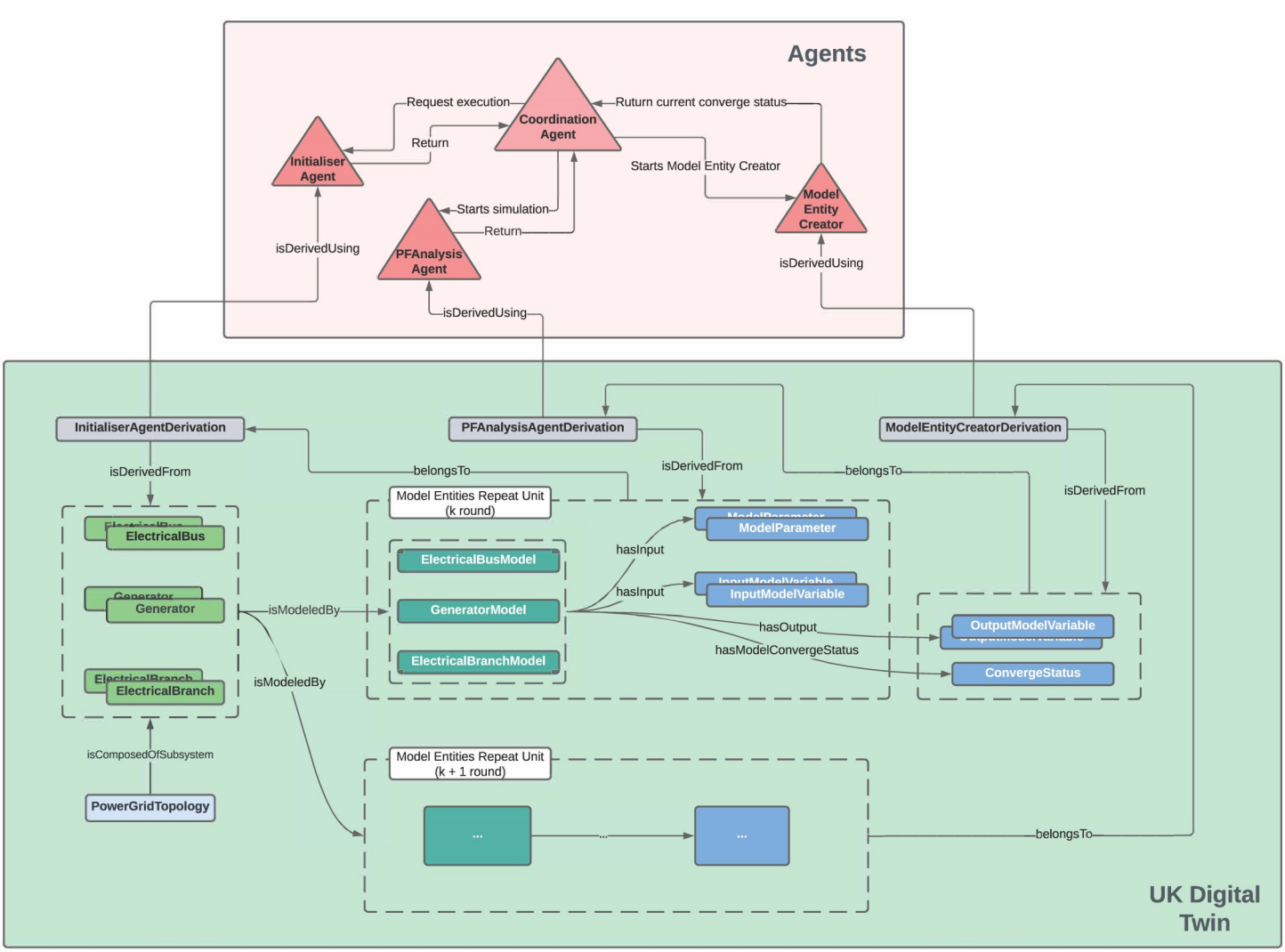


Figure 6.7: Power flow analysis agent acting on the knowledge graph-based digital twin of the UK.

Mr John ATHERTON (PhD student, CAM) has performed a systematic review of the UK's power generation infrastructure. The review resulted in a mapping across the Balancing Mechanism Reporting Service (BMRS), Energy Industries Council (EIC), and pre-existing Digest of UK Energy Statistics (DUKES) data sources to create a consolidated database of UK power stations and power generation units. The mapping process also rates the confidence of the matches. He has also developed two scripts to read power output data and visualise the data. Due to this automation, previously siloed data sources can have their data combined when mapped. Examples of such data include the capacities and outputs of numerous dispatchable energy sources and wind power plants/farms.

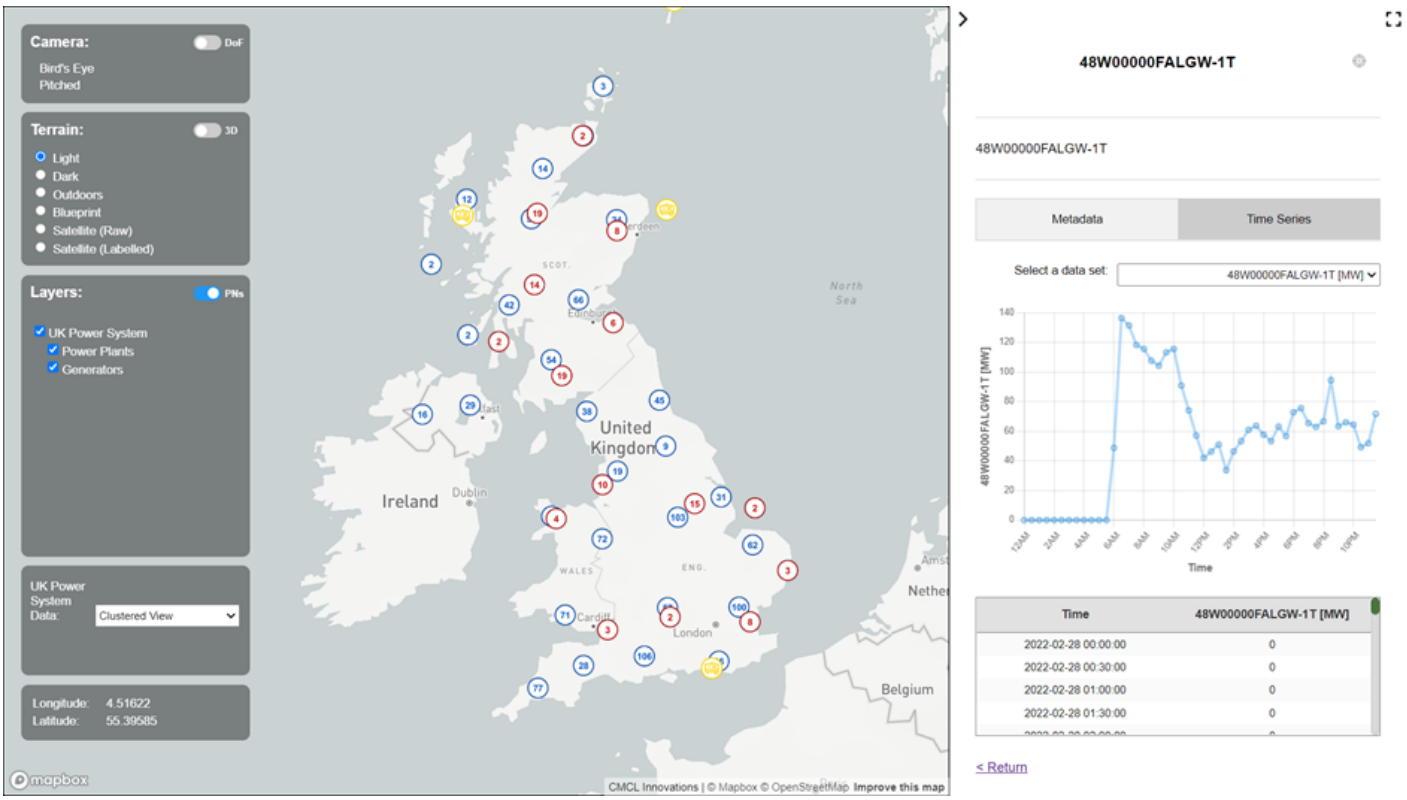


Figure 6.8: The left figure visualises the geo-spatial distribution of UK power stations and power generation units. The right figure displays the time series data of a selected generation unit's output.

Update on work package JPS.4

Model analysis and visualisation

Dr Vishvak KANNAN (Research Fellow, CARES), **Dr Jingya YAN (Research Fellow, CARES)**, **Mr Lerh Feng LOW (Computer Scientist, CARES)** and **Ms Srishti GANGULY (Project Engineer, CARES)** have collected and instantiated building data in the knowledge graph for Singapore. The building data was obtained from a public data source. The collected data were visually checked for accuracy and completeness, before being instantiated in the knowledge graph. The data contained approximately 13,755 residential and commercial buildings in CityGML Level of Detail 3 (LOD3).

Mr Low has also created over 6,000 LOD1 models for structures on Singapore Jurong Island, along with documenting their heights, owners, and land lot numbers, among other information. Working in conjunction with Ms Ganguly, this information has been instantiated into the knowledge graph. Mr Low is in the process of incorporating information about the chemicals produced on Jurong Island, that is where and how they are produced.

Dr Andreas EIBECK (IRP JPS) and **Ms Shaocong ZHANG (Software Developer, CARES)** have been working on the improvement of the performance of an automated instance matching framework. This involves proposing and integrating a new algorithm for unsupervised instance matching called 'AutoCal'. AutoCal consists of three main steps based on heuristics and statistics: 1) computes maximum similarity vectors on subsets of paired instances sharing equal tokens; 2) uses their empirical marginal distributions to derive calibrated property scores and 3) estimates a matching threshold for the aggregated property scores. The performance of AutoCal was evaluated with six different settings for instance matching: two new settings with power plant instances exhibiting a mixture of properties with short string, numerical, and missing values, as well as four settings from domains that are

Figure 6.9: Visualisation of the CityGML LOD3 building model in Singapore mainland.

frequently used in the literature (containing a large portion of text). AutoCal achieves results competitive to recently proposed unsupervised instance matchers from the field of Machine Learning and is specifically well-suited for use in an automated environment.

Mr Xiaochi ZHOU (PhD student, CAM) has been working on the review of the impact of Blockchain technology on the chemical industry and research. A review paper entitled 'Blockchain Technology in the Chemical Industry' was accepted by *Annual Review of Chemical and Biomolecular Engineering*. Figure 6.10 shows the word cloud generated from this review paper. The review paper first analysed the motivation for the trend of integrating Blockchain technology into industry systems. Due to the rapid growth in the number of devices, controllers, and sensors integrated and connected to industry systems, it is challenging for centralised systems to provide prompt and robust control. Consequently, the trend of adopting decentralised systems is inevitable. However, without centralised control, it is even more crucial to guarantee the integrity of data, prevent malicious action, safeguard transactions and so forth. Blockchain being the most prevalent solution for autonomous distributed controls in decentralised systems is therefore selected for implementing the trust layer. The paper also thoroughly introduced the technical details of Blockchain and Blockchain-based smart contracts such as how data are stored in the Blockchain, how peer-to-peer (P2P) networks are structured, and how consensus mechanisms are implemented. Various mainstream implementations of Blockchains, including Bitcoin, Ethereum, Cardano, NEO, Tezos, Ripple, and MultiChain; and different consensus mechanisms, for example, Proof-of-Work (PoW) and Proof-of-Stake (PoS) mechanisms are introduced as well. A quantitative analysis was also conducted on the publications of relevant articles.

Furthermore, the review paper discussed the concepts of industry systems and the application of Blockchain technology and/or smart contracts and its impact on the chemical industry as a whole, and on specific key topics. The key topics include the Internet of Things, Industry 4.0, P2P energy markets, emission trading, and smart cities. For each key topic, the review paper examined the motivation for adopting Blockchain technology or smart contracts, and provided a list of related applications and research.

Figure 6.10: Word cloud generated from all the articles collected in the review paper entitled 'Blockchain Technology in the Chemical Industry'.

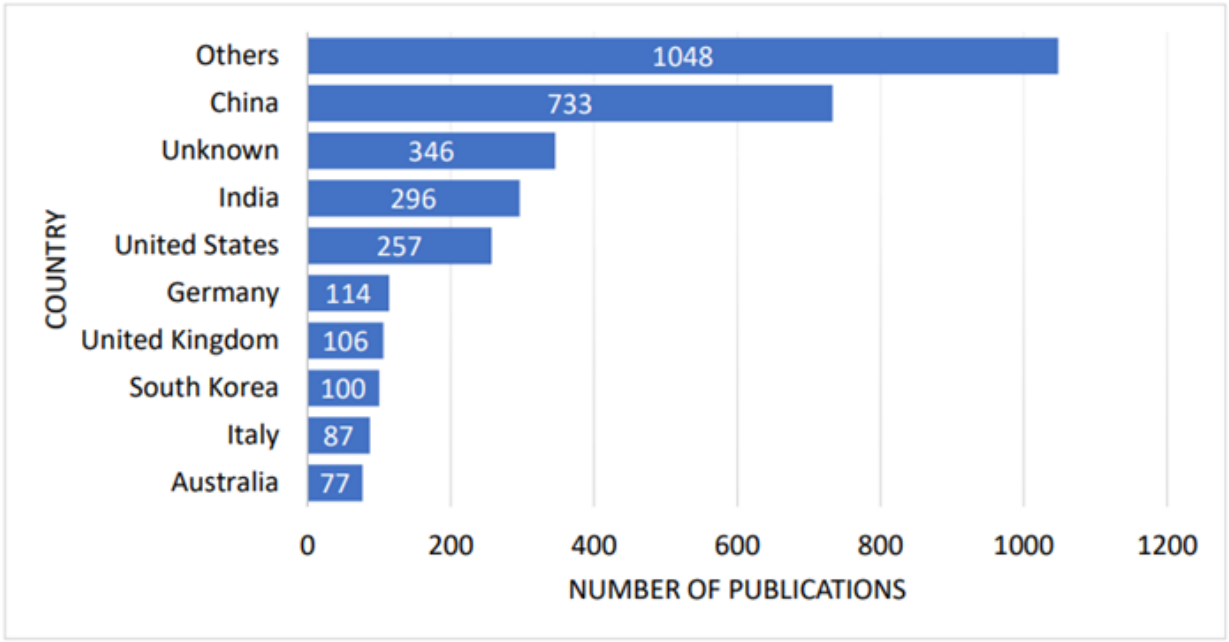


Figure 6.11: Number of publications per country on the topics of Internet of Things, Industry 4.0, P2P energy markets, emission trading, and smart cities.

Other activities and achievements

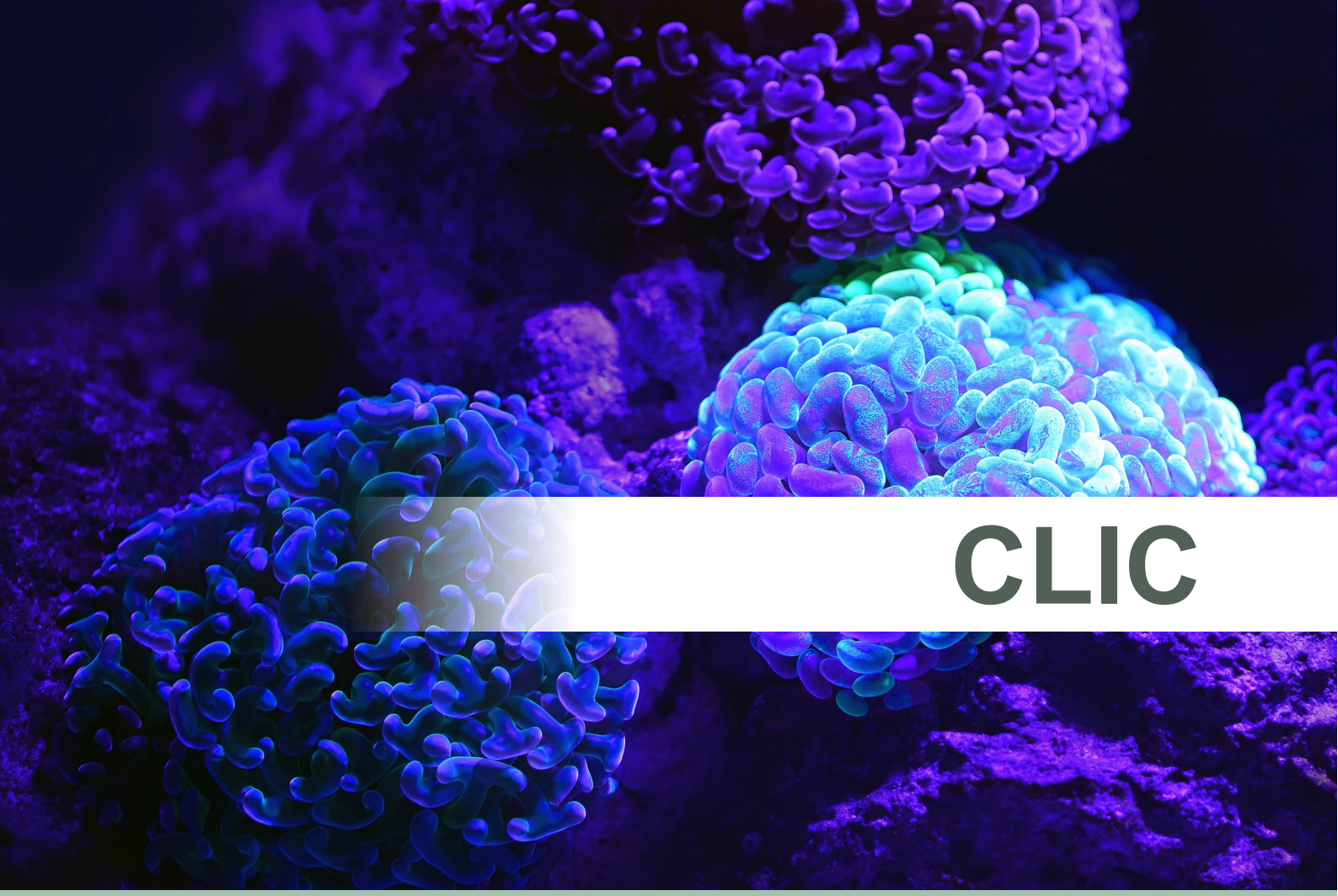
Prof Markus KRAFT (PI, CAM) gave a keynote talk at the Cambridge Zero Virtual Research Symposia on 17 November 2021 entitled 'Intelligent Decarbonisation and The World Avatar Project'. The talk explained the methodology behind The World Avatar project and highlighted its potential benefits. Prof Kraft gave a presentation called 'The Universal Digital Twin – accessing the world of chemistry' for the AI3SD Autumn Seminar Series at the University of Southampton on 24 November 2021. The presentation outlined the Universal Digital Twin and some of its applications in the realm of chemistry.

Prof Kraft presented at the International Symposium of Life-Cycle Emissions of Future Vehicles and Mobility (LIEF) on 30 November 2021. The talk titled 'A thermodynamic digital twin approach for future fuels, combustion modes and emissions', introduced a thermodynamic digital twin approach for more efficient combustion.

Prof Kraft gave a presentation at the Centre for Liveable Cities (CLC) on 15 February 2022. The presentation titled 'Digital Twins and Semantic Technology' gave an overview of The World Avatar project.

Prof Kraft was also announced as a Turing Fellow by The Alan Turing Institute on 12 January 2022. Turing Fellowships are awarded to established scholars with proven research excellence in data science, artificial intelligence, or related fields.

Mr Markus HOFMEISTER (PhD student, CAM) will be presenting his work at the International Conference on Evolving Cities 2022, which will be held July 13-15 in Southampton, UK.



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 **Social and Cognition Workgroups** have been working together to begin extensive data-collection for the WP0.1 Adult Study. The teams have optimised the task battery, with the additions of new tasks in the area of inhibition and working memory, and online scoring for verbal and creativity tasks. Data analysis is harmonised across adult and adolescent studies through the efforts of the Computational Modelling discussion group, which is co-led by the Cognition and School Workgroups. In addition to developing standardised pipelines for data processing and analysis, the computational modelling team has also set up a CLIC GitHub repository as a collaboration platform for data analysis. A pre-registration report for the WP0.1 Adult Study was submitted in Dec 2021.

To address hypothesised inter-relations between cognitive flexibility subcomponents and structure learning, the Cognition Workgroup is developing observer models of structure learning and applying hierarchical Reinforcement Learning (RL) models to extract specific learning and flexibility parameters from the executive function paradigms.

In November 2021, the CLIC **Social Workgroup** welcomed the arrival in Singapore and guidance of Professor Henriëtte Hendriks (Social Workgroup PI and Deputy Director, CAM), who aided in testing and pre-registration preparation for the study and helped finetune Standard Operation Procedures. She also conducted a series of workshops for the research team and helped optimise task administration.

Currently, the Social Workgroup has implemented JavaScript to code for the social decision-making tasks in the Qualtrics platform for task refinement. The team is also using R scripts to perform data quality checks, pre-processing of the data, and analysis of the social questionnaires and social decision-making tasks. The team has prepared a pre-registration for the hypotheses on associations between social decision-making, structure learning and cognitive flexibility in healthy young adults. A data codebook for WP0.1 Adult Study has been completed, while codebooks for WP0.1 adolescents' and WP0.2 study are in progress.

The **School Workgroup** team conducted a 4-day data collection pilot of the CLIC WP0.1 study with a class of Normal (Technical) Secondary school students in October 2021. The team will be returning to the school in May 2022 to gather data from 300 students for the main study. Improvements have been made on task delivery and protocol to increase engagement in the Structure Learning task by developing a backstory, accompanied by a video and activity sheets. The School Workgroup is also designing and validating a new measure of creativity, involving the creation of a three-dimensional creative product suitable for a naturalistic classroom setting.

The School Workgroup also organised a professional development workshop for Singapore teachers on Cognitive Flexibility and how skills in Executive Function affect learning. The School Workgroup also led a training workshop for all CLIC researchers on Electroencephalography (EEG) methodology and gold standards for data acquisition.

The team from the **Neuroimaging Workgroup** has completed two pilot studies for the WP0.2 Structure Learning Intervention Programme.

Findings from these pilot studies suggested further adjustments for the cognitive and social measures battery to be administered for equating the intervention and passive control groups, as well as adjustments of parameters of the training task used for the intervention. A third pilot has been conducted to iron out data collection issues as well as to test the intervention design and measure of flexibility. Results from Pilot Study 3 are pending and will help to inform the effects of the new intervention design of CLIC's complete cognitive battery. Planning and coordination is ongoing for the upcoming data collection for WP0.2. The MRI pilots have been conducted to finalise the imaging protocol. The development of the MRI analyses pipelines is progressing steadily under the close supervision of CLIC's neuroimaging leads from both Cambridge and NTU.

The CLIC Data Storage (CLIC Network-Attached Storage-NAS and CLIC Google Workspace) infrastructure for secure storage and sharing of research data between CLIC and Cambridge personnel is now fully operational. A framework for data management has been developed, along with a Personal Data Inventory Map, and data on -boarding and off-boarding procedures. All CLIC personnel and collaborators (National Institute of Education and LKC Medicine) have now been briefed on data handling guidelines and obligations to ensure secure use and access to CLIC's data.

Finally, in November 2021, a CLIC Social Media Team was formed. Information regarding the study and cognitive neuroscience of cognitive flexibility for learning will be disseminated through accounts established via Twitter, Facebook, LinkedIn, and Instagram. This will provide an avenue to provide visibility of the ongoing CLIC projects and engage with the public on current topics relevant to our research activities.

The CLIC team are actively progressing with data collection and study preparation, including the upcoming Data Analysis Bootcamp in June with colleagues in Cambridge. The team are on course with updated milestone projections of the study and are steadily working towards future objectives.

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

The Cognition Workgroup has been working actively together with the Social Workgroup to launch large-scale data collection for the WP0.1 Adult study (target N=400 adult participants). **Dr Ke TONG (Research Fellow, NTU)** has been instrumental in coordinating the setup and optimisation of the WP0.1 adult study task battery, including the addition of new inhibition and working memory tasks, and online scoring for certain verbal and creativity tasks. He has also led the pre-registration of the WP0.1 Adult study on the Open Science Framework (OSF) platform. One journal manuscript on the CLIC WP0.1 adult study research protocol (see Figure 7.1) is currently in preparation for submission.

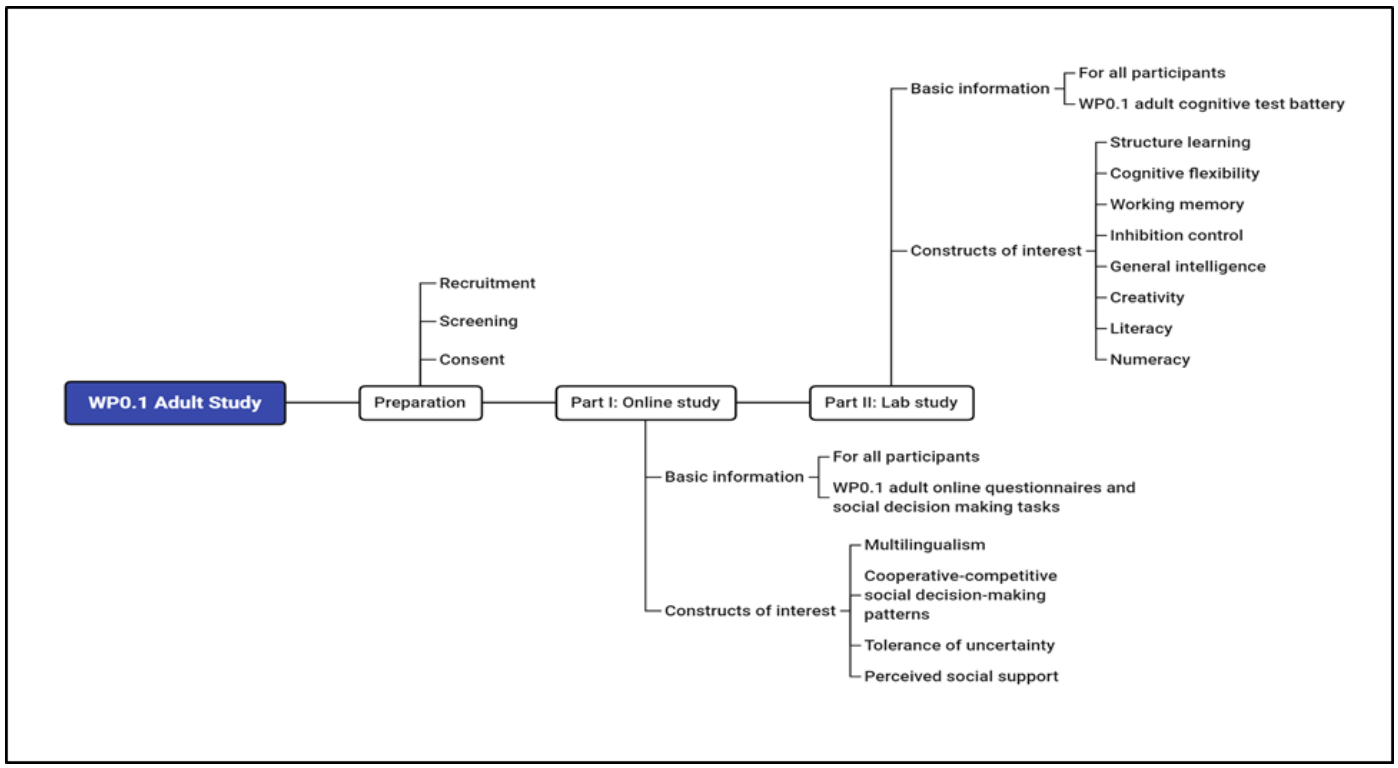


Figure 7.1: Overview of the test components of the WP0.1 adult study

The Cognition Workgroup also co-leads a Computational Modelling discussion group with contributors from all CLIC workgroups as well as external collaborators. The discussion group, co-led by Dr Tong (Cognition) and **Dr Ryutaro UCHIYAMA (Research Fellow, NTU)** (School), is responsible for developing standardised pipelines for data processing and analysis. Toward this aim, the discussion group has already formalised the data pre-processing pipeline for the CLIC WP0.1 study. A CLIC GitHub repository has also been set up as the collaboration platform for data analysis.

Specifically, Dr Tong is working on observer models of structure learning and the application of hierarchical Reinforcement Learning (RL) models to common executive function paradigms (e.g., Wisconsin Card Sort Test, Probabilistic Reversal Learning, Inter-Extra Dimensional Set Shift). This approach will help to address – at the fundamental construct level - the hypothesised inter-relations between cognitive flexibility subcomponents and structure learning. Figure 7.2 shows a hypothetical illustration of how RL models may be used to identify underlying constructs in relation to switching and learning).

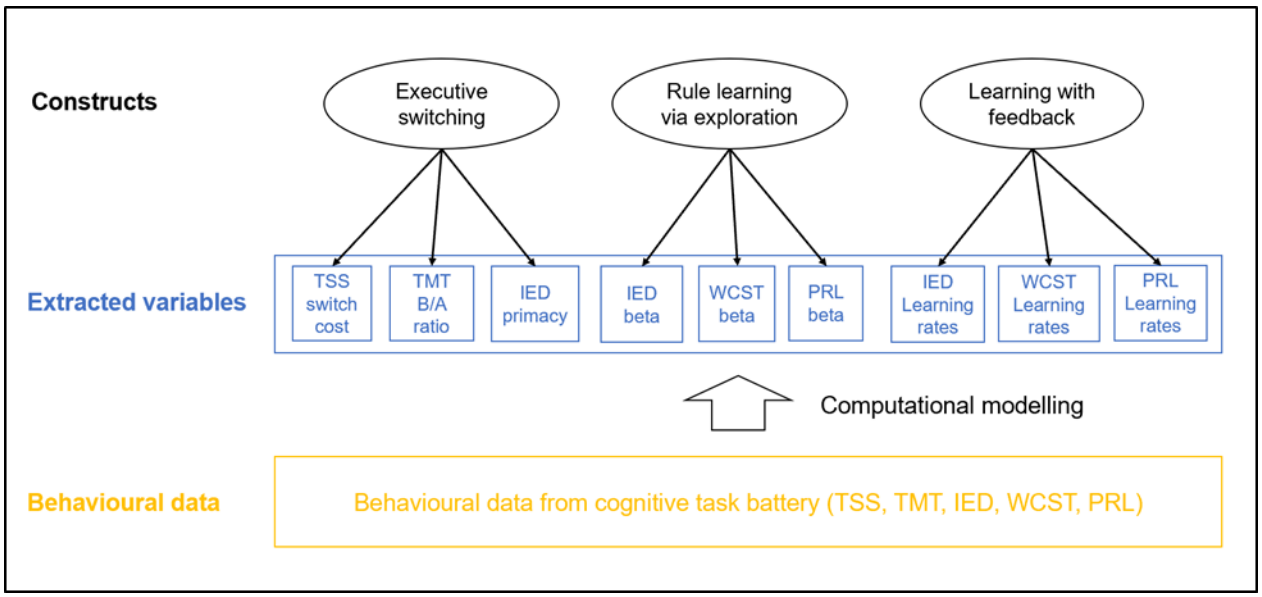


Figure 7.2: Illustration of RL modelling of common EF behavioural tasks to extract constructs in relation to switching and learning

Mr LEE Kean Mun (Research Assistant, NTU) joined the CLIC Cognition team in March 2022 and has been working under the supervision and guidance of **Assoc Prof Victoria LEONG (PI and Deputy Director, NTU)**. Mr Lee contributes to data collection and data quality checks for the WP0.1 Adult study. He is actively involved in administering cognitive tasks and is responsible for the scoring of the Torrance Test of Creative Thinking. He is under training to take on more roles in monitoring data collection status and data analysis.

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 Social Workgroup

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

Since September 2021, the Social Workgroup has worked towards launching data collection for WP0.1 and data collection is currently ongoing. At the time of writing, 83 adult participants have been recruited and 57 adult participants have fully completed the WP0.1 study (both the online and face-to-face portions). While the Research Assistants have been collecting data, the Research Fellows and PhD student have been checking the quality of the incoming data - for example by checking participants' attention while completing the online surveys, tracking any missing data, and monitoring participants' straight-lining behaviour. Any issues with the online Qualtrics survey platform are also being monitored. The Social Workgroup has also been preparing and has recently submitted the pre-registration for the hypotheses pertaining to the socio-cognitive variables in the adult's study. The Social Workgroup is particularly focused on the constructs pertaining to language, tolerance of uncertainty, perceived social support, social decision-making, and career development (see Figure 7.3).

Prior to the launch of data collection, **Prof Henriëtte HENDRIKS (PI and Deputy Director, CAM)** came for a visit to Singapore as stipulated by the CLIC grant. She arrived in Singapore for a residential stay of approximately 7 weeks (28 November 2021-14 January 2022). During her stay, she met with **Ms Christine AYE (CLIC Administrator, NTU)**, **Prof Annabel CHEN (PI & Director, NTU)**, and **Assoc Prof Victoria LEONG (PI & Deputy Director, NTU)**. She also met with the Singapore Social Workgroup in person, including **Assoc Prof Georgios CHRISTOPOULOS (PI, NTU)**, and became acquainted with all Research Assistants and the newly brought in Research Fellow through a number of social events and work meetings. She was also handed over some preparatory work for the organisation of face-to-face testing of the cognition battery and the de-

Outcome Variables

Construct	Examples of Questionnaires
Creativity	Creative Achievement Questionnaire (CAQ)
	Creative Self-Efficacy (CSE)
	Creative Mindset (CM)
Empathy	Empathy Quotient (EQ)
Theories of Intelligence	Implicit Theory (Intelligence)
Perseverance towards goals	Grit
Career	Future Work Self
	Career Exploration
	Job Search Efficacy
	Work Self-Efficacy Scale
	Perceived Employability
	Vocational Identity
	Career Decidedness

Sociocognitive variables

Multilingualism	Clip-Q Singapore Language History Questionnaire
Perceived Social Support	Provisions for Social Relationships and Adaptations to Stress
	Multidimensional Scale of Perceived Social Support
Tolerance of Uncertainty	Racial Essentialism Scale
	Receptiveness to Opposing Views
	Need for Closure Scale
Social Decision Making	Decision Making Tasks (Prisoner's Dilemma and similar decision making tasks)
	Social Value Orientation
	Cooperativeness and Competitiveness Personality Scale
	Independent/Interdependent Self-Construal Scale
	Coopetition-Oriented Mindset Scale
Personality	Big Five Inventory
	Individual Adaptability (I-ADAPT)

Figure 7.3. Sample of variables and questionnaires investigated by Social Workgroup (not exhaustive)

velopment of the Standard Operating Protocols (SOPs) for these purposes as **Dr Kastoori KALAIVANAN (Research Fellow, NTU)** was leaving. She coordinated further preparations of the face-to-face testing (including the order of the tasks, timing of the tasks, and issues of best practice with participants), which is largely conducted by the Research Assistants in the Social Workgroup. She ran a number of workshops and gave feedback on how best to organise and run the various cognitive tasks and oversaw the fine-tuning of the SOPs after test-runs had taken place. She is very closely involved in the running of the face-to-face data collection and joins the weekly meetings of both the Social Workgroup and the larger WP0.1 team. She has also helped prepare pre-registration documents for both the overall study and the social part of the study.

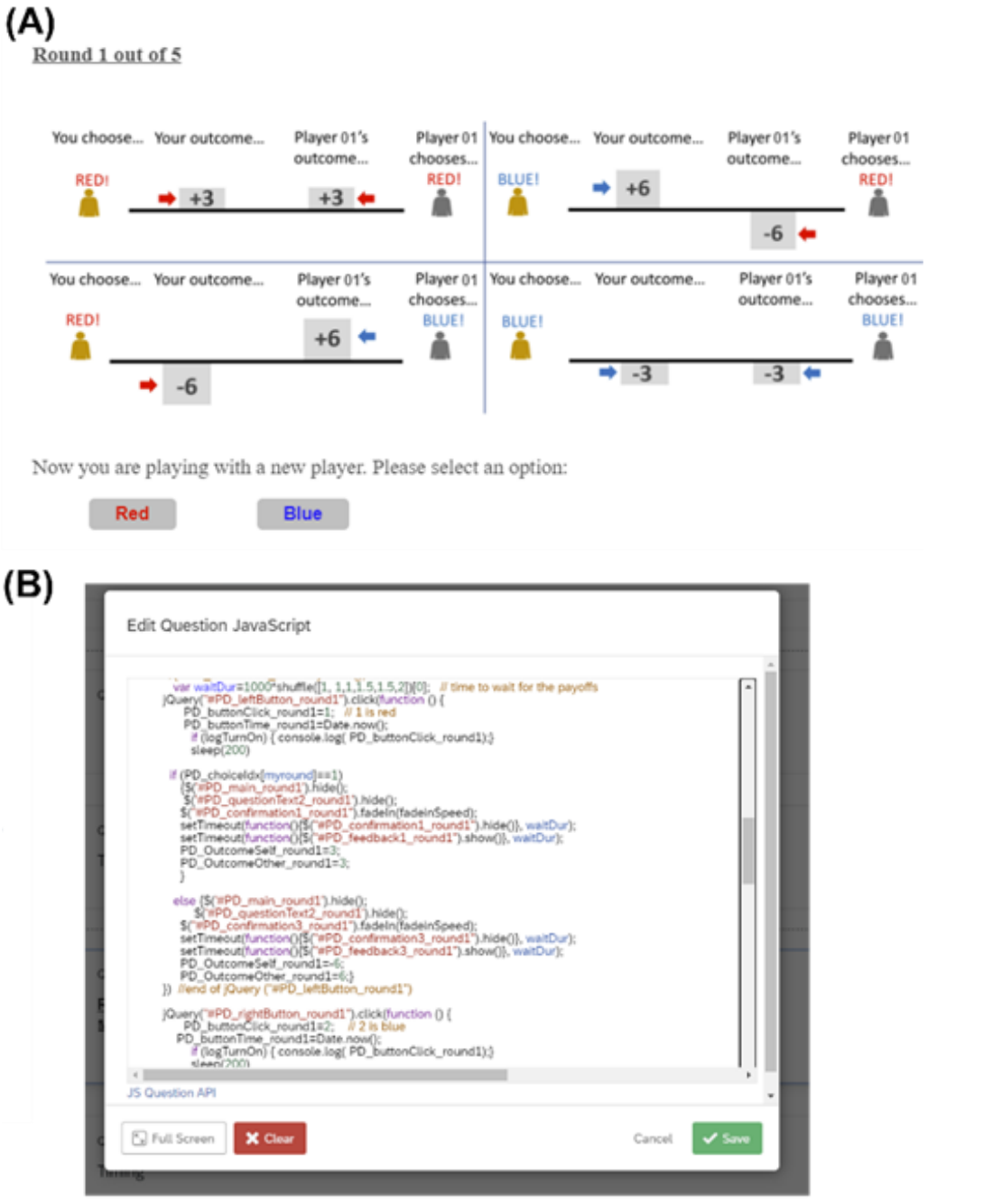


Figure 7.4: The interface of the prisoner's dilemma game and its JavaScript code. (A) Participants were instructed to click the button Red or Blue. A partner also chose between the two options. Both players' choices determined their outcomes. After they have made choices, the outcomes would be shown. (B) JavaScript code was implemented in the Qualtrics platform to add the flexibility of giving feedback depending on participants' choices.

Assoc Prof Georgios CHRISTOPOULOS (PI, NTU) has been managing the preparation of the WP0.1 studies for data collection, particularly the social factors such as social decision making, co-operation-competition, and tolerance of uncertainty. He is now overseeing the data collection process for the adult study, including participant recruitment, administration of the studies, and data quality checks, as well as the related pre-registrations. He is managing the activities of the group of researchers mentioned below.

Dr FENG Shengchuang (Research Fellow, NTU) has designed the social decision-making tasks for the WP0.1 studies. He implemented JavaScript coding for the social decision-making tasks in the Qualtrics platform to refine the tasks and make them more easily understandable to both adult and adolescent participants. Social decision-making tasks, which had been traditionally delivered in-lab, were administered online through the Qualtrics platform. The programming language JavaScript was used to code the interactive web-based tasks. Participants' choices and response time were recorded for each task and they were shown feedback about the number of points they won or lost. Figure 7.4 shows the interface of one of the tasks – the prisoner's dilemma game and its JavaScript code.

Dr Feng also prepared R scripts for data quality checks, pre-processing of the data, and analysis of the social questionnaires and social decision-making tasks. He has also prepared a pre-registration for the hypotheses regarding the associations between social decision-making and structure learning and cognitive flexibility in healthy young adults. In addition, he has also been assisting and mentoring others regarding data analysis and modelling methods. For example, he gave a talk titled "Markov Chain Monte Carlo methods to estimate parameters of reinforcement learning models" to other Research Fellows within CLIC.

Dr Nadhilla VELDA MELIA (Research Fellow, NTU) has taken over the duties for data organization and is the Variable Naming and Data Codebook Lead of the Social Workgroup after **Ms TAN Yan Fen (Research Assistant, NTU)** left. She has completed the data codebook and variable naming for the WP0.1 adult study and is now in charge of preparing the data codebook for the WP0.1 adolescents' study and WP0.2 study. She is also running data quality checks and preparing R scripts for data analysis for the social questionnaires, particularly those pertaining to language, tolerance of uncertainty, and perceived social support. For example, she has generated heatmaps (see Figure 7.5) to investigate potentially problematic datapoints, such as participants' straight-lining behaviours or excessive missing data.

Ms Emma SAM Yoke Loo (PhD Student, NTU) has contributed to the general logistical and administrative planning for WP0.1, such as the pre-registration and data analyses. She is also assisting with participant recruitment for the WP0.1 study by collating demographic characteristics of targeted populations to help monitor the demographic profile of the recruitment sample.

Ms Sam is also responsible for the sub-study under WP0.1 which is focused on the association between cognitive flexibility and career development. Specifically, she has prepared R scripts for performing data analyses for WP0.1 (in particular the career variables), examining the quality and distribution of the data and normal distribution, and establishing scale validity and reliability.

Ms Irene MELANI (Research Associate, NTU) contributed to the general research planning for the WP0.1 project. Specifically, she led the preparation of and submitted the pre-registration outlining the research proposal, aims, and plans (e.g., statistical approaches) addressing key research questions of interest to the Social Workgroup under the WP0.1 project on the Open Science Framework. In addition, she was also involved in the preparation of the pre-registrations for the main WP0.1 projects recruiting samples of Singaporean young adult and adolescents. She was involved in the early stages of data quality checks, in which she examined the descriptive statistics and distributional properties of the data to guide decisions on data exclusion criteria for the variables of interest to the Social Workgroup. Furthermore, she also supported the

general administrative and logistical planning, as well as data collection for the WP0.1 project.

Ms Melani is also a member of the CLIC Social Media Team. In November 2021, she contributed to the launch of CLIC's social media accounts on Twitter, Facebook, LinkedIn, and Instagram, aimed at building awareness for the CLIC project and engaging the general public in communication and conversations on current topics relevant to CLIC's research activities. Prior to the launch of CLIC's social media, she was heavily involved in the discussions on developing CLIC's social media identity, sharing her input on the appropriate logo, banner design, and handle names for each social media platform. A recent review of CLIC's social media performance suggests that CLIC's LinkedIn and Twitter accounts have increasingly garnered visitors and followers who are mostly professionals from the higher education and research sectors, as well as academics. To further harness the publicity gained from this profile of followership, she and her team members are continually planning, crafting, and releasing posts to attract further interests from professionals or academics of similar backgrounds,

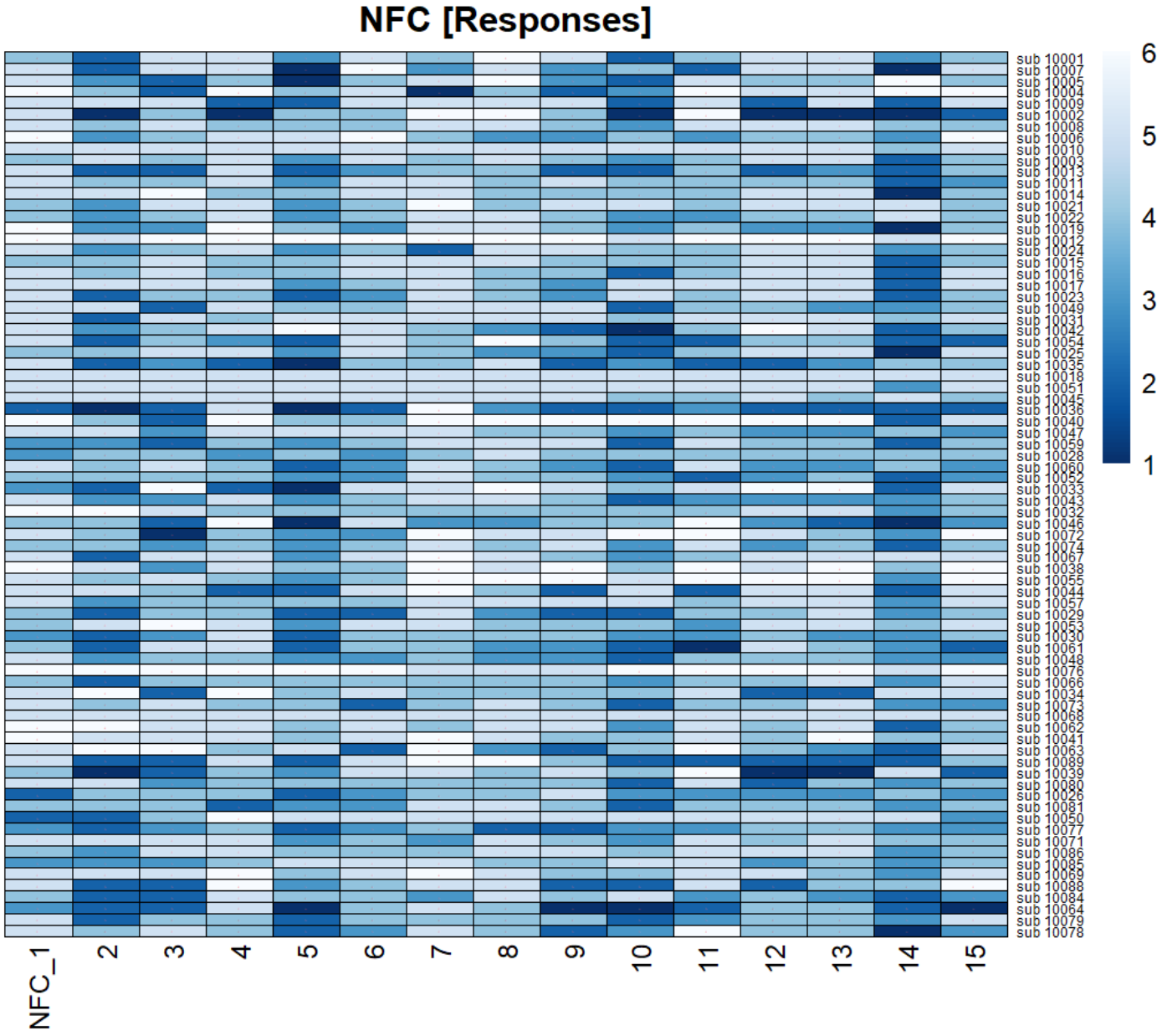


Figure 7.5: Heatmap of responses for the Need for Closure scale (N = 78)

and to further CLIC's social media reach to the general public.

Ms YAP Hui Shan (Research Assistant, NTU) contributed to the general logistical and administrative planning for WP0.1, such as the setup of multiple survey forms for data collection for both the WP0.1 adults and adolescents study and designing ways to allow for some questionnaires to be administered online. She also helped to draft and update portions of the SOP for administering the cognitive tasks to participants. In addition, she conducted data collection for a pilot study which was used to inform the design of the social decision-making tasks used for the WP0.1 and WP0.2 studies. She is also involved in the data collection for WP0.1 adults study where she mostly handles data collection for the online portion of the study.

Ms LEE Li Ling (Research Assistant, NTU) contributed to the general logistical and administrative tasks for WP0.1. She is part of the recruitment team and the lead coordinator of the face-to-face portion of the study which includes various tasks, such as drafting the SOP for administering the cognitive tasks to participants, session scheduling, and compensating participants.

Ms CHAN Yuan Ni (Research Assistant, NTU) assisted in the general logistical and administrative planning for WP0.1, such as setting up the online survey forms, designing the decision-making games, as well as updating the relevant SOP and manuals. She is also currently involved in data collection for the WP0.1 adults study.

Ms PEI Jia Ying (Research Assistant, NTU) is part of the recruitment team for WP0.1 where she handles part of the logistics and administrative planning, such as screening and recruiting eligible adult participants for the study. She provides primary supervision and training for undergraduate student assistants to administer various computerised and cognitive tasks to assist with the data collection process. Additionally, she is the Data Management lead of the Social Workgroup and ensures that the social group adheres to the data compliance guidelines.

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 Schools Workgroup

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

In October 2021, the School Workgroup conducted a 4-day data collection pilot of the CLIC WP0.1 study with one class of Normal (Technical) secondary students at their school. The research team will be returning to the school in May 2022 to collect data from 300 students for the main study.

Dr Ryutaro UCHIYAMA (Research Fellow, NTU) has been leading the analysis of the adolescent data, both in conducting statistical analysis of extant data, and in establishing the analytic protocol by writing the pre-registration. He has also been co-leading (together with Dr Tong) a bi-weekly discussion group on advanced computational methods for data analysis, involving CLIC members and affiliates from both NTU and Cambridge. Dr Uchiyama has been involved in various logistical issues, involving choice of devices to use for testing, designing the testing battery, and determining appropriate settings for the individual tasks. He also co-presented a seminar in November 2021 on CLIC's activities to the SOLEC (Science of Learning in Education) group of the National Institute of Education (NIE; an autonomous institute within NTU).

Under the guidance of **Prof David HUNG (PI, NTU/NIE)**, **Dr TEO Chew Lee (Co-I, NTU)**, and **Dr Peter SEOW (Co-I, NTU/NIE)**, **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** has been assigned to coordinate the School Workgroup team and to liaise with Adults' Working Groups (i.e. Cognition and Social teams) to ensure that data collection procedures, coding and analysis are properly aligned across the Working Groups. She joined the team in conducting a 4-day data collection pilot of the CLIC WP0.1 study with one class of Normal (Technical) Secondary students in their classroom and enabled a nested cognitive assessment and individual testing through an online video platform to comply with COVID safety measures. After the pilot, she was involved in refining the implementation of various tasks, as well as logistics for upcoming data collection for WP0.1 in schools and in the laboratory setting.

Dr Lopes Fischer also delivered a professional development workshop to 60 Singapore teachers on how Cognitive Flexibility and additional Executive Function skills may affect learning. Additionally, she conducted additional Professional Development Workshop sessions at CLIC about

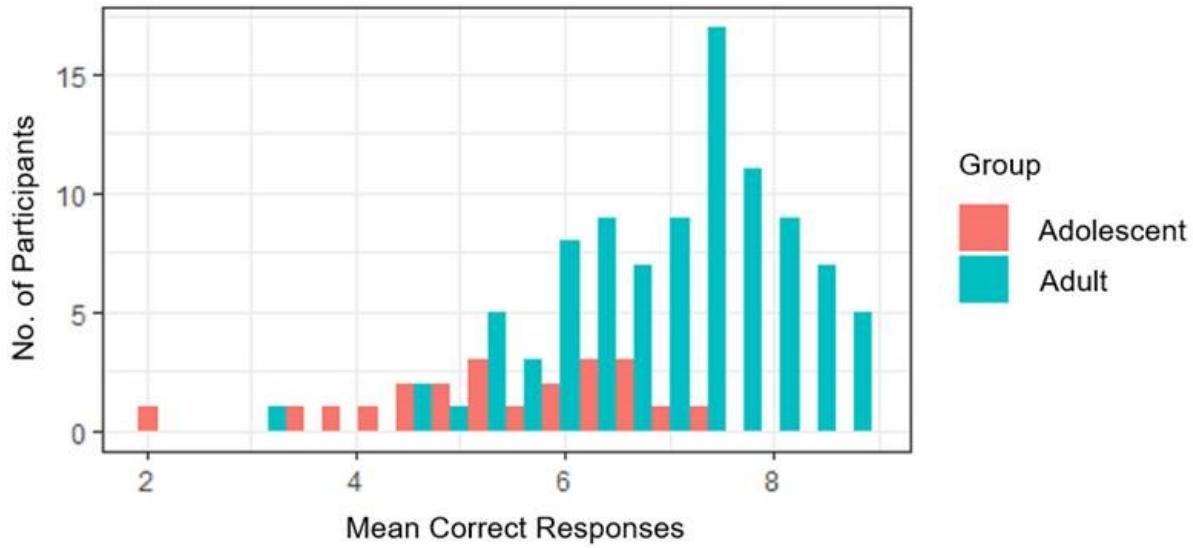


Figure 7.6: A comparison of adult and adolescent performance on the Wisconsin Card Sorting Test, a classical test of cognitive flexibility

the Electroencephalography (EEG) methodology, which comprised hands-on sessions regarding gold standard operational procedures for EEG data acquisition. Finally, under the guidance of **Assoc Prof Victoria LEONG (PI and Deputy Director, NTU)**, Dr Lopes Fischer has been involved in establishing new computational modelling methods applied to analyse infants' electroencephalographic (EEG) signals and unveil the neural processes behind new language patterns assimilation.

Since the last report, **Mr Timothy LEE (Research Associate, NTU)** has been involved in data collection and analysis for the School Workgroup under the guidance of **Prof David HUNG (PI, NTU/NIE)**, **Dr TEO Chew Lee (Co-I, NTU/NIE)** and **Dr Peter SEOW (Co-I, NTU/NIE)**. Mr Lee joined the School Workgroup in conducting the pilot WP0.1 study and was involved in the planning and setup of research platforms, and managed troubleshooting at the school. Following this, he has been primarily involved in data processing and analysis of the pilot data and refining the implementation of various tasks, as well as logistics for upcoming data collection for WP0.1 in schools and in the lab.

Mr Lee also played a leading role within the School Workgroup in crafting a professional development workshop on executive function and learning, delivered to 60 Singapore teachers, and developing this workshop into a mixed-methods study on teachers' knowledge of executive function and its influence on their teaching practice.

In addition, under the guidance of **Assoc Prof Victoria LEONG (PI & Deputy Director, NTU)** and **Prof Henriëtte HENDRIKS (PI and Deputy Director, CAM)**, he has been leading CLIC's data management framework with **Dr CHUNG Sheng Hung (Research Engineer, NTU)** and **Dr CHENG Xiaoqin (Research Fellow, NTU)**. Working with this core team from the Data and Communications Workgroup, Mr Lee has developed a CLIC data onboarding briefing for all CLIC members, setup a role-based access control system for CLIC's data storage resources, and managed day-to-day data protection issues.

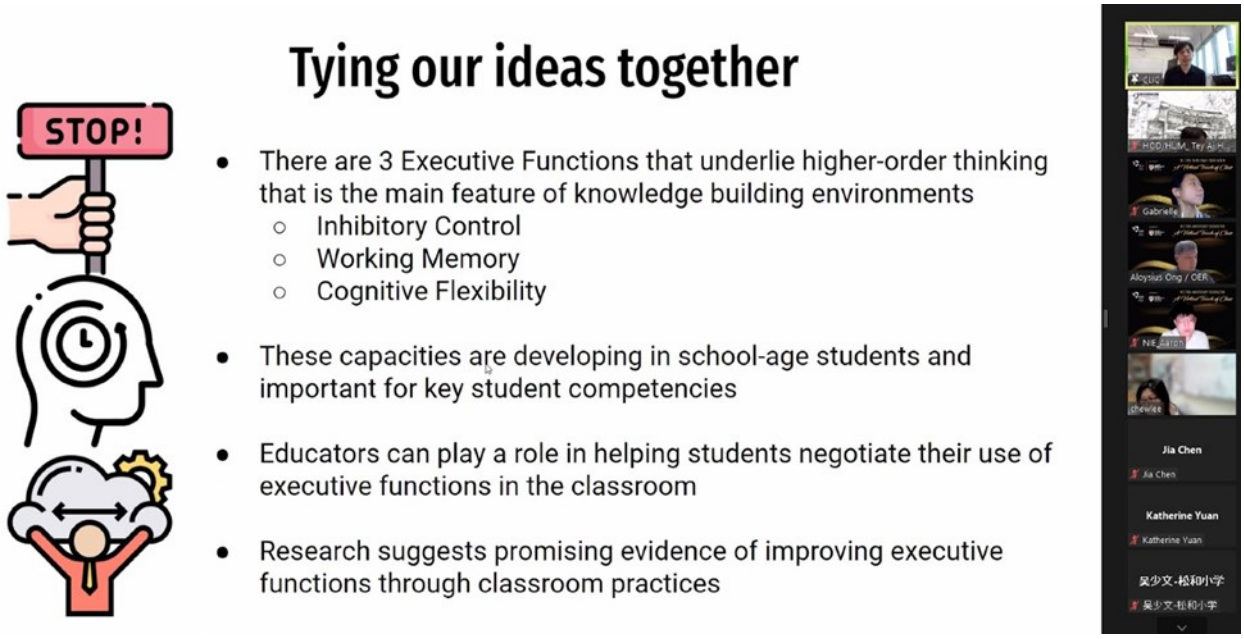


Figure 7.7: Screen-capture of the professional development workshop for executive function and influence on teaching practice.

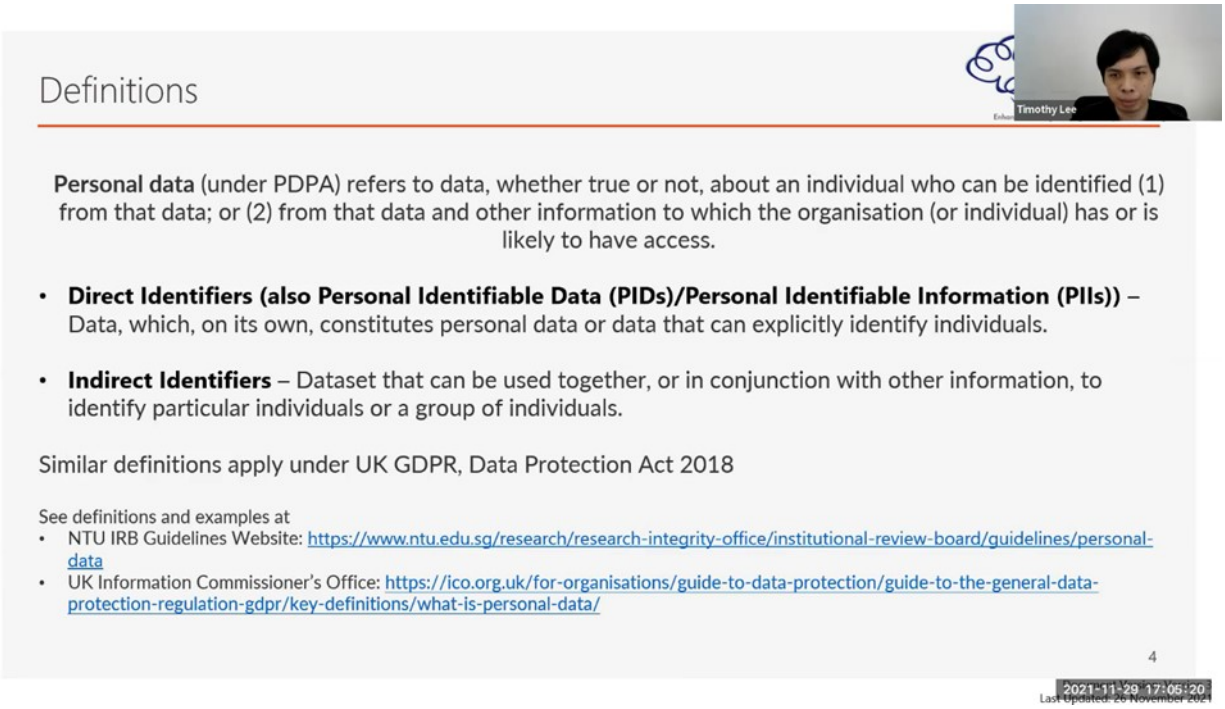


Figure 7.8: Screen-capture of CLIC's data onboarding briefing

Ms CHUI Yingqi (Research Assistant, NTU) joined the School Workgroup in September 2021 under the supervision of **Prof David HUNG (PI, NTU/NIE)**, **Dr TEO Chew Lee (Co-I, NTU/NIE)** and **Dr Peter SEOW (Co-I, NTU/NIE)**. She was involved in the organisation and execution of the pilot WP0.1 data collection where she helped code and score participant task responses. Ms Chui has been involved in motivating and engaging students in the school setting through the development and design of a reward system. She is working on the improvement of task delivery and protocol, through the development of a comprehensive set of Standard Operating Procedures. In particular, she has created a backstory, a video, and activity sheets to increase students' engagement in the Structure Learning task.

Under the guidance of **Dr TEO Chew Lee (Co-I, NTU/NIE)**, **Dr Peter SEOW (Co-I, NTU/NIE)**, and **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)**, Ms Chui has also been working on the design and validation of a new creativity measure that can be used in naturalistic classroom settings. This measure would involve the creation of three-dimensional creative products, which will be scored using a coding system she is developing.

Figure 7.9: Screen-capture of the video created for the Structure Learning task.

Ms Phillis FU (Research Associate, NTU) has been involved in data collection protocol development, and in planning and executing the pilot CLIC WP0.1 study. Her work contributed to the success of the School Workgroup in translating the administration of a suite of neuropsychological and cognitive tasks in a classroom setting. This 4-day data collection (The Brain Camp) also served to introduce teachers to the concept of neuropsychological and cognitive testing. Ms Fu is currently in-charge of planning the upcoming data collection camp in May 2022, which will involve over 300 students.

Ms Fu, along with Ms Chui, are leading the recruitment and training of student assistants for intensive data collection events. The student assistants are a valuable manpower resource for the different workgroup as they are actively involved in the School Workgroup and Adult Team's data collection. Ms Fu has advertised, interviewed, and recruited students from NTU to train them in task administration. She produced training materials that were used in the other workgroups, supported the training of new CLIC members, and has been helping with the adult data collection.

Under the guidance of **Prof Henriëtte HENDRIKS (PI & Deputy Director, CAM)**, Ms Fu and **Ms Irene MELANI (Research Associate, NTU)** formed CLIC's social media team representing CLIC on various social media platforms. The team's creation of the CLIC Twitter account managed to gain 10.7K impressions from December 2021 to March 2022.

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 Neuroimaging Workgroup

Neuroimaging: Structure Learning Training and Cognitive Flexibility

The neuroimaging workgroup ran and completed two pilot studies to pilot the WP0.2 Structure Learning Intervention Programme. Data analyses for Pilot 1 and 2 have been completed by **Dr CHENG Xiaoqin (Research Fellow, NTU)** and **Ms TEO Jia Li (Research Assistant, NTU)**. Results of the two pilots were used to tweak the intervention design after numerous consultations with **Prof Annabel CHEN (PI & Director, NTU)**, **Prof Zoe KOURTZI (PI & Director, CAM)**, **Prof Barbara SAHAKIAN (Co-I, CAM)**, **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM)** and **Assoc Prof Victoria LEONG (PI & Deputy Director, NTU)** (see Figure 7.10 for current intervention design). A new measure for cognitive flexibility was proposed for implementation at both pre and post-test so that baseline pre-test scores are matched between intervention and control groups. Pilot 3 was hence planned to smooth out potential data collection issues in the main study and to test out the new intervention design and flexibility measure. At present, Pilot 3 is still in progress and the neuroimaging team will be using results from Pilot 3 to examine potential effects of the new intervention design on CLIC's full cognitive battery that includes all tasks on cognitive flexibility, working memory and inhibition. Matching procedures and scripts that will be used for the main study have also been tested out in Pilot 3. The operations and data collection of all three pilots are led by **Ms CHOO Boon Linn (Research Associate, NTU)**, Dr Cheng, and Ms Teo, with strong support provided by CLIC's new research fellow, **Dr LIU Chia-Lun (Research Fellow, NTU)**, for Pilot 3.

In addition, the neuroimaging workgroup are also actively planning and coordinating the upcoming intense data collection for WP0.2 main study which will include pre and post-test MRI scans. In preparation for the main study, Dr Cheng, Ms Teo, and Ms Choo, conducted another round of hiring to recruit more student assistants for the upcoming data collection that will start in May 2022. An 8-hour long research training programme spread across four days was developed and conducted for 15 part-time NTU undergraduate student research assistants. These student assistants are currently assisting with WP0.2 Pilot

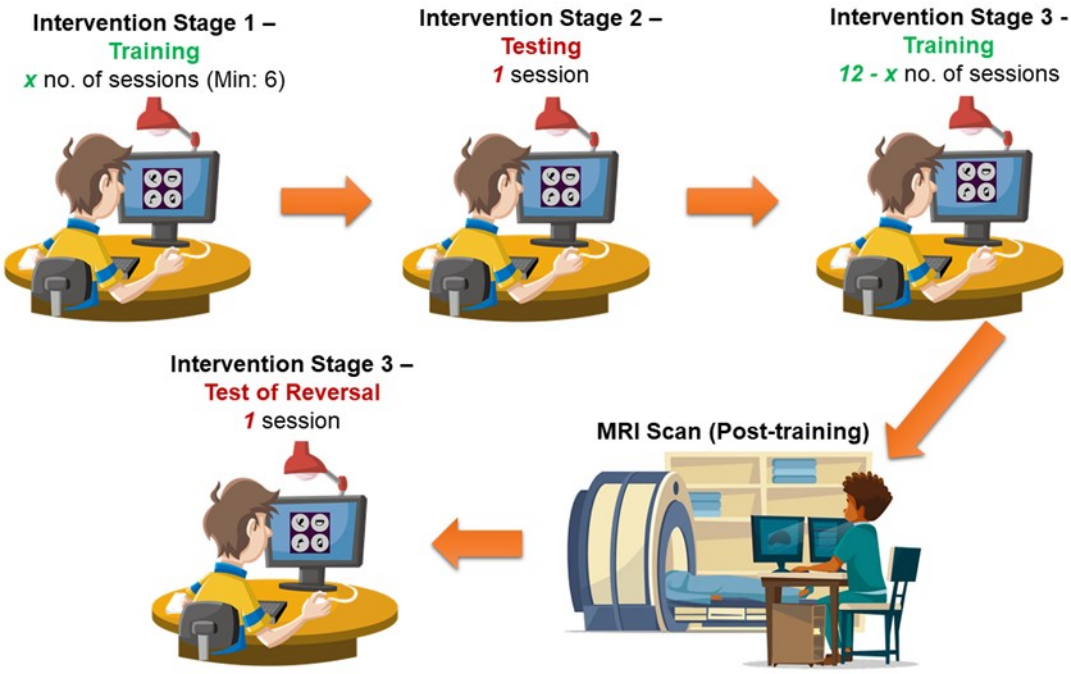


Figure 7.10: Intervention Design Used for Pilot 3. The neuroimaging team is currently evaluating the effects of this design on behavioural measures.

3 data collection and they will also be involved in the main study data collection. Furthermore, the neuroimaging team have also commenced preparation work for the main study.

Ms Teo is presently tasked with drafting standard operating procedures, checklists for the actual operations, scripts for automation of various operations and behavioural data checks, alongside with managing the neuroimaging team's student assistants and Pilot 3's ongoing data collection. Dr Liu and Dr Cheng are coordinating scanning schedules with CoNiC so that the tight MRI data collection schedule can be carried out smoothly.

In view of the substantial changes in the study design for WP0.2, Dr Cheng is amending the preregistration draft in accordance with these changes. The neuroimaging team will be forwarding the drafts to relevant PIs for their comments and are aiming for submission of WP0.2 preregistrations on NIH ClinicalTrials.gov before the commencement of the main study.

Substantial progress on the development of the MRI analyses pipelines were made by the neuroimaging workgroup. Dr Liu is currently spearheading the development of pipelines for multiparameter mapping (MPM, see Figure 7.11) and resting-state fMRI while Dr Cheng is working on the analyses pipelines for magnetic resonance spectroscopy (MRS) with close supervision from CLIC's neuroimaging leads, **Prof John SUCKLING (PI, CAM)** and **Prof Balázs GULYÁS (PI, NTU)**, alongside critical inputs from **Prof Annabel CHEN (PI & Director, NTU)** and **Prof Zoe KOURTZI (PI & Director CAM)**. Dr Liu and Dr Cheng will be running two additional MRI dry runs at CoNiC in May before the start of the actual scans in June. With the help of Ms Teo and Ms Choo, Dr Liu and Dr Cheng have started developing a short MRI training course for the neuroimaging team's student assistants and drafting the MRI scan operating protocol.

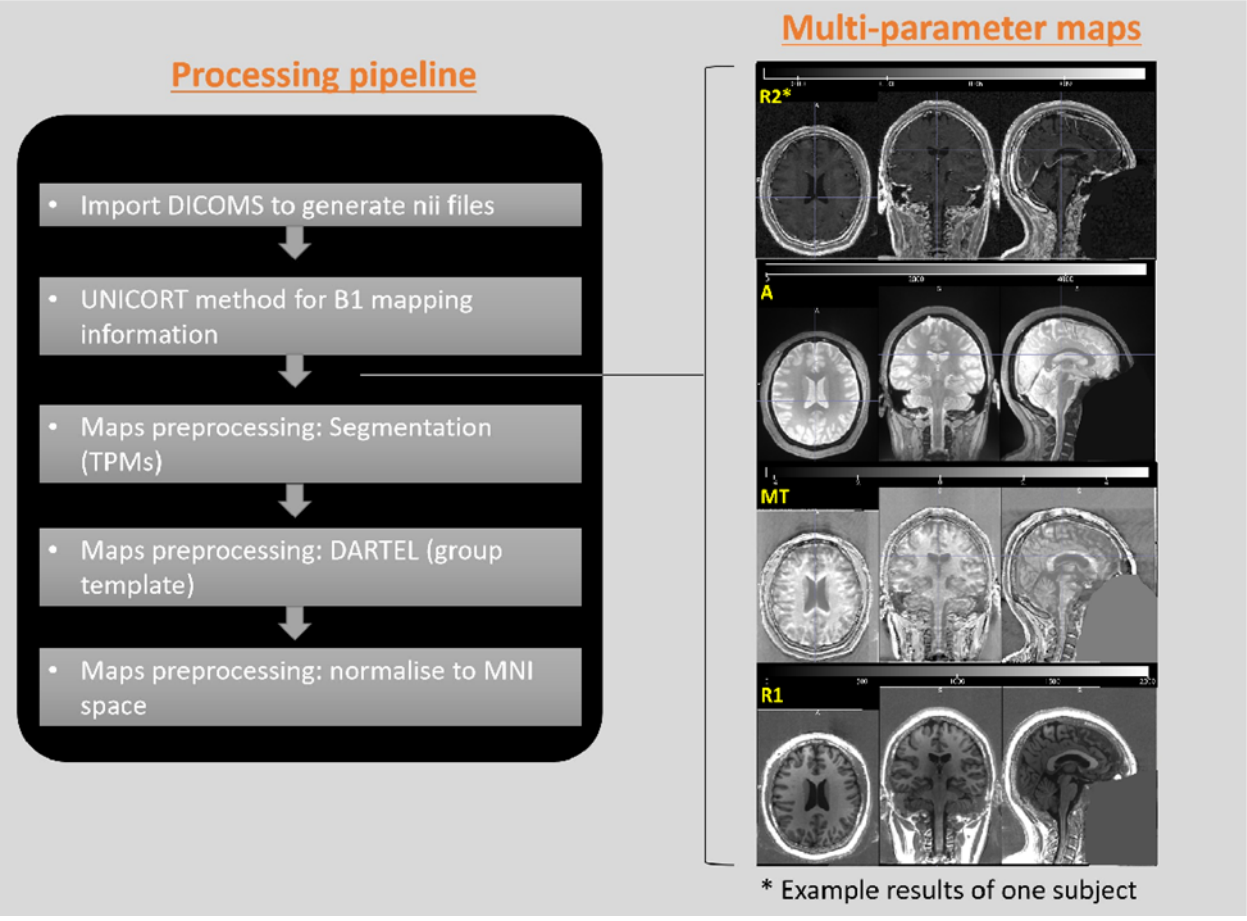


Figure 7.11: Multiparameter Mapping Preprocessing Pipeline.

In anticipation of heavy computational needs of WP0.2, the neuroimaging team commenced on the configuration of CLIC's Linux analysis servers which Ms Choo previously procured.

Dr Liu and Dr Cheng are discussing on the best way to configure and manage analysis softwares in the Linux servers e.g., via Docker containers and Ms Choo is currently assisting in the implementation and exploration of its feasibility. Furthermore, Dr Liu and Dr Cheng are also setting up the file structure for WP0.2 data in accordance with the Brain Imaging Data Structure (BIDS).

Apart from developing research protocols, preparation for and implementation of studies for WP0.2, the team also supports WP0.1 and CLIC's main operations in various ways. Dr Liu and Dr Cheng are assisting WP0.1 with a validation of the anti-saccade task (one of the inhibition tasks in CLIC's cognitive battery) using an eyetracker (Eyelink). Ms Choo is the main personnel leading the setup of the REDCap web server and has been instrumental in navigating and resolving the various network complexities that arose from the setup. She is currently working on extending the different expiry dates of CLIC's IT infrastructure and exploring various backup solutions for CLIC's data in the various servers.

CLIC IT Computing Infrastructure and Resources

Dr Chung supported the setup of computational modelling servers with necessary software and packages for research computation and analysis. The computational modelling servers, hosted in Windows and Linux provide platforms for analysis and facilitates distributed processing of computational modelling for CLIC researchers. He has helped to setup CLIC Data Storage (CLIC Network-Attached Storage-NAS and CLIC Google Workspace) for a secure storing of research data used by CLIC and Cambridge researchers. As CLIC PDPA Manager, Dr Chung has actively supported the development of the Personal Data Inventory Map and impact assessment to assess various personal data processing activities. Dr Chung has also conducted Data Onboarding/Offboarding Procedure briefings during November and December 2021 to all CLIC personnel and collaborators (National Institute of Education and LKCMedicine) to brief the CLIC data handling guidelines and obligations to ensure safe usage and access to CLIC's data storage platform.

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 publications generated by CLIC during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

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

Irene Melani, George Christopoulos, Henriëtte Hendriks, Shengchuang Feng, Yoke Loo Sam, Nadhilla Melia, Yap Hui Shan, Ke Tong, Ryutaro Uchiyama, Xiaoqin Cheng, Victoria Leong, Barbara Sahakian, Trevor William Robbins, Zoe Kourtzi, and Annabel Chen, *OSF Registries*

DOI: 10.17605/OSF.IO/AY9GR

Description: The present project is part of a larger project aimed at examining cognitive flexibility, executive functions, and learning in healthy young adults in Singapore. The present pre-registration aims to address specific hypotheses of interest derived from the larger project that might not be described here in detail. Cognitive flexibility involves the mental ability to switch or shift amongst different conceptual representations in response to the dynamic environment. It is considered to be a component of executive functioning and is critical to behavioral success. Despite being an executive function, prior research showed that cognitive flexibility could be distinguished from other executive functions, such as working memory and inhibitory control that were commonly found to be highly correlated with each other. One of the primary aims of the larger project is to examine the separability of cognitive flexibility from other main executive functions, such as working memory and inhibitory control. In the present project, we examine the potential links between cognitive flexibility and socio-cognitive aspects of interest (to be referred to as socio-cognitive variables), namely: (1) multilingualism, (2) cooperative-competitive social decision-making patterns, (3) tolerance of uncertainty, and (4) perceived social support, which lack direct empirical tests, especially in Singapore's context, in addition to these socio-cognitive variables' potential relations with outcome variables of interest (i.e., creativity, literacy, numeracy, and problem solving/critical thinking).

Other activities and achievements

Prof. Annabel CHEN Shen-Hsing (PI & Director, NTU) gave a virtual presentation titled "Helping the Adult Brain Learn Better for Lifelong Learning" at the Neuroplasticity—Rewiring Our Brain for Learning conference at the Singapore University for Social Sciences (SUSS) on 14 October. She is also an Editorial Board Member for Psychology Research and Behaviour Management, Neuropsychology Review, Aging, Neuropsychology and Cognition; and an Associate Editor for Frontiers in Human Neuroscience, and Human Brain Mapping.

She has received the following grant awards:

- Defence Science Organisation (DSO) National Laboratories (Temasek Lab) (PI) Cognitive, Neural and Social Factors involved in the Perception of Real vs. Fake Information (2022-2025)
- Defence Science Organisation (DSO) National Laboratories (Temasek Lab) (PI) Proud to be Singaporean: An Investigation into the Neural and Cognitive Processing of National Identity and National Belonging (2021-2025)

Assoc Prof Victoria LEONG (PI & Deputy Director, NTU) has received the following grant/ awards since the last report:

- 2022 FABBS Behavioural & Brain Sciences Early Career Impact Award (ICIS)
- A*STAR Human Health Potential Prenatal/Early Childhood Grant — A Sociometric AI Screening Tool to Risk-Stratify Infant Neurodevelopment Trajectories

Prof Barbara SAHAKIAN (Co-I, CAM) was awarded the 2021 Lifetime Achievement Award. This award is presented to individuals with an international recognition for their contribution and impact to psychopharmacology.

Prof Trevor ROBBINS (Senior Scientific Advisor, CAM) was awarded the William James Fellow in 2022. This highest award of the Association for Psychological Science (APS) recognises members internationally for outstanding contributions to scientific psychology.

The CLIC team are actively working with the Cambridge Adaptive Brain Group under **Prof Zoe KOURTZI (PI & Director, CAM)** to develop the iABC research platform for future deployment of gamified training interventions. i-ABC is a computerised application for online profiling of learning ability and cognitive flexibility.

The Schools Workgroup has delivered a Professional Development Workshop (The Neuroscience and Psychology of Learning Workshop (25-26 Oct 2021)) to teachers led by **Mr Timothy LEE (Research Associate, NTU)**. This 3-hour interactive workshop introduced teachers to executive functions, their underlying neurobiology, and related psychological constructs that impact students' learning in the classroom.

Dr Nastassja LOPES FISCHER (Research Fellow, NTU), **Ms Phillis FU (Research Associate, NTU)**, and **Mr Timothy LEE (Research Associate, NTU)** are core-team members on an NIE-MOE Working Paper titled "How Science of Learning can help enhance student's emotional engagement during learning, motivate them to learn and the development of their metacognitive abilities" currently in the planning phase.

New Collaborations

The neuroimaging team has submitted a joint grant application for the Workforce Development Agency Research Fund (WDARF) grant with NUS, Department of Nursing to examine the role of cognitive flexibility in adult learners. In addition, there are also plans to submit a grant proposal to the MOE Tertiary Education Research Fund (TRF) with our collaborators at NUS, Department of Nursing. This TRF grant proposal would be a follow-up to the WDARF grant and utilises neuroimaging to examine potential brain changes after the proposed intervention. CLIC's MRI protocol, together with some of the flexibility tasks in CLIC's cognitive battery (e.g., structure learning) will be implemented so that some cross comparison of the results can be performed with WP0.2 data. In addition, the neuroimaging team are in discussions with their Cambridge collaborators to apply for an Intra-CREATE grant in August 2022.

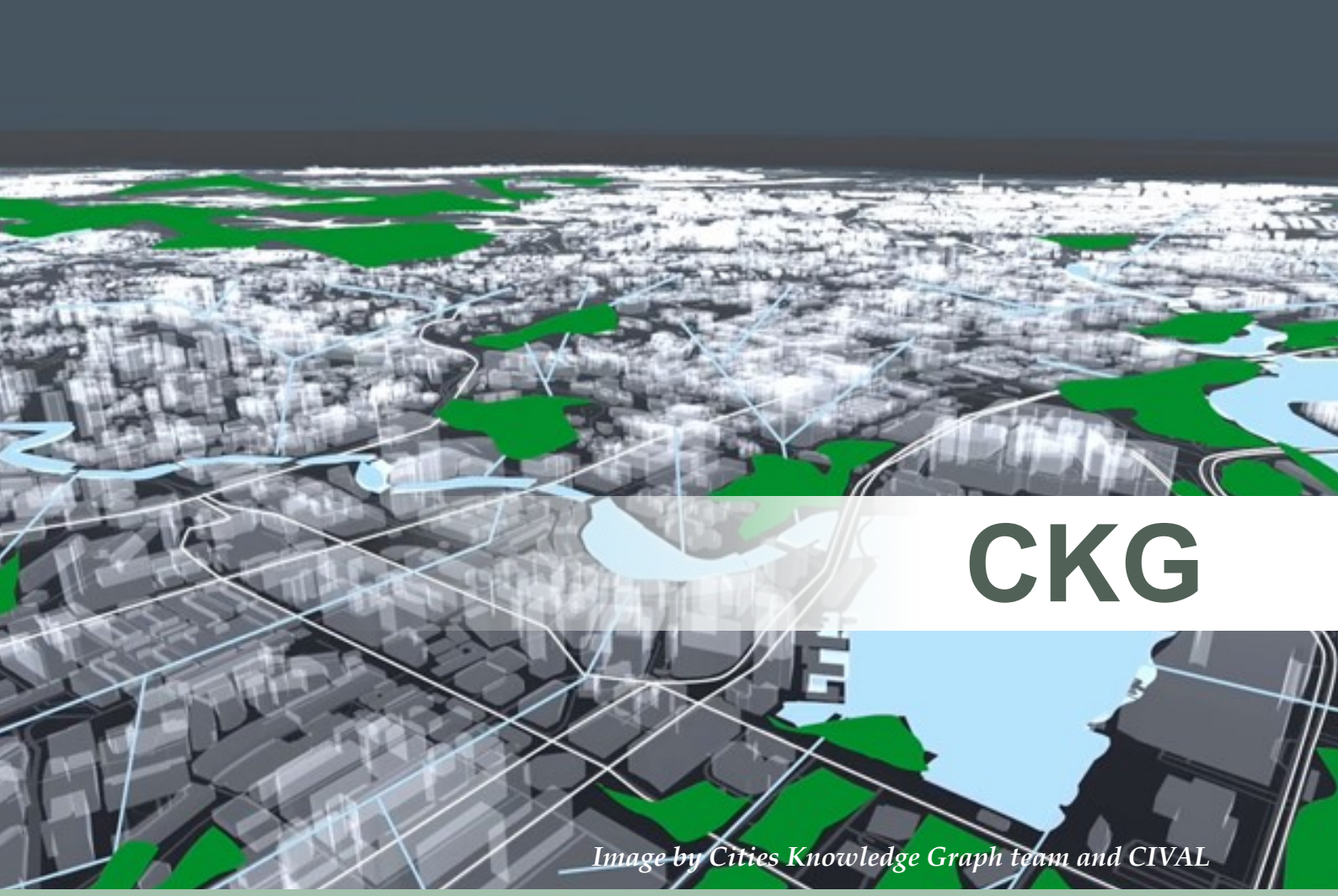


Image by Cities Knowledge Graph team and CIVAL

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, creating an unprecedented knowledge graph for city planning.

CKG Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Stephen CAIRNS
ETH Zürich

OVERVIEW

Cities Knowledge Graph (CKG) is an Intra-CREATE Thematic Grant project in the 'Cities' thematic area. The project brings together expertise from Cambridge 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 Principal Investigators from the University of Cambridge (Prof Dr Markus Kraft) and ETH Zürich (Prof Dr Stephen Cairns). Dr Pieter Herthogs (Senior Researcher, SEC) is the Co-Investigator and Project Leader. Dr Aurel von Richthofen (Team Leader Cities, Arup Berlin) and Dr Franziska Sielker (Lecturer, University of Cambridge) are Co-Investigators of the project.

Over the past six months, we have expanded the ontology of mixed-use zoning types to cover all thirty-two zoning types found in the Singapore Master Plan. This new OntoZoning ontology now describes the zoning and land use domain primarily through 32 zoning type classes, 101 land use classes that are allowed in each zoning type, and 345 programme classes that are or may be allowed in each land use class. The OntoZoning ontology is also extended with ontoMixedUse-Zoning ontology, which defines 163 archetypes of mixed-use development in Singapore, derived from Google Place data as well as Urban Redevelopment Authority (URA) plot and zoning data using clustering and multivariate linear regression. These archetypes, providing programme distributions and gross floor area (GFA) estimates for different combinations of zoning types and gross plot ratios, have been shown to augment urban building energy modelling workflows for energy demand forecasts and energy supply system design, and have many potential urban planning applications beyond energy modelling.

We have also developed a Thematic Surface Discovery Agent (TSDA). The objective of the agent is to upgrade buildings of LOD1 to LOD2, converting the geometry tree describing the exterior shell to an array of _BoundarySurface entities describing the exact same exterior shell geometry, but semantically differentiated into the different surface types. This process is referred to as 'thematicisation'. Specifically, the TSDA classifies the polygons in the direct surface geometry trees of buildings into wall, roof and ground polygons. It transforms their surface geometry trees to an OntoCityGML-compliant wall surface-, roof surface-and ground surface-based hierarchy while preserving as much of the original tree structure as possible.

Furthermore, in conversations with the URA's Design and Planning Lab, we have scoped three use cases for assistive applications supporting land-use planning activities: (1) a 'site regulations advisor' to demonstrate the ability to display relevant city planning regulations for the selected sites (land plots); (2) a 'suitable site selector' to demonstrate CKG innovations in site selection and recommendation based on automated Strengths, Weaknesses, Opportunities, and

Threats (SWOT) analysis and evaluation for desired development programmes and planning goals; and (3) a 'future scenarios builder' to assist planners in setting up, simulating, analysing, and managing multiple scenarios in parallel. These use cases cover the horizontal breadth and vertical depth envisioned in this project. As a first step, we are developing a demonstrator that supports the first and second use cases. The 'programmatic plot finder' extends on the allowable land use queries enabled by the OntoZoning ontology, integrating URA legislations that determine the maximum allowable GFA of plots. The resulting demonstrator will assist users in finding plots that could house their particular desired combinations of land uses and programmes (types and amounts).

Moreover, we have implemented a tiling approach for the visualisation of large city models with the web-based front-end 3DCityDB-Web-Map-Client. The generated tiles are loaded and unloaded dynamically based on the camera view to allow users to navigate smoothly when visualising large city models. Visualisation demonstrations of regions where data are readily and publicly available (Berlin, Pirmasens and King's Lynn) have been prepared and deployed using this approach.

Professor Markus Kraft, PI
University of Cambridge

Professor Stephen Cairns, PI
ETH Zürich

Update on work package 1

Developing master-planning ontologies

Ms Heidi SILVENNOINEN (Researcher, SEC), supported by **Dr Pieter HERTHOGS (Senior Researcher, SEC)**, **Dr Zhongming SHI (Postdoctoral Researcher, SEC)**, **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)** and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, has expanded the ontology of mixed-use zoning types to cover all thirty-two zoning types found in the Singapore Master Plan. This new OntoZoning ontology now describes the zoning and land use domain primarily through 32 zoning type classes, 101 land use classes that are allowed in each zoning type, and 345 programme classes that are or may be allowed in each land use class. While zoning types and land uses are specific to Singapore and are sourced exclusively from the Urban Redevelopment Authority (URA) documents, programmes are universal land uses, activities or types of development that may be allowed in each land use. Examples of programmes include, 'Restaurant', 'Tennis', and 'Printing press'. In addition to URA documents, programmes are also derived from Google Places and an existing land use ontology called LBCSv2–which is based on an American land use classification system. The ontology is also central to the 'programmatic plot finder' demonstrator, described in Work Package 6.

The OntoZoning ontology forms the basis of a paper entitled 'Multi-criteria site selection using an ontology: the OntoZoning ontology of zones, land uses and programmes for Singapore', which has been preprinted and submitted to a journal. The pre-print investigates how the ontology may be used for multi-criteria site selection and describes how linking the ontoZoning ontology to geospatial data on Singapore's plots enables querying for plots where it is possible to place specific programmes, or combinations of programmes (Figure 8.1). By linking the plot data to other data in the knowledge graph, such as building footprints and heights, gross plot ratios and Mass Rapid Transit (MRT) station locations, it is possible to perform complex queries. An example of a query combining multiple data sources is 'where can I find plots that allow building flats or condominiums, are adjacent to a park, and have unused gross floor area?' (Figure 8.2)

Dr Shi, Ms Silvennoinen, Mr Chadzynski, and Dr Herthogs have extended the OntoZoning ontology with the ontoMixedUseZoning ontology, which defines 163 archetypes of mixed-use development in Singapore, derived from Google Place data as well as URA plot and zoning data using clustering and multivariate linear regression. These archetypes, providing programme distri-

```
PREFIX ocgml: <http://www.theworldavatar.com/ontology/ontocitygml/citieskg/OntoCityGML.owl#>
PREFIX zo: <http://www.theworldavatar.com/ontology/ontozoning/OntoZoning.owl#>
SELECT ?zone ?id ?geometry
WHERE {
      GRAPH <http://127.0.0.1:9999/blazegraph/namespace/singaporeEPSG4326/sparql/ontozone>{
            ?use1   zo:allowsProgramme | zo:mayAllowProgramme          zo:Tennis.
            ?use2   zo:allowsProgramme | zo:mayAllowProgramme          zo:PrintingPress.
            ?zone   zo:allowsUse | zo:mayAllowUse                      ?use1;
                    zo:allowsUse | zo:mayAllowUse                      ?use2.
            ?id     zo:hasZone                                         ?zone.}

    GRAPH <http://127.0.0.1:9999/blazegraph/namespace/singaporeEPSG4326/sparql/surfacegeometry/> {
          ?s1   ocgml:cityObjectId  ?gco_id ;
                ocgml:GeometryType ?geometry.
          BIND ( strafter( STR(?gco_id), "genericcityobject/" ) as ?gco_id2 ).
          BIND ( strbefore( ?gco_id2, "/" ) as ?gmlid ).}

    GRAPH <http://127.0.0.1:9999/blazegraph/namespace/singaporeEPSG4326/sparql/cityobject/>
        { ?s2   ocgml:gmlId  ?gmlid ;
                ocgml:id     ?id.}
}
```

Query to select zone types, plot ids and plot geometry

Condition that the zone types must allow uses, that in turn allow developments containing Tennis activities and a Printing Press

Find plot geometry from a separate graph

Figure 8.1: Blazegraph interface displaying a SPARQL query for the geometry and ids of plots that allow programmes 'Tennis' and 'Printing press'.

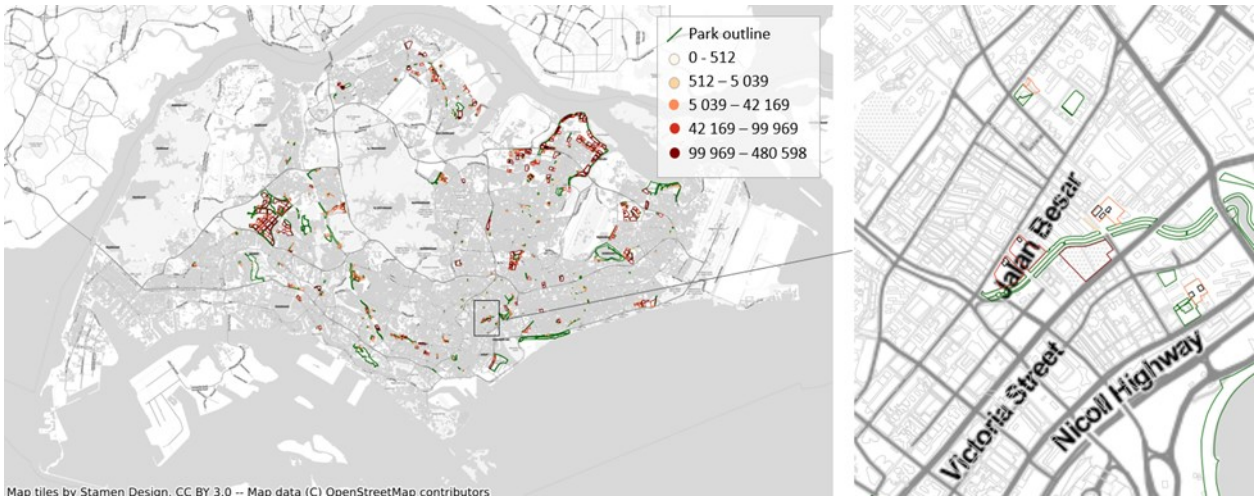


Figure 8.2: Visualisation of results for the query: 'where can I find plots that allow condominiums or building flats, are adjacent to a park, and have unused gross floor area?' The plots are coloured in shades of red according to their unused gross floor area.

butions and gross floor area (GFA) estimates for different combinations of zoning types and gross plot ratios, have been shown to augment urban building energy modelling workflows for energy demand forecasts and energy supply system design, and have many potential urban planning applications beyond energy modelling. Representing and storing the archetype definitions using a machine-readable ontology encourages its adoption by other researchers and contributes to building an automated workflow. This work has been published as a pre-print entitled 'Defining archetypes of mixed-use developments for improved urban building energy modelling' and has been submitted to a journal.

Ms Grišiūtė, Ms Silvennoinen, and Dr Herthogs have worked on categorising the urban planning regulations that determine the allowed GFA and regulations that affect allowable land uses and programmes in addition to the Singapore Master Plan. The categorisation allowed filtering of regulations applicable to urban parameters determining GFA at approximately Level of Detail 1 (LOD1), e.g. building height, setback or site coverage, and informed about necessary extensions for OntoZoning ontology, such as the semantic representation of use quantum.

In addition, Ms Grišiūtė has worked on mapping mobility simulation output data generated by Multi-Agent Transport Simulation Toolkit (MATSim) with iCity Transportation Planning Suite of Ontologies (TPSO) concepts. This process maps existing data sets to the vocabulary of the ontology to disambiguate the data and make them semantically explicit. She also used the data mapping and TPSO concepts to instantiate MATSim mobility simulation data in the knowledge graph. This will allow the formulation of queries about city objects, such as plots, that would not be possible based on single-domain data alone.

Dr Emily LLOYD (Research Fellow, CARES), **Dr Jingya YAN (Research Fellow, CARES),** and Dr Shi have developed an ontology called ontoUBEM-MP to link two domains: urban building energy modelling (UBEM) and master planning (MP). Interoperability between the domains of UBEM and MP is enabled through machine-readable links between equivalent or related concepts in the two knowledge domains. Aside from enabling interoperability, such an ontology can also be applied to automate building energy performance analyses on a given MP proposal, as the ontology represents all necessary concepts and knowledge in a machine-readable way. Dr Shi and Dr Lloyd are in the process of preparing a journal publication pre-print to describe this work.

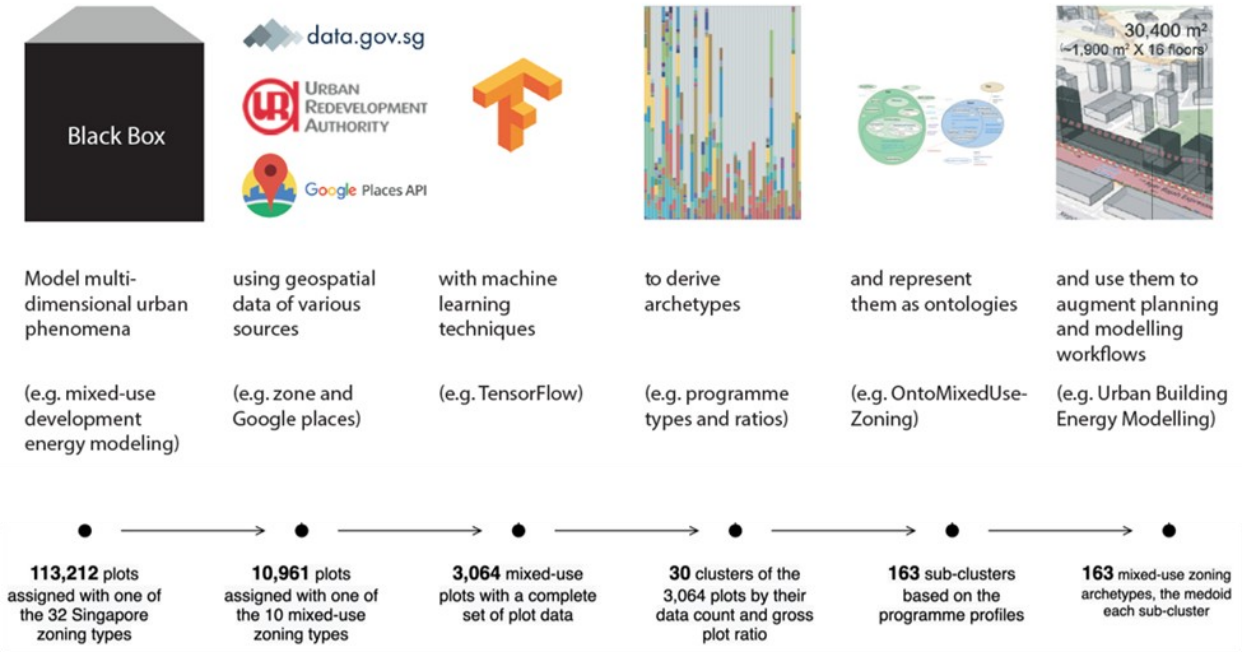


Figure 8.3: Methodology to derive mixed-use archetypes from various urban datasets and use them in planning simulation workflows.

Update on work package 2

Developing the knowledge graph's architecture

Ms TAI Huay Yi (Software Developer, CARES), in close collaboration with **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, completed a feature to import coordinate reference system (CRS) information into the knowledge graph by adding a SPARQL UPDATE to set the spatial reference identifier (SRID) and srsName attributes of the dataset as triples. This feature streamlines the import process by setting the CRS information in the knowledge graph via the 3D City Database Importer/Exporter tool interface, or automatically via the CityImportAgent. To support this feature, information on various CRSs obtained from PostGIS were translated into triples and added to the knowledge graph's 'public' namespace. SPARQL SELECT queries were also added to the 3D City Database Importer/Exporter tool to retrieve information from the 'public' namespace using SRID values, and to query the CRS of a selected namespace.

Ms Shiying LI (Software Engineer, SEC), in close collaboration with Ms Tai and Mr Chadzynski, implemented a tiling approach for the visualisation of large city models such as Berlin, Germany (around 500,000 buildings) with the 3DCityDB-Web-Map-Client. Due to the limitations of the platform, large models can only be partially loaded on the 3DCityDB-Web-Map-Client for visualisation. Hence, a post-processing step was developed in the CityExportAgent to tile large Keyhole Markup Language (KML) files. This involves reorganising the exported KML files into geospatially ordered tiles, where each tile consists of one new KML file with information on buildings physically located within the tile (as shown in Figure 8.4). Tiling is performed after a city model is exported from the knowledge graph into the KML files but before the city model is visualised on the 3DCityDB-Web-Map-Client. Using the existing 3DCityDB-Web-Map-Client feature, tiles are loaded and unloaded dynamically based on the camera view to allow users to navigate smoothly when visualising large city models.

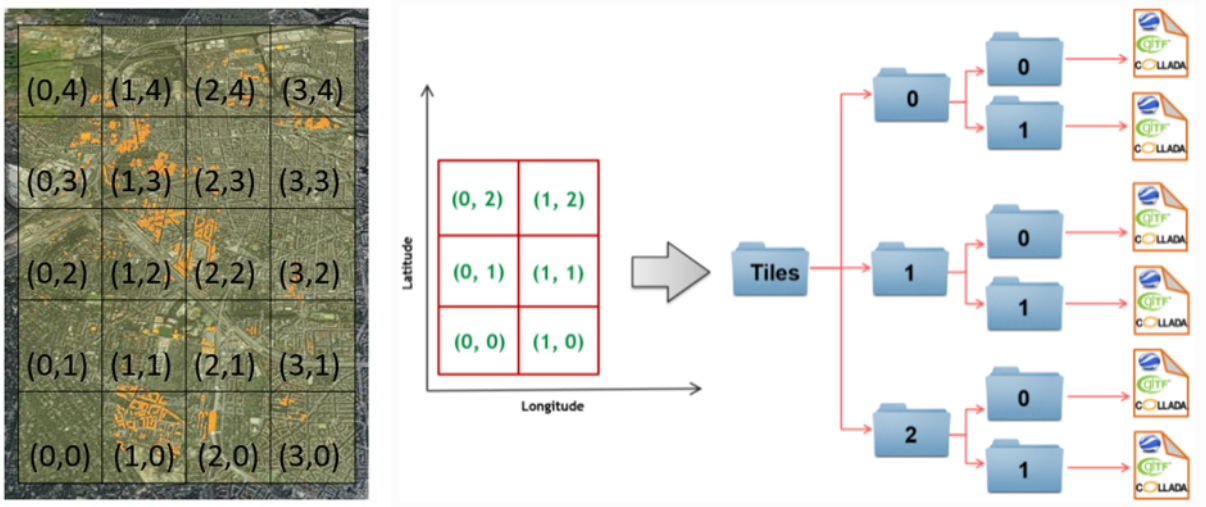


Figure 8.4: The left figure illustrates the tiling grid for large city models where each tile is represented as a bounding box. The right figure illustrates the re-arranged KML files' structure according to the tiling grid that facilitates the dynamic loading of tiles for the visualisation of large city models. The right figure is reproduced from the 3dCityDB documentation.

Dr Jingya YAN (Research Fellow, CARES) implemented a feature to export full geometry data from the knowledge graph into a KML format for visualisation. This feature includes two main parts. The first part was to query geometry data of buildings from the knowledge graph. If the geometry data contains no thematic surface types, the surface geometry data will be directly queried. On the other hand, if the geometry data contains different types of thematic surface, the type of thematic surface will first be queried, and then followed by the related surface geometry data. The second part was to format the display style in the KML data structure. This is necessary because Cesium (the application 3DCityDB-Web-Map-Client is based on) only supports World Geodetic System (WGS) 84 in its visualisation, and therefore, the CRS transformation must occur before formatting the KML file. Dr Yan used the Geospatial Data Abstraction Library (GDAL) to transform the CRS and based on the thematic surface type information, the different display styles are set in the KML file.

Ms Li optimised the query execution time required by the KMLExporter (a component of the CityExportAgent) when acting on large datasets. This involves optimising the formulation of the queries to reduce the number of complex operators and refactoring particular complex queries into several simpler queries, as well as using java code to post-process the results to reduce the computational load on the server side. The post-processing step replaces complex SPARQL operators such as UNION and FILTER with other processing and filtering functions implemented in the 'OptimizedSparqlQuery' class. With this optimisation, the query execution time of certain queries can be reduced from thirty minutes to a few hundred milliseconds.

Alpha release of the project, codenamed Primary One, which contains three agents: CityImportAgent, CityExportAgent and DistanceAgent, has been prepared to automate instantiation of large city models in the form of semantic triples in the knowledge graph (CityImportAgent), export the city models data into the KML format for visualisation (CityExportAgent), as well as showcase basic analytical capabilities by calculating distances of interest between city objects (DistanceAgent). Dependencies on the JPS Base Library from The World Avatar (TWA) code repository have also been included in this release. In particular, the agents now utilise TWA agent framework, the routed and technology-agnostic knowledge graph access capabilities included in the library.

Figure 8.5: Visualisation of exported Pirmasens Level of Detail 1 (LOD1) building data (left), with surfaces coloured based on their types, and Singapore LOD3 building data (right).

Update on work package 3

Developing agents to operate software and integrate data

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES), in close collaboration with **Ms Shiying LI (Software Engineer, SEC)** and **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)**, continued to work on the development of a system of autonomous intelligent software agents (CityImportAgent, CityExportAgent and DistanceAgent), based on a cognitive architecture, that is capable of automated instantiation, visualisation and analysis of multifaceted City Information Models in dynamic geospatial knowledge graphs. The agents successfully created a semantic model of Berlin in Level of Detail 2 (LOD2), consisting of 419,909,661 triples, that are described using OntoCityGML and are compliant with CityGML 2.0 standard. The system of agents also visualised and analysed the city model by autonomously tracking external interactions with the 3DCityDB-Web-Map-Client, automatically calculating distances between city object representations, as well as enriching the city model by adding new information to the knowledge graph. A paper describing this work entitled 'Semantic 3D City Agents – An intelligent automation for dynamic geospatial knowledge graphs' has been prepared and published in the journal *Energy and AI*.

Ms Li together with Mr Chadzynski added the newly developed code to a single dependency management system – Maven. Unit tests providing complete coverage of the new features have also been developed. A dependency management system executes unit tests before code compilation and project builds to make sure the intended functionality is unchanged after code development. All newly implemented features are tested for compatibility with the graphical user interface managed by Gradle (another dependency management system) and the agent system managed by Maven.

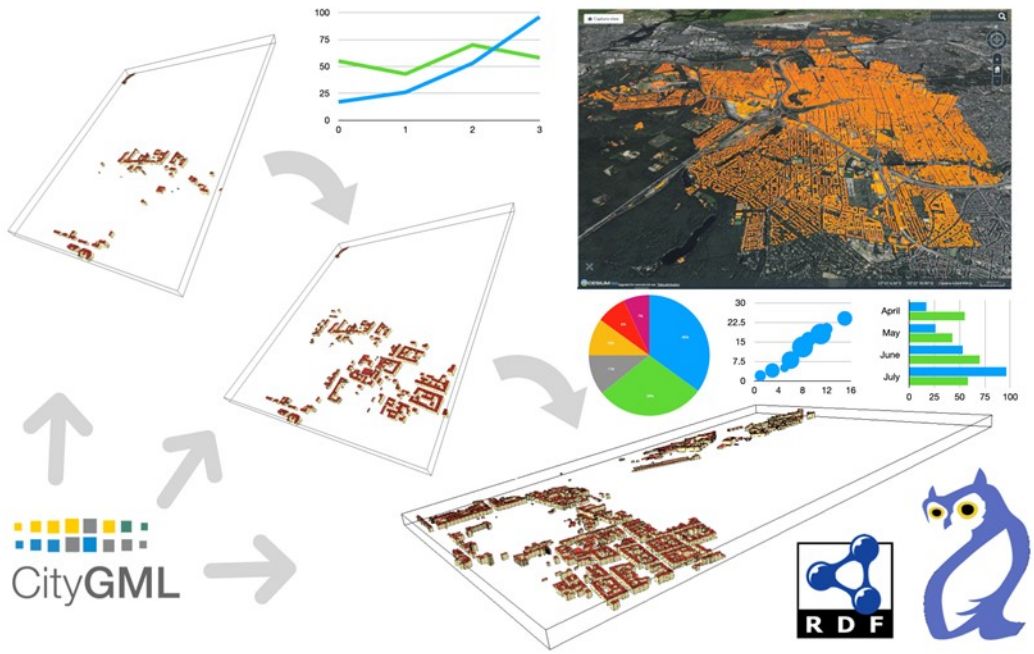


Figure 8.6: Graphical abstract of the paper entitled 'Semantic 3D City Agents – An intelligent automation for dynamic geospatial knowledge graphs'. The paper describes the work on a system of autonomous intelligent software agents (CityImportAgent, CityExportAgent and DistanceAgent), based on a cognitive architecture, that is capable of automated instantiation, visualisation, and analysis of multifaceted City Information Models in dynamic geospatial knowledge graphs.

Ms Grišiūtė, in close collaboration with Ms Silvennoinen and Mr Chadzynski, has developed the City Information Agent (CIA) which retrieves related semantic city object information from the knowledge graph upon receiving a POST request with a given city object ID. The CIA processes the query results into an informative output that is then visualised via the 3DCityDB-Web-Map-Client interface (as shown in Figure 8.7). The CIA design reuses elements from the ongoing development of CityGML object representations in Java.

Dr Emily LLOYD (Research Fellow, CARES), in close collaboration with **Dr Zhongming SHI (Postdoctoral Researcher, SEC)** and Mr Chadzynski, has developed the City Energy Analyst (CEA) agent which will allow automation of building energy analyses. This involves packaging the CEA software as an agent that uses the city object ID in the POST request sent to it, to query for the geometric information of the building from the knowledge graph. This is achieved through a SPARQL query sent to the knowledge graph via the access agent. The CEA agent converts the retrieved geometric information into the format required by the CEA software and then runs the CEA with the input data. The output data produced by the CEA demand and photovoltaic programs, such as buildings' energy demands and their photovoltaic energy potential, are extracted by the CEA agent and added to the knowledge graph. This is achieved either via a SPARQL update passed to the access agent or, for time series data, via the time series client by means of a link to a relational database storing the data.

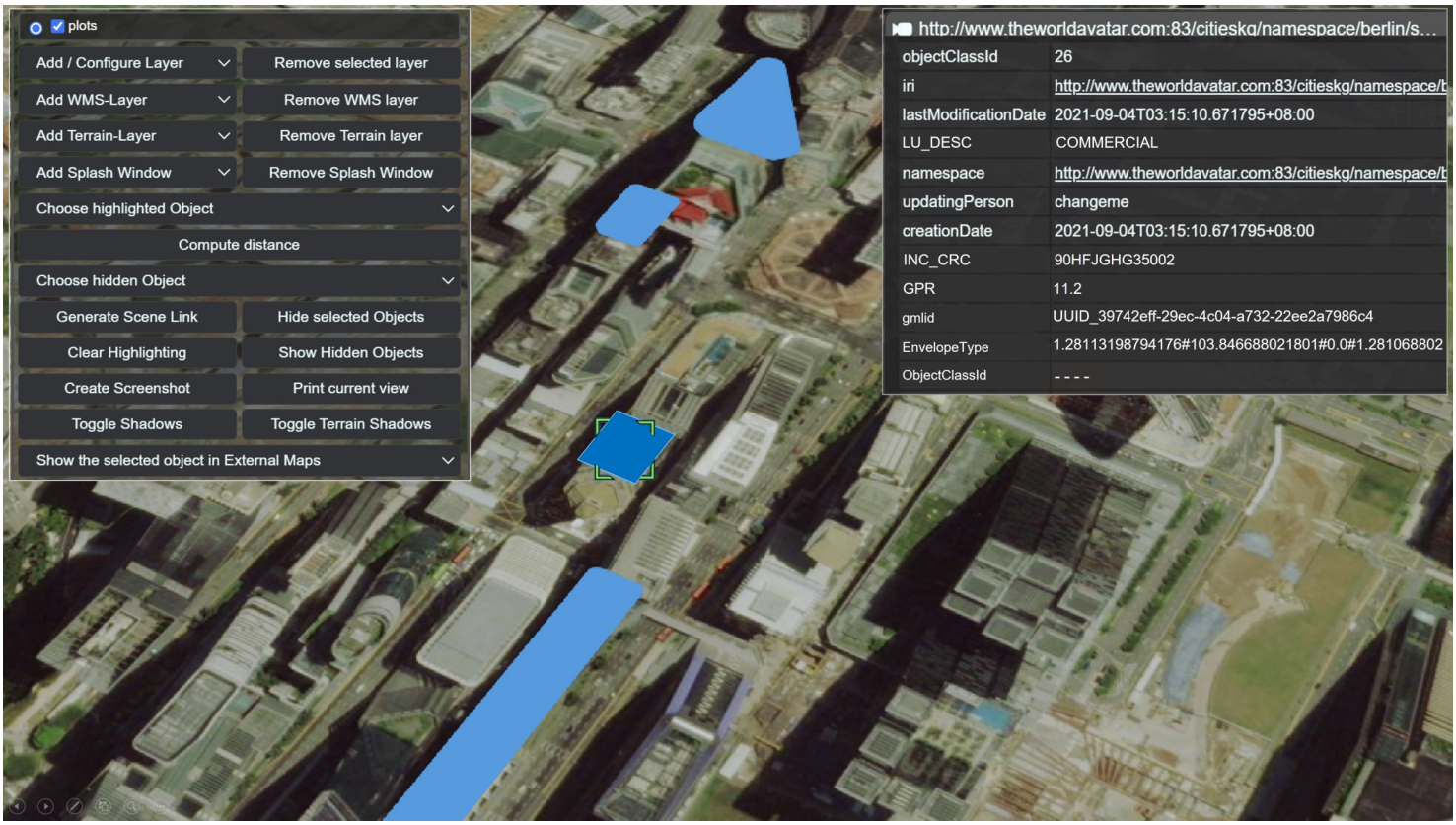


Figure 8.7: The 3DCityDB-Web-Map-Client interface with several plots in Downtown Singapore and the retrieved semantic information from the knowledge graph by the CIA for one of the plots.

Mr Jefferson CHUA (Non-C4T student, University of Cambridge), in close collaboration with Mr Chadzynski, developed the Thematic Surface Discovery Agent (TSDA). The objective of the agent is to upgrade buildings of LOD1 to LOD2, converting the geometry tree describing the exterior shell to an array of _BoundarySurface entities describing the exact same exterior shell geometry, but semantically differentiated into the different surface types. This process is referred to as 'thematicisation'. Specifically, the TSDA classifies the polygons in the direct surface geometry trees of buildings into wall, roof and ground polygons. It transforms their surface geometry trees to an OntoCityGML-compliant wall surface-, roof surface- and ground surface-based hierarchy while preserving as much of the original tree structure as possible. The scope of valid inputs are buildings with top-down topography, i.e. theoretically encodable in heightmaps of rooftop (and base) elevation, with no overhangs or interior geometry and well-conditioned winding order, i.e. polygon coordinate sequences consistently indicate the direction of face normals by a right- or left-hand rule. The TSDA is nevertheless executable on buildings of different levels of detail that do not satisfy the topographical requirement, but may result in errors. However, this may still be useful for some applications which do not require high precision, e.g. estimating the total area of roof.

Ms Mehal AGARWAL (Software Developer, CARES) validated the performance of the TSDA by running the TSDA to identify the thematic surfaces of city objects in a database of Berlin and by comparing the surface geometries the TSDA identified with the given surface geometries in the database. She is in the process of understanding the TSDA to improve its accuracy and efficiency.

Algorithm 1: Surface theme identification algorithm for a single building.

Input: Array of surface polygons of a building, S.
Output: Array of surface-theme pairs, R.

begin
  for $s_i \in S$ **do**
    Project the polygon of s_i to a metric projection, EPSG:25833.
    Calculate the vector area $\vec{s}_i$ of the metric polygon using the shoelace formula in each of the xy, xz and yz planes.
    Calculate the normal $\hat{n}_i$ by normalising $\vec{s}_i$.
    if $|\hat{n}_z| <$ tolerance **then**
      Append (s_i, "wall") to R.
    else
      if $\hat{n}_z > 0$ **then**
        Append (s_i, "roof") to R.
      else
        Append (s_i, "ground") to R.
      end
    end
  end
  Calculate the average centroid r of "roof" surfaces.
  Calculate the average centroid g of "ground" surfaces.
  if $n_{\text{inv}} > n_{\text{up}}$ **then**
    Switch all "roof" entries in R to "ground" and vice versa.
  end
  return R.
end

Figure 8.8: Surface theme identification algorithm for a single building.

Update on work package 4

Developing interfaces and planning libraries for the CKG

Ms TAI Huay Yi (Software Developer, CARES) together with **Ms Srishti GANGULY (Project Engineer, CARES)**, have prepared and deployed the visualisation demonstrations of Berlin, Pirmasens, and King's Lynn building data on the web-based front-end 3DCityDB-Web-Map-Client, as data are readily and publicly available for these regions. This work can easily be extended and applied to other regions where such 3D building data are publicly available, in particular Singapore. **Ms Shiying LI (Software Engineer, SEC)** and Ms Tai also prepared the visualisation demonstrations of 2D public plot data for Singapore using the 2019 Master Plan.

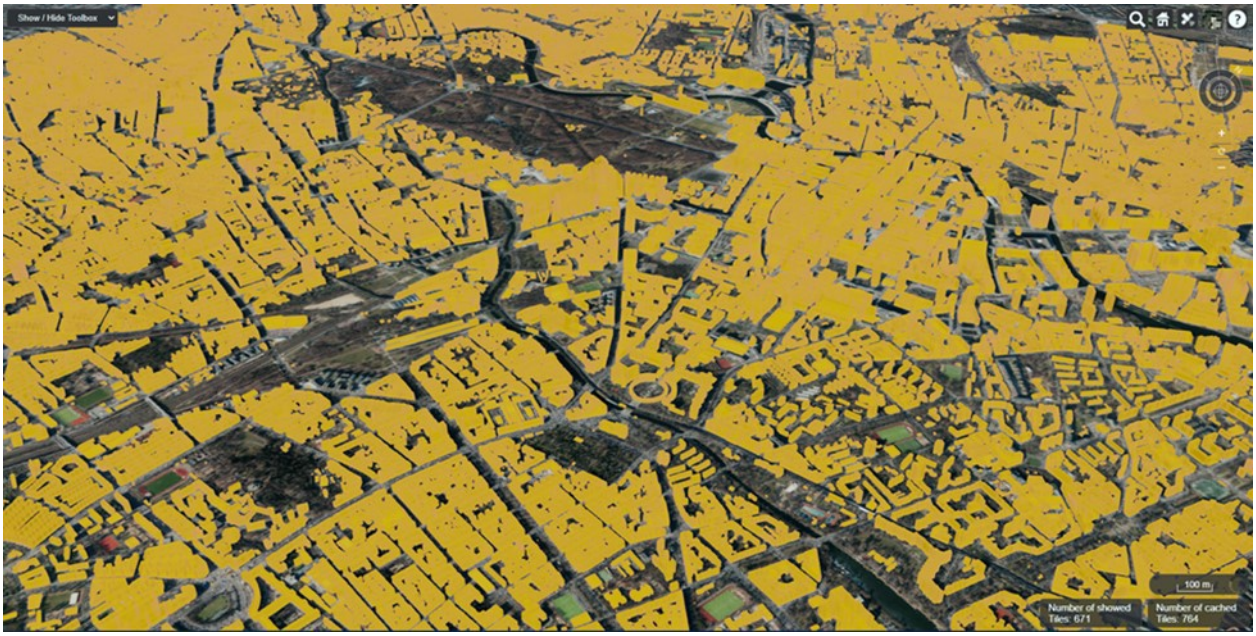


Figure 8.9: Visualisation of exported models of Berlin building data on the 3DCityDB-Web-Map-Client.

Figure 8.10 Visualisation of exported models of Pirmasens building data on the 3DCityDB-Web-Map-Client.

Figure 8.11: Visualisation of exported models of King's Lynn building data on the 3DCityDB-Web-Map-Client.

Figure 8.12: Visualisation of Singapore's plot data (2019 Master Plan URA) on the 3DCityDB-Web-Map-Client, focusing on the Central Area.

Update on work package 5

Developing Design Informatics Functions

Ms Ayda GRIŠIŪTĖ (Researcher, SEC), together with **Dr Pieter HERTHOGS (Senior Researcher, SEC)**, has improved and extended previous work done on a use case of Strengths, Weaknesses, Opportunities, and Threats (SWOT) analysis for assessing the potential of on-site solar energy use for plots in Singapore. This experimental use case is developed to explore how the knowledge graph can be combined with a SWOT analysis framework to inform planners of how a variety of urban planning metrics may impact Sustainable Development Goals (SDG) related planning targets, such as assessing the on-site solar energy potential. The improvements include extending the automated SWOT analysis to diverse regions in Singapore, namely key growth areas; an improved SWOT score aggregation for measuring, monitoring and comparing different performance indicators; and positioning this work within the context of SDGs. The progress on this use case has been translated into a conference paper and was presented at the 27th International Conference of the Association for Computer-Aided Architectural Design Research in Asia 2022 (CAADRIA2022), which was held April 9-15 in Sydney, Australia.

Dr Herthogs has also been developing an ontological framework for design goals and their evaluation, structuring nine goal types into three interrelated hierarchical levels. It is a mid-level, domain agnostic ontology defined in relation to top-level ontology Basic Formal Ontology (BFO).

Figure 8.13: The geospatial distribution of overall SWOT analysis scores across four chosen regions in Singapore. The overall SWOT analysis score is defined as the difference between aggregated SO and WT. Positive scores (i.e. SO) that outweigh WT are coloured in blue shades while negative scores (i.e. WT) that outweigh SO are coloured in red shades. These maps show that our automated SWOT analysis framework is consistent across use cases with different topological features, development phases and information coverage.

Figure 8.14: One of the four regions' SWOT analysis results: a) score composition of four example plots; b) distribution of overall SWOT analysis results; c) distributions of separate SWOT descriptors. S and O primarily cluster in areas of developed plots with high-rise buildings, while W and T cluster in areas that are not yet developed; d) bar chart of SWOT analysis results for all plots. Most plots balance negative and positive factors and only very few plots are highly suitable or highly unsuitable for solar panel installation (when considering geometrical, geographical and urban morphological criteria).

Update on work package 6

Demonstrators: horizontal and vertical use cases

In conversations with the Urban Redevelopment Authority (URA)'s Design and Planning Lab, the team scoped three use cases for assistive applications supporting land-use planning activities: (1) a 'site regulations advisor' to demonstrate the ability to display relevant city planning regulations for the selected sites (land plots); (2) a 'suitable site selector' to demonstrate CKG innovations in site selection and recommendation based on automated Strengths, Weaknesses, Opportunities, and Threats (SWOT) analysis and evaluation for desired development programmes and planning goals; and (3) a 'future scenarios builder' to assist planners in setting up, simulating, analysing, and managing multiple scenarios in parallel. These use cases cover the horizontal breadth and vertical depth envisioned in this work package.

As a first step, the team led by **Dr Pieter HERTHOGS (Senior Researcher, SEC)** is developing a demonstrator that supports the first and second use cases. This 'programmatic plot finder' extends on the allowable land use queries enabled by the OntoZoning ontology, integrating URA legislations that determine the maximum allowable gross floor areas (GFA) of plots. The resulting demonstrator will assist users in finding plots that could house their particular desired combinations of land uses and programmes (types and amounts).

This illustration of multi-domain queries supporting planning tasks builds on the ontology and queries presented in the pre-print 'Multi-criteria site selection using an ontology: the OntoZoning ontology of zones, land uses and programmes for Singapore', described in Work Package 1. The goal of the demonstrator is to implement a smooth and efficient workflow for executing and visualising the queries described in the pre-print, including the query of plots allowing hotel and gym developments (as shown in Figure 8.15). As part of this development process, the team addresses some of the gaps and limitations identified in the original version of the ontology. This includes extending the OntoZoning ontology to enable the retrieval of allowed land uses and programmes, and the automated estimation of the buildable amounts (GFA) of these programmes based on applicable urban planning regulations in Singapore that regulate built volume.

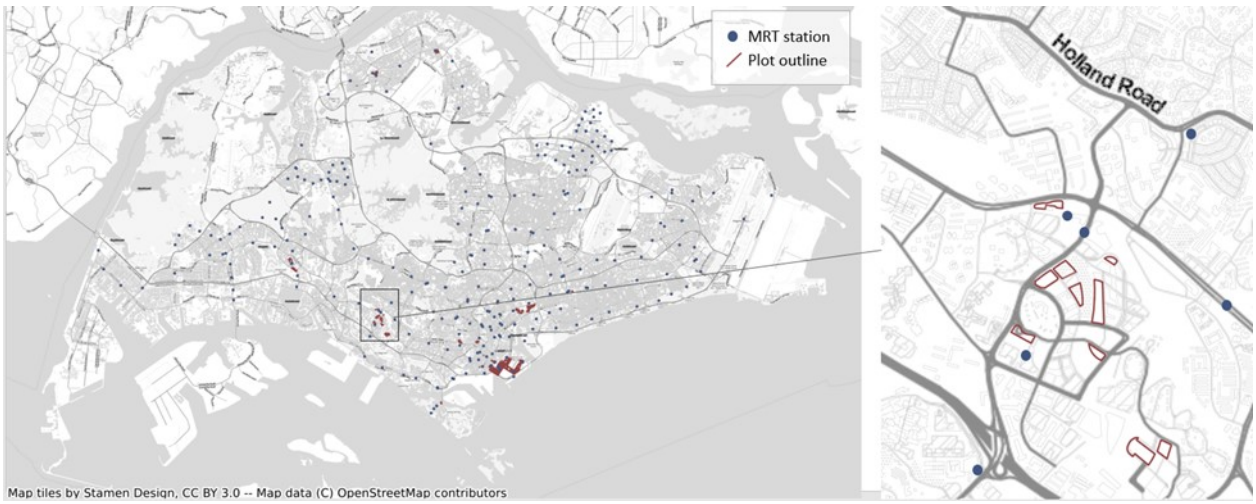


Figure 8.15: Visualisation of query result displaying all plots located within 1,000m of a Mass Rapid Transit (MRT) station which are currently empty and allow the building of a gym and a hotel.

In particular, **Ms Heidi SILVENNOINEN (Researcher, SEC)** is updating the OntoZoning ontology to add allowed use quanta for each land use type in a given zone. This is essential for enabling queries of where it is possible to place a given floor area of a programme or land use (as shown in Figure 8.16). The revised ontology also aims to account for interrelations between allowed land uses (for example, a plot allows building a store but only if a hotel is also built), and exceptions to allowed land uses based on a plot's context. **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)** is developing a query component for the retrieval of the allowable amount (area) of programmes in the form of an estimated plot GFA. This involves automating the retrieval of local urban planning regulations applicable to urban parameters that affect GFA and estimating its value for every plot. **Ms Shiying LI (Software Engineer, SEC)** is developing a user interface for the demonstrator to allow users to select desired programmes and their amounts and only plots that meet the constraints are visualised in the 3DCityDB-Web-Map-Client interface. The team is also exploring how to make the land use and programme queries more user-friendly, for example, by adding labels to each class in the ontology, and possibly by linking the ontology to a synonym dictionary. Ideally, users would be able to make queries to the knowledge graph using natural language.

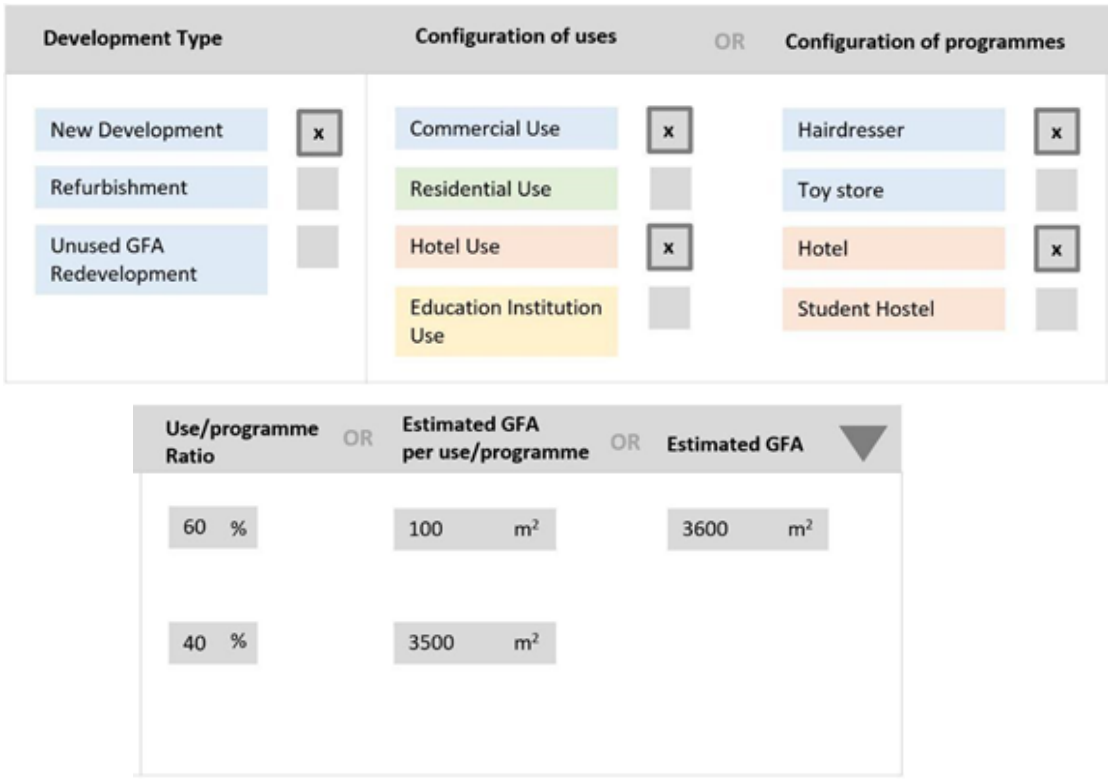


Figure 8.16: An interface wireframe for programmatic plot finder functionalities. The user can define the types of plots to search for, e.g. built, unbuilt or plots with unused GFA. The user can also select the desired programme or land use combinations and input the desired amounts.

Scientific output

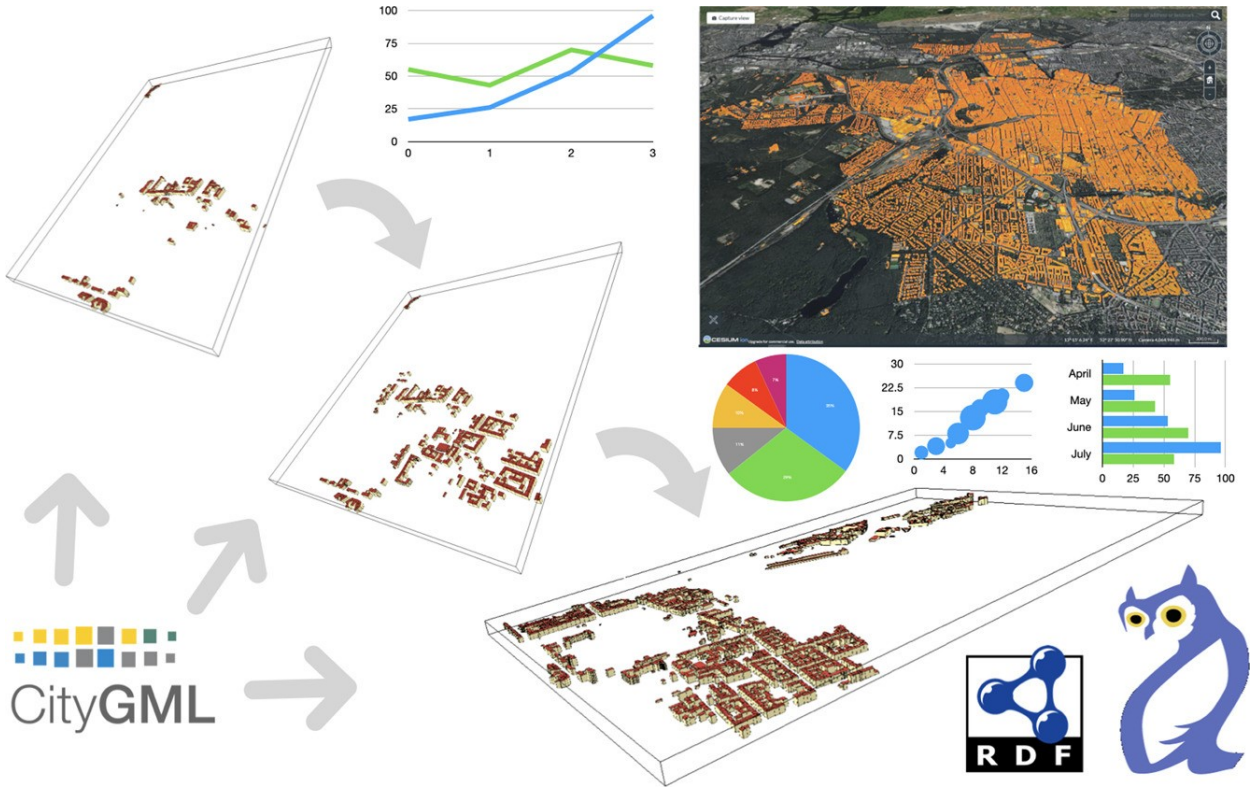
The following are the CREATE-acknowledged publications generated by CKG during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Semantic 3D City Agents—An intelligent automation for dynamic geospatial knowledge graphs

Arkadiusz Chadzynski, Shiying Li, Ayda Grisiute, Feroz Farazi, Casper Lindberg, Sebastian Mosbach, Pieter Herthogs, and Markus Kraft, *Energy and AI*

DOI: 10.1016/j.egyai.2022.100137

Abstract: This paper presents a system of autonomous intelligent software agents, based on a cognitive architecture, capable of automated instantiation, visualisation and analysis of multifaceted City Information Models in dynamic geospatial knowledge graphs. Design of JPS Agent Framework and Routed Knowledge Graph Access components was required in order to provide backbone infrastructure for an intelligent agent system as well as technology agnostic knowledge graph access enabling automation of multi-domain data interoperability. Development of CityImportAgent, CityExportAgent and DistanceAgent showcased intelligent automation capabilities of the Cities Knowledge Graph. The agents successfully created a semantic model of Berlin in LOD 2, compliant with CityGML 2.0 standard and consisting of 419 909 661 triples described using OntoCityGML. The system of agents also visualised and analysed the model by autonomously tracking interactions with a web interface as well as enriched the model by adding new information to the knowledge graph. This way it was possible to design a geospatial information system able to meet demands imposed by the Industry 4.0 and link it with the other multi-domain knowledge representations of The World Avatar.



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, such as the Urban Redevelopment Authority (URA) in Singapore. Further exchanges took place with URA's Design & Planning Lab, to discuss potential CKG use cases.

Prof Dr Stephen CAIRNS (PI, SEC) was invited to present the CKG project at 'Future Towns and Districts', an event by the Centre for Liveable Cities (CLC), with Housing Development Board (HDB) and URA, in January 2022. **Dr Pieter HERTHOGS (Co-I, SEC)** gave a guest lecture on the CKG project and the importance of knowledge representation at ETH Zurich in March 2022.

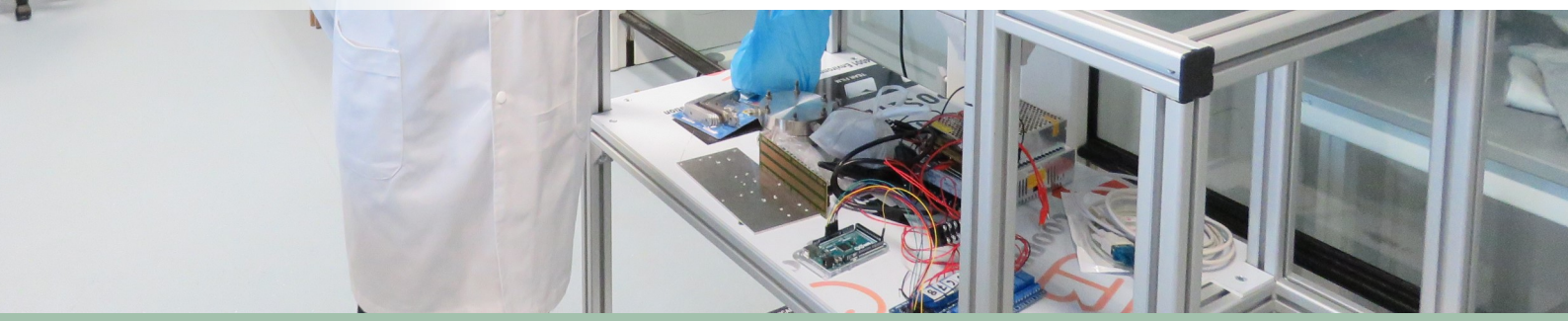
Dr Herthogs met with the Smart City Project Office (Smart Nation and Digital Government Office) and URA's Design & Planning Lab in March 2022, presented project updates, and discussed a proposed collaboration to initiate broader stakeholder engagement workshops to explore and scope future possibilities of knowledge graph technology as an enabler for smart and sustainable city initiatives (beyond city planning). Mr Genki UNNO (Visiting Researcher, Takenaka Corporation), advised by Dr Herthogs, is developing a thematic evaluation framework for Smart City projects and visions, specifically introducing criteria for context-adaptation.

Dr Franziska SIELKER (Co-I, CAM) headed a collaborative initiative of a position paper on the need for interoperability in smart city governance. This work has been published as a pre-print entitled "The Conundrum in Smart City Governance: Interoperability and Compatibility in an ever-growing digital ecosystem". All the authors, including **Dr Aurel VON RICHTOFEN (Co-I, Arup Berlin)**, **Prof Markus Kraft (PI, CAM)**, and **Dr Pieter HERTHOGS (Co-I, SEC)** also contributed to the special session 'Towards smart city planning – digital twins and parallel world scenarios to support better public policies?' at the conference 'Data for Policy 2021' held in September 2021 by University College London.

A literature review paper by Dr von Richthofen, Dr Herthogs, Prof Kraft, and Prof Dr Cairns entitled 'Semantic City Planning Systems (SCPS): A Literature Review' was published in January 2022 in the *Journal of Planning Literature*. The paper posits the term 'Semantic City Planning Systems' as the use of Semantic Web Technologies to support City Planning practices.

Under the leadership of Dr von Richthofen and Prof Dr Kraft, Arup and Computational Modelling Pirmasens GmbH (CMPG) have been awarded the project 'DATEN:RAUM:FREIBURG' for the digital urban twin for the city of Freiburg im Breisgau in Southern Germany. The project will be based on the same open data platform used by the CKG project. The project is part of Germany's ambitious programme for 'Smart City Modellprojekte' funded by the German Federal Ministry of the Interior (BMI).

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 smaller projects are also often a good opportunity for interns (such as Mr Aman SINGHAL, pictured above during his time working on the RINGs project in 2019) to have a novel experience of research and technology development not easily available during their undergraduate degrees.

The current CARES small projects include three funded by the private-public partnership Pharmaceutical Innovation Programme Singapore (PIPS) and Consumer Energy Usage Data in Smart City Development (CEUS, an Intra-CREATE seed grant project). CARES is now collaborating with the Singapore-ETH Centre on Cooling Singapore 2.0 and an update on this work is included.

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.

Consumer Energy Usage Data in Smart City Development (CEUS)
Intra-CREATE seed grant

CEUS commenced in October 2020 and is a seed funded Intra-CREATE collaborative project between Cambridge CARES and the Singapore-ETH Centre. CEUS aims to lay the groundwork for Singapore consumers to manage their energy usage and cost. It will also outline ways for local government to make informed decisions based on real-time energy use for smarter city planning. The project is led by Principal Investigators **Dr Franziska SIELKER (PI, CAM)** and **Dr VSK Murthy BALIJEPALLI (PI, SEC)** and supported by other researchers at Cambridge CARES, the Singapore-ETH Centre, Nanyang Technological University (NTU) and ETH Zürich.. **Mr QUEK Hou Yee (Research Associate, CARES)** was the funded researcher at CARES at the grant close date of March 31st 2022.

Urban management has always been concerned with managing immense information flows between the growing network of stakeholders from diverse fields. The immense data flows offer a multitude of new opportunities to address the challenges associated with an ever-growing world of "data" and complexities. One example is the recent liberalisation of Singapore's residential electricity market. Consumers have now been given more choice and flexibility in selecting suitable electricity retailers and pricing plans to meet their needs. Given the growing complexity of smart city systems, the immense information streams generated are often overwhelming to the average consumer who lack knowledge, tools, and interest in analysing and optimising their electricity consumption usage. This leads to a lower level of consumer engagement and competition that counteracts the original intentions for a more consumer-oriented electricity market.

CEUS aims to develop a knowledge-enabled, data-driven, user-friendly, common platform on Singapore's real-time consumer energy usage. The CEUS platform would provide real-time information about consumer energy usage to enable the public service and individual consumers to make more informed decisions and promote more active participation in the energy market.

The outcomes from CEUS are summarised below:

- Developed a Singapore-specific City Information Modelling (CIM) grammar based on the Enterprise Architect tool and IEC TC57 specifications to standardise representation of consumer energy data.
- Integrated the CIM grammar with CARES' J-Park Simulator for seamless and efficient data exchange.
- Created instances of the relevant technologies, consumers, electrical, and energy components etc. utilised in the frameworks and incorporated them into the JPS knowledge graph.
- Internet of Things (IoT) hardware setup having micro-components to capture the energy usage data of different consumer appliances in real-time has been successfully accomplished and made available in the public domain at http://ceus.live.
- Identified the value of CIM technologies inclusive of the digital twin, Building Information Modelling (BIM), and Geographic Information System (GIS), and their integration with the semantic web technologies (ontologies, knowledge graph) to establish more intelligent robust urban management systems and sustainable city developments.

Work Package 1: Standardised representation of consumer-level CIM grammar

Led by SEC, this work package developed a standardised CIM grammar in Singapore's energy consumer domain to empower consumers and encourage active consumer participation in the electricity market. CIM is a well-established open standard for information modelling in the power systems domain by providing standard, unambiguous definitions and representations of various energy-related concepts. CIM has been considered an enabler of smart grids with a robust

framework for accurate data sharing, merging, and transformation into reusable information. Based on a thorough literature review, the developed CIM grammar for Singapore's consumer energy domain is built on the Enterprise Architect tool and IEC TC57 specifications. Parameters defined in the energy usage information and grid parameters are used as inputs for the CIM grammar development process.

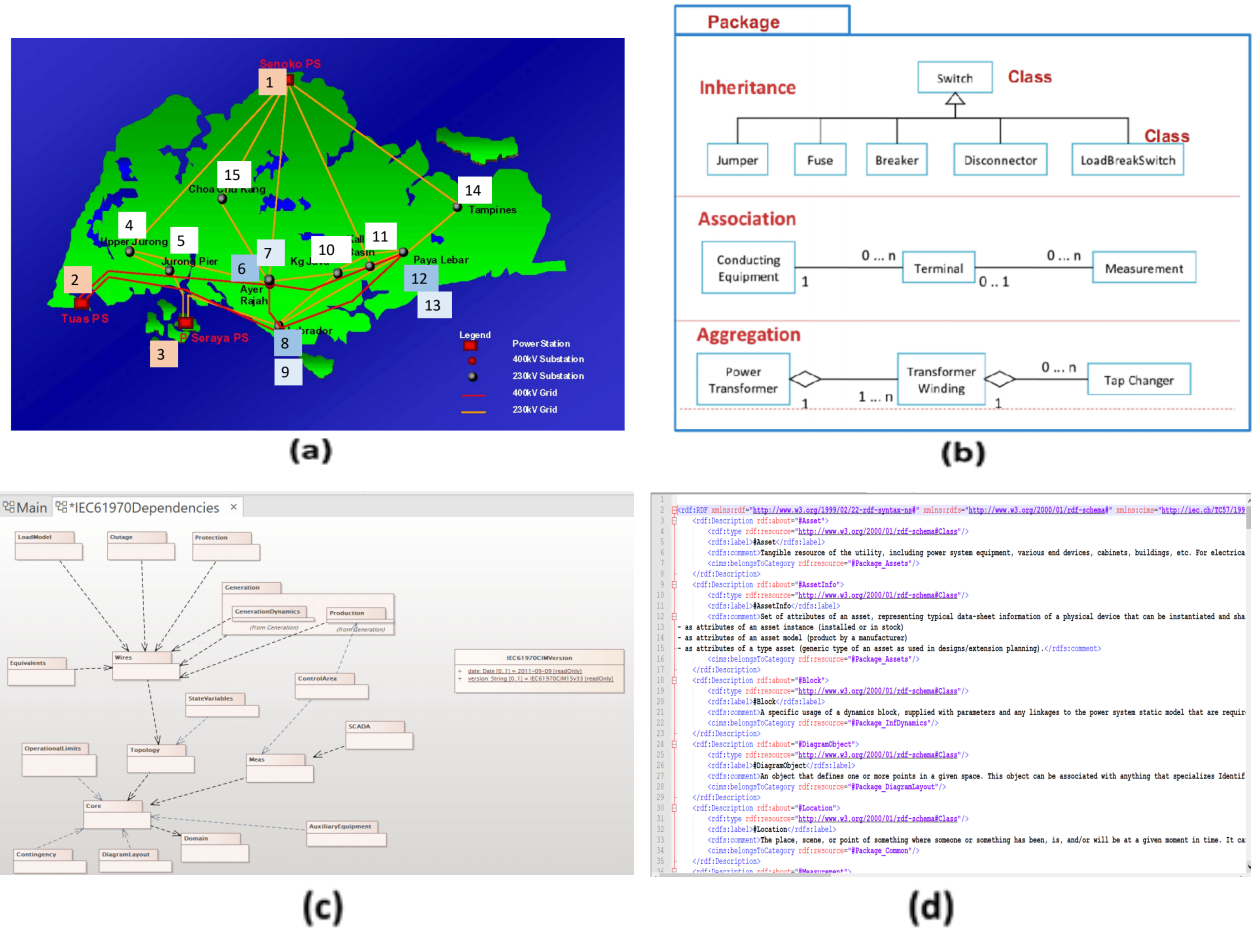


Figure 9.1 (a) Horizon scan of electricity consumer space for knowledge gathering. (b) Describing relationships between different electricity parameters. (c) Developing UML diagrams and establishing upstream link with CIM. (d) Schema XML file generation.

Work Package 2: Knowledge graph and ontology development

The literature review shows that the CIM grammar only provides formal definitions and does not encode the necessary contextual information to carry out complex tasks such as automation and reasoning. Led by CARES, this work package aimed to enhance the expressivity of the CIM grammar developed in WP1 by creating a knowledge base and ontology schema for Singapore's consumer energy domain. This work establishes the relationships between the CIM concepts and integrates them within the CARES JPS framework for further elaboration in WP3. The JPS agent architecture can utilise the energy consumption data to automatically execute specific tasks within the electricity domain, such as analysing consumption patterns for market participation and presenting energy savings through an ontology-based model-driven knowledge approach.

Although the JPS is envisaged as eventually being a fully autonomous digital twin, current iterations of these digital tools are reliant on manual inputs and visualisation, partly to assure their human users of their competency and accuracy. In building a digital twin for the consumer energy domain, it is necessary to incorporate City Information Modelling technologies such as BIM and GIS alongside the developed CIM grammar.

As per the findings of WP4, these technologies would visualise and support the developments within the energy domain for smarter sustainable infrastructures, inclusive of energy grids.

As a start, the team have tested the JPS knowledge graph's interoperability with GIS and CIM through a case study. A CityGML LOD4 model for a housing unit was generated from images of the apartment block's escape plans, floor plans, and building façades. This model was then instantiated through the OntoCityGML ontology, reflecting the CityGML 2.0 standard, alongside the sensors' location, into the JPS knowledge graph. The real-time consumer data measured by the sensors were also instantiated through the consumer energy ontology into the JPS knowledge graph. By generating a LOD4 model as illustrated in Figure 9.2, users can visualise and identify the sensors' positions and the corresponding power consumption of different appliances within the household. By knowing the appliances and sensors' geospatial information, this approach could expand the understanding of current energy consumption patterns for different households and different appliances at a more granular level. This understanding would empower consumers with recommendations to optimise their interior layout, including the appliances and furniture, to reduce energy consumption and enjoy energy savings.

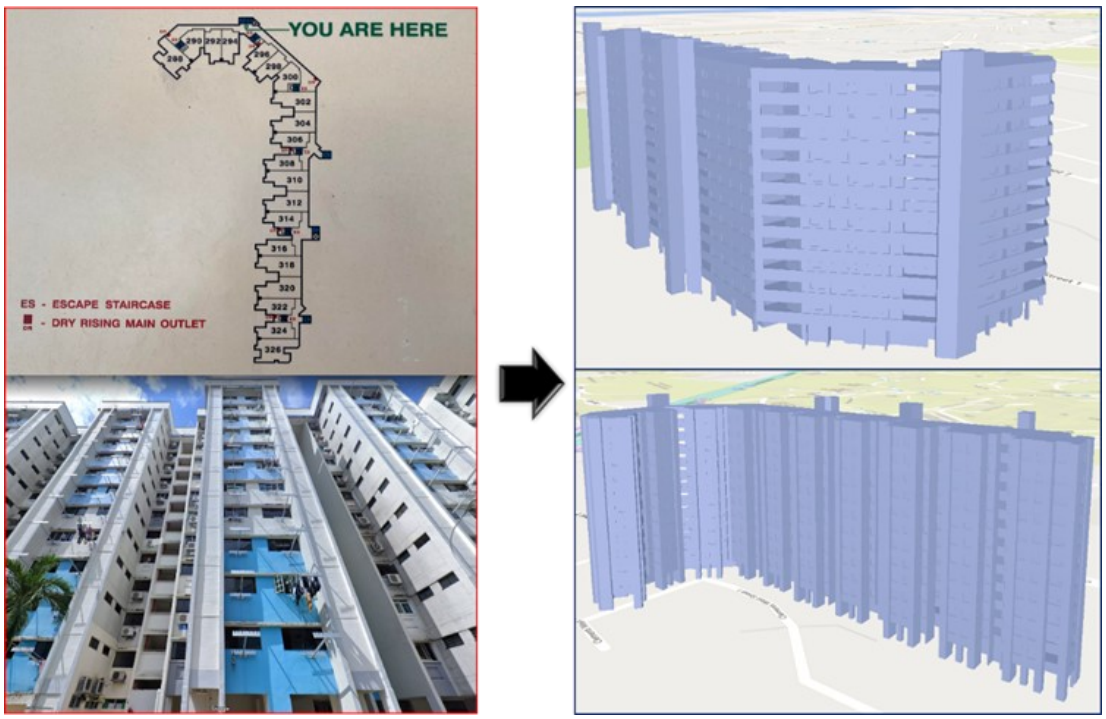


Figure 9.2: The LOD4 model of the selected HDB block in JPS.

Nevertheless, GIS is insufficient to represent and analyse granularity at the consumer appliance level that is relevant to the use case in WP3 with BIM being a more appropriate tool. CEUS proved that integrating BIM into JPS is possible, and the CEUS team is working with other CARES members to continue exploring BIM integration into the JPS, to enable a more seamless integration between GIS, CIM, and BIM.

The consumer appliance optimisation module of WP3 is demonstrated in the JPS architecture through another case study. This case study involves a fridge equipped with multiple sensors located within the CARES laboratory in one of the CREATE buildings on the NUS campus. The fridge's electric voltage, current, power, energy consumption, and power factor data is measured through the sensors and an agent in JPS is set up to retrieve and convert the data into an ontological time series format based on the CIM grammar in the knowledge graph. Another agent utilises this data alongside price data from other sources

as inputs to the optimisation module to identify the optimal schedule and cost for the fridge, as illustrated in Figure 9.3, and sends signals to turn it on or off. This example investigates the potential of incorporating automated facility management capabilities into the JPS within the context of a chemistry laboratory. In the long term, this test would be expected to extend to more appliances within the lab and support the development of a use case in lab automation. By offloading menial lab management tasks currently undertaken by the lab users, their time and attention could then be focused solely on the experiments, and hopefully, lead to new discoveries, insights, and innovation.

The experiences in WP2 reflect the findings of the literature review on BIM-GIS integration. First, the seamless data exchange between the two data schemas is still unsuccessful for higher granularities. This is due to the difficulties in aligning and linking the disparate geometric and semantic attributes of both schemas. In our attempt, the key bottleneck occurs at the geometry level and cannot be overcome with the capabilities of existing tools. Moreover, the two schemas are most distinct at smaller scales e.g. at the appliance level, in which GIS has limited representation capabilities of both semantic and geometric information. Second, there is an absence of coordination and benchmarking between various research streams. Attempting to test these tools for the conversion of BIM to GIS highlights the redundancies and overlaps between existing and ongoing procedures.

This perpetuates an ever-growing, distributed number of BIM-GIS methodologies that are difficult to identify and subsequently to benchmark. Lastly, these developments often neglect the practicalities required for these applications. In the CEUS context, we collaborated from the outset in the development of the CIM grammar and considered their applications and outcomes using ontologies at the smart city context. This streamlined the development process and reduced duplicate work by tailoring existing standards to Singapore's context rather than starting from scratch.

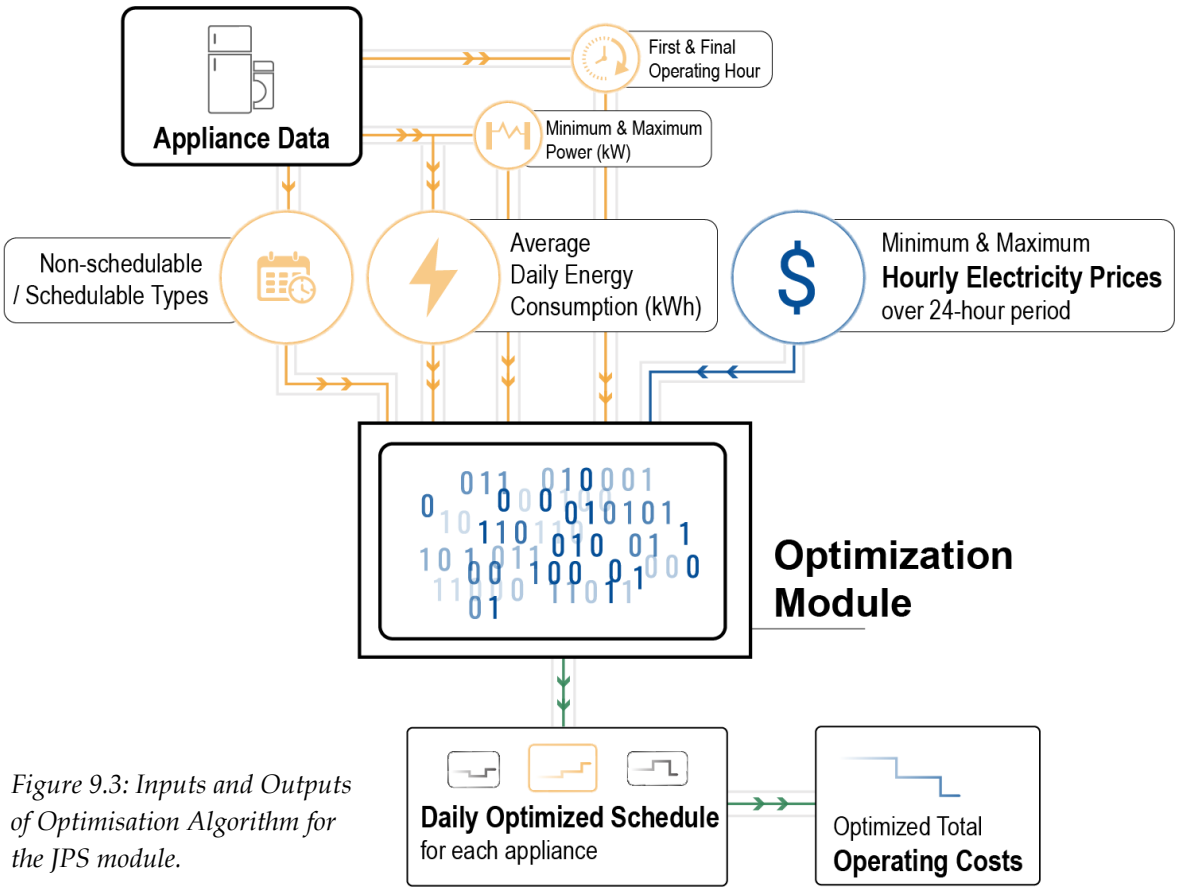


Figure 9.3: Inputs and Outputs of Optimisation Algorithm for the JPS module.

Work Package 3: Real-time consumer energy usage data exchange interface

Led by SEC, this work package handled the development and the implementation of the use case as a real-time consumer energy usage data exchange interface for scheduling home appliances. Real-time consumer energy data is integrated with the consumer energy ontology developed in WP2 to become a part of the JPS knowledge graph to run on consumer applications. The knowledge from the use case can be used to make an informed decision on infrastructure provision or energy policies at the consumer level. For example, real-time energy consumption patterns provide input to policies that reduce urban heating and increase consumer uptake of smart city solutions. Deliverables of this work package are a presentation file describing the outcomes and UML diagrams, available in Appendix C.

The researchers have successfully established the IoT hardware setup using micro-components to capture the energy usage data of different consumer appliances in real-time. The sensors provide real-time measurements of parameters such as indoor temperature and electricity usage (consisting of power, voltage, and current). This data is then collected every 100 milliseconds and aggregated to a live dashboard interface, and is made available in the public domain at http://ceus.live.

An optimisation algorithm has been developed for a consumer benefit aggregator that determines the optimal schedule for consumer appliances in real-time to maximise consumer benefits and comfort while minimising energy consumption at any moment. The algorithm utilises the data on daily energy consumption by appliance, electricity prices, operating time, and other data as data inputs. By considering the anticipated demand, supply, and prices, the algorithm generates optimal schedules and costs for consumer appliances as outputs. Based on these outputs, the aggregator would send dynamic schedule signals to the relevant appliances to either turn on, off, or modify their outputs if possible. This optimal schedule reduces energy consumption and is translated into energy savings for the consumer.

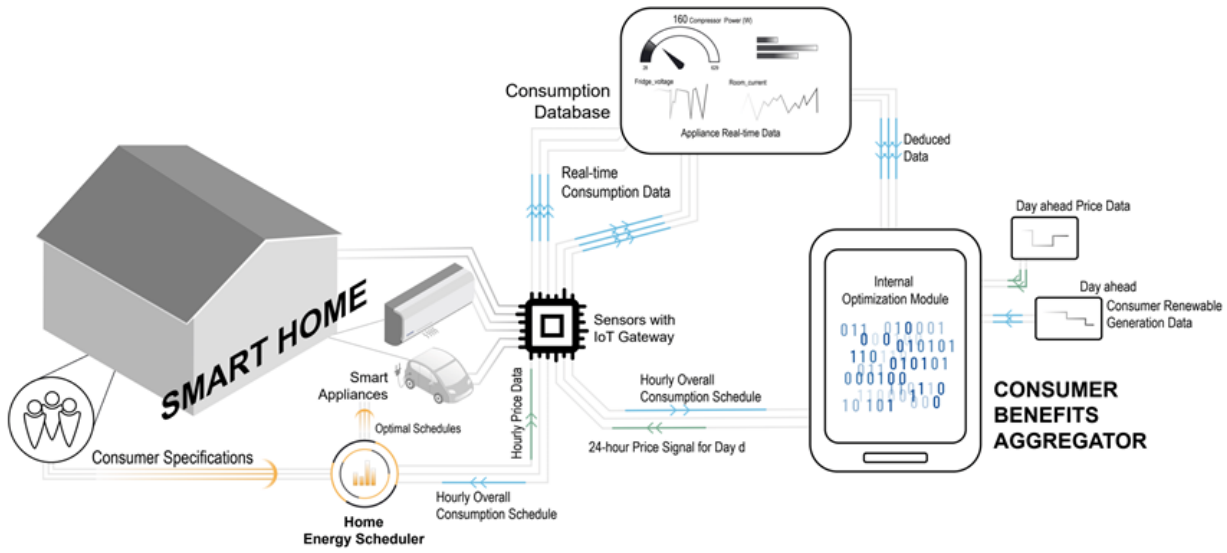


Figure 9.4: Overview of the use-case implementation and information flow.

Work Package 4: Planning for cities—integration of consumer energy data in city information modelling

Adding an urban planning and policy perspective, this work package complements the technological developments in WPs 1 to 3. Cities are complex evolving interdependent living systems with various intangible influences (policy, human behaviour, commercial interests) that are difficult, if not impossible, to capture through data and digital technologies. Without a thorough understanding of urban governance issues, it remains unclear how the benefits proposed by current technology-driven approaches will be delivered and sustained at any scale.

Given this background, it is crucial to re-acknowledge the mediatory role of urban planning to untangle and accommodate the complex network of actors and their conflicting interests involved in the city's development across disciplines and scales for more sustainable outcomes. Specifically, the concept of City Information Modelling is relevant to scrutinise the capacity of these digital planning tools and systems to support deliberative participatory planning processes and generate interdisciplinary insights to make more informed decisions for a sustainable smart city.

By providing a thorough analysis of Singapore's energy and city planning governance model, WP4 aims to understand the value of City Information Modelling in city planning and energy systems, how City Information Modelling could enable interoperability with the diverse urban information systems available and how it can be implemented in practice for the knowledge graph to become a one-stop solution with the potential for a consumer digital twin.

The key publication and outreach activities are as follows:

- [Conference paper] "Evolution of power system CIM to digital twins—a comprehensive review and analysis" was published in *2021 IEEE PES Innovative Smart Grid Technologies Europe*. DOI: 10.1109/ISGTEurope52324.2021.9640174
- [Journal article] "The Conundrum in Smart City Governance: Interoperability and Compatibility in an ever-growing digital ecosystem." was submitted to *Data & Policy* on 30 Nov 2021.
- [Journal article] "Are urban planners late to the game? A Literature Review on BIM, GIS, and Semantic Web Integration" has been submitted to *Sustainable Cities and Society Journal*.
- [Journal article] "Interactive Scheduling of Consumer Appliance Usage in the Home - A Real-time Deployment Usecase" and "Digital Twin in Energy Consumer Choice Modelling – A Systems Perspective" to be submitted to *IEEE Systems Journal* in April 2022.
- The CARES led paper titled "Are urban planners late to the game? A Literature Review on BIM, GIS, and Semantic Web Integration." has been submitted to the Annual Congress of the Association of the European Schools of Planning (AESOP) 2022 for review.
- **Dr Franziska SIELKER (PI, CAM)**, initiated and moderated the panel session (inclusive of a pre-conference online presentation) at the *Data for Policy 2021 Conference*, and the subsequent conference paper in publication. Other invited contributions during the conference days for presentation were led by **Prof Markus KRAFT (CARES Director)**, Mr Amit BHAVE from CMCL Innovations, **Dr Pieter HERTHOG (Co-I for CKG, SEC)** from Singapore-ETH Centre, and Dr Timea NOCHTA from Centre for Smart Infrastructure and Construction.

Data2Knowledge in the Digital Manufacture of Pharmaceuticals

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

Data2Knowledge in the Digital Manufacture of Pharmaceuticals is a project funded under the Pharma Innovation Programme Singapore (PIPS) programme led by Prof Alexei Lapkin and Prof Markus Kraft. This is a 15-month (now extended to 21-month) project that commenced in December 2020. The project aims to develop a full digital framework for automated experiments within a digital laboratory.

In this reporting period, **Mr Jiaru BAI (PhD student, CAM)** revised a perspective paper on a thorough literature review of the current state-of-the-art practices in lab automation, which led to hypothesising that knowledge graph technology, orchestrating semantic web technologies, and multi-agent systems, will be the driving force to transform data to knowledge, evolving the way of automating the laboratory. The perspective paper has been accepted for publication in *JACS Au*.

Mr Bai and **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)** have been working on conceptualising and implementing a dynamic knowledge-graph-based framework of an existing automated closed-loop optimisation setup, which was originally demonstrated as part of the PIPS C4 project. The complete knowledge graph consists of two aspects: ontologies abstracting the knowledge in the flow chemistry experiment, and agents operating the experiment based on the semantic-enriched data.

The ontology development started with instantiating the digital twin of the physical elements of the experimental system, with the long-term goal of fully digitalising the chemistry laboratory. Figure 9.5 illustrates the PIPS C4 project hardware system. In brief, the system consists of a "Vapourtec Module", which comprises pumping modules, a robotic liquid handler, the tubular reactor used in the specific experiments, a four-way valve that is used to send the end product for analysis during the experiments, and a back pressure regulator (BPR). The system is controlled via a programmable interface, 'Flow Commander', supplied by the vendor (Vapourtec Ltd). In addition, the overall system includes an analytical instrument – a high-performance liquid chromatograph (HPLC), specifically an Agilent 1260 Infinity system equipped with a G1311B quaternary pump, Eclipse XDB-C18 column (Agilent product number: 961967-302), and G1314F variable wavelength detector (VWD).

The ontological instantiation was done based on the principles behind the Internet of Things (IoT) Smart Applications REFerence (SAREF) ontology. In this project, SAREF was adopted and extended to meet the specific implementation for the Vapourtec module and for the HPLC instrument. The key concepts and relationships are formulated into OntoLab ontology.

Two additional ontologies were developed to cover knowledge in chemical reactions, OntoRxn, and the design of experiment practice, OntoDoE. The development of OntoRxn is based on a thorough review of the current reaction schema and chemical ontologies, which was done as part of

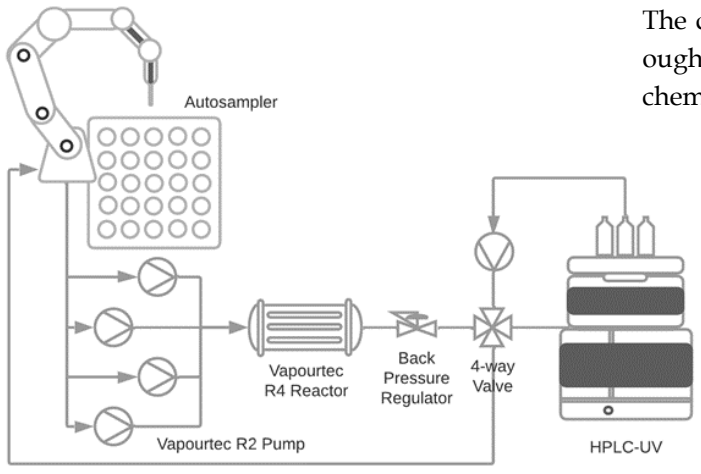


Figure 9.5: Schematic diagram of the experimental system.

the perspective paper aforementioned. In particular, we are inspired by Open Reaction Database (ORD), Unified Data Model (UDM), ChemRxnExtractor, and OntoCAPE.

Figure 9.6 demonstrates the automated Design of Experiment (DoE) exercise supported by OntoDoE and DoE Agent. It marks up the DoE configuration with OntoDoE, which triggers the operation of the DoE Agent to retrieve the experiment data from the knowledge graph, make suggestions about the next experiments, and populate those suggestions back to the knowledge graph.

Three other agents were also developed as a breakdown and re-implementation of the control codes from the PIPS C4 project, namely the Execution Agent, the PostProc Agent, and the HPLCInput Agent. The control codes in the PIPS C4 project have been taken apart and transformed into agents. Mr Bai is in the process of assembling the developed agents into one framework in silico, which will lead to real experiments in the upcoming months.

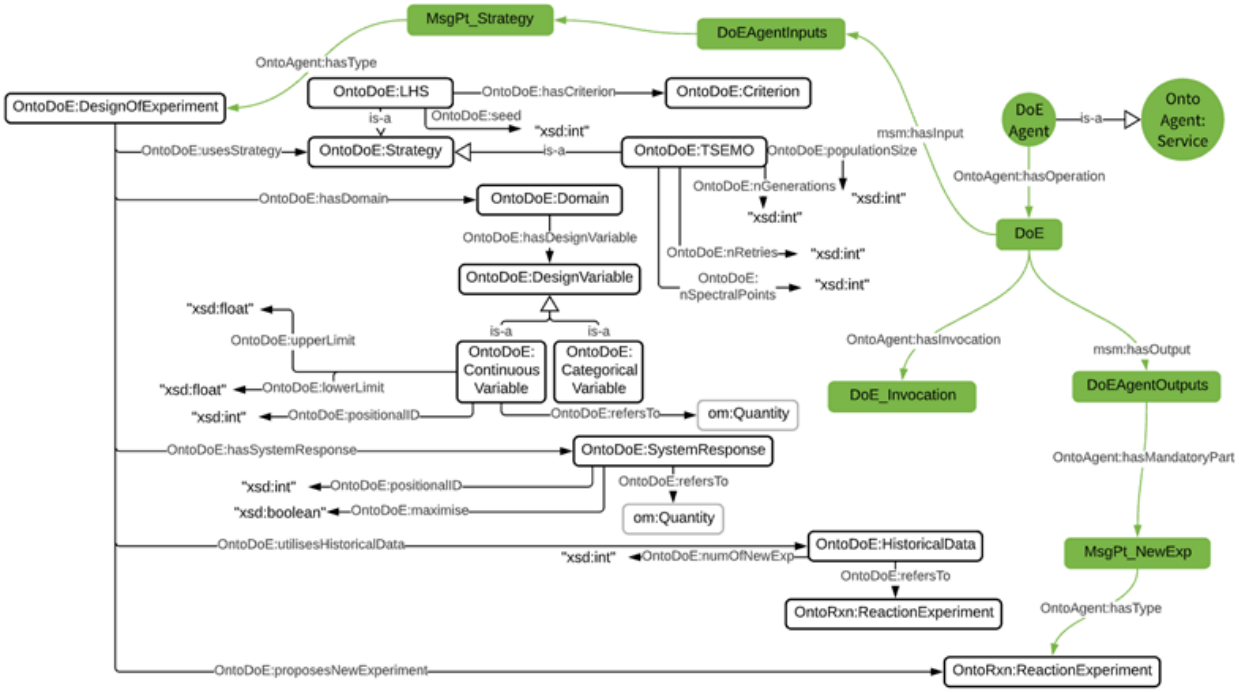


Figure 9.6: Ontological markup for the design of experiment (OntoDoE) and the agent that automates the design of experiment exercise (DoE Agent).

Development of Multi-Step Processes in Pharma

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

Development of Multi-Step Processes in Pharma is funded under the Pharma Innovation Programme Singapore (PIPS) programme and led by Prof Alexei Lapkin. This is a three-year project which commenced in June 2019.

For a given active pharmaceutical ingredient (API), the complexity of the multi-step chemical synthesis and purification, and the enormous number of possible reagent and reaction condition combinations are significant bottlenecks for rapid large-scale manufacturing. The work conducted by **Dr Simon SUNG (Research Fellow, CARES)** and **Dr Mohammed JERAAL (Research Fellow, CARES)** are focused on developing a novel automated self-optimising system that can rapidly identify sustainable and high yielding multi-step chemistry and purification routes in tandem. This will be achieved by combining pro-

grammable chemical handling equipment, analytical tools and machine learning (ML).

Earlier in the project, Dr Sung and Dr Jeraal developed an optimisation algorithm for the multi-step optimisation of chemical processes for multiple simultaneous objectives. The end-to-end machine learning pipeline collectively utilises a range of supervised and unsupervised learning methods for a synergised approach to the representation and optimisation of chemical systems. In the last 6 months, the optimisation workflow has been augmented to improve access to a broader range of optimisation strategies.

Following extensive computational testing, the duo have seamlessly integrated the improved algorithm into a fully autonomous robotic platform for the optimisation of multi-step chemical synthesis and purification processes. The practical application of this digital workflow in the optimisation of both single and multi-step chemical optimisation processes has led to marked increases in yield and optimisation times for their respective chemical processes. Together with visiting researcher Dr Jannik BURRE (RWTH Aachen University), the algorithm has been further developed to include simulation of downstream processes, thus permitting the holistic optimisation of entire chemical manufacturing workstreams.

Dr Magda BARECKA (Research Fellow, CARES) has been involved in this programme since July 2021, working towards the development of first principle models that will be used together with Machine-Learning automatic process optimisation. Her main research interest lies in understanding how to extract maximum process knowledge from a minimum number of automatised experiments, so that different phases of the process design can be accelerated. She has been developing a method that allows for a stepwise screening of the data generated by a platform for reaction optimisation in order to determine the limiting phenomena for the given reaction. The basic concept of the method was tested with several literature case studies (Figure 9.7).

Besides the engagement in PIPS, she has been working further on development of novel concepts for isotopes manufacturing, and continuing her core work on the development of CO_2-based production methods that are scalable and viable in the current market.

In this reporting period, she co-authored a paper titled "Accelerating Net Zero from the Perspective of Optimizing a Carbon Capture and Utilization System" that was published in *Energy & Environmental Science*. She also gave an in-person presentation titled "Disrupting the carbon cycle without interruption to chemical plant operations" at the ACS Spring Meeting in San Diego on 21st March 2022. She visited Lawrence Berkeley National Laboratory on 1st April 2022 and gave a presentation on "Techno-economic analysis of emerging CO_2 electrolysis technologies".

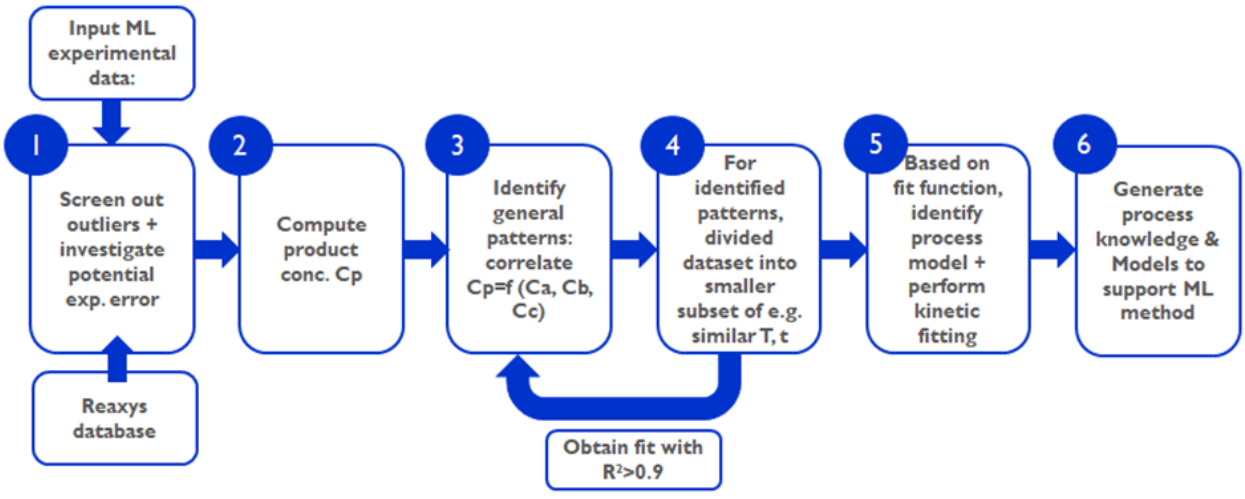


Figure 9.7: Overview of the process design methodology developed within PIPS. *Dr Magda BARECKA*

Digital Workflow and Continuous Processing in Pharmaceuticals Manufacturing

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

Digital Workflow and Continuous Processing in Pharmaceuticals Manufacturing is funded under the Pharma Innovation Programme Singapore (PIPS) programme and led by Prof Alexei Lapkin. This is a two-year project which commenced in January 2021.

Transformation of manufacturing in the pharmaceutical industry to new emerging business models (on demand, customisation, sustainable manufacturing, etc.) is heavily dependent on the development of supporting technologies, such as a novel manufacturing paradigm of fully continuous processes and digital tools for support of R&D and manufacturing.

A number of current challenges in the supporting technologies are interlinked. Thus, development of effective flow processes and the use of continuous flow technology in manufacturing requires innovation in process modelling, reactor technology/reactor manufacturing, process data monitoring and knowledge management. This requirement spans the areas of synthesis, process engineering, process control, data science and artificial intelligence.

Dr Dogancan KARAN (Research Fellow, CARES) recently joined in March 2022 as a part of PIPS-Pfizer. Currently, Dr Karan is working on an industrially relevant batch-to-continuous process transformation for the synthesis of an active pharmaceutical ingredient (API). He has developed first principle models that will be used along with machine learning algorithms to optimise the process parameters for flow reactor development. The main goal of this work is to develop robust workflows for pharmaceutical companies which can be adopted as a standard protocol for batch-to-continuous flow process transformation.

DR CHEN Guoying (Research Fellow, CARES) reports that flow chemistry has been widely known as a good approach in process chemistry. In the pharmaceutical industry, several drugs have been manufactured in continuous flow way. Dr Chen's project collaborates with Pfizer to transfer batch chemistry to flow chemistry. Recently, he has studied different synthetic routes to the drug. With flow equipment, he has evaluated the synthetic route which is more practical, less costly, and environmentally friendly for large scale manufacturing (Figure 9.8). The current results show very good conversion. He also evaluated different types of reactors which all yielded satisfying results. In future, he will apply machine learning tools to optimise the synthetic process and achieve better yield.

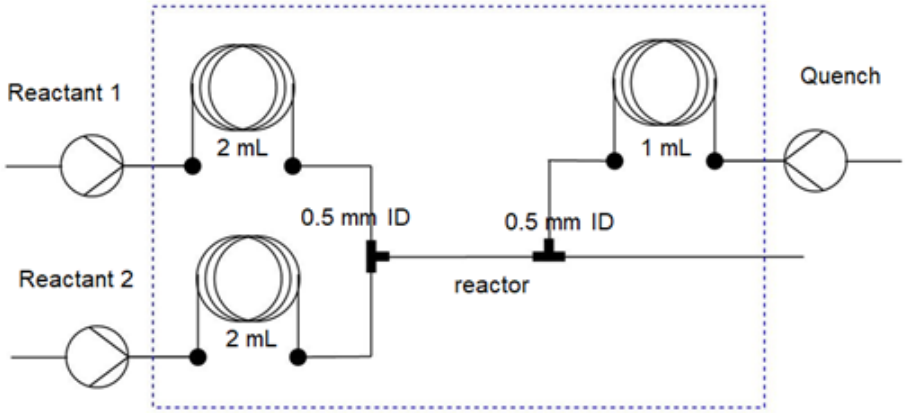


Figure 9.8: Flow reaction for the drug

Dr CHEN Guoying

Cooling Singapore 2.0

In collaboration with the Singapore-ETH Centre

Cooling Singapore 2.0 aims to construct a Digital Urban Climate Twin for Singapore. This platform will bring together several computational models (environmental, land surface, industrial, traffic, building and energy) as well as climate models to investigate ways to reduce Singapore's urban heat and mitigate its effects. The Digital Urban Climate Twin will also allow researchers to trial various scenarios and predict the impact they may have on urban heating.

CARES' contribution to Cooling Singapore 2.0 is to evaluate anthropogenic heat emissions from Industry in Singapore by developing computational energy models using The World Avatar Knowledge Graph. Ultimately, these energy models will be fed into the Digital Urban Climate Twin. We will also develop models to simulate the effect of potential mitigation solutions on the anthropogenic heat emissions from Industry in Singapore.

Dr Vishvak KANNAN (Research Fellow, CARES) developed a cross-domain query agent that demonstrates a proof-of-concept to query and process information from knowledge graphs of two different domains. The agent executes a federated query to retrieve entities based on their geo-spatial and other properties that are stored in different knowledge graphs. In this proof-of-

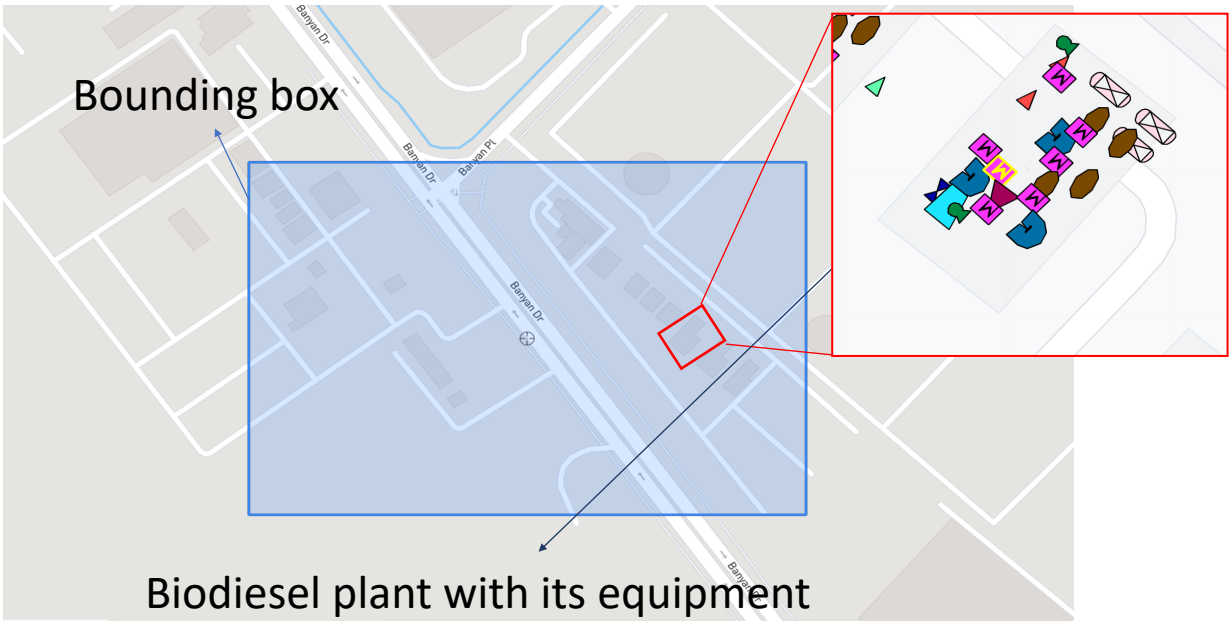



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Figure 9.9: Federated query to retrieve entities with cost greater than $30,000 within a bounding box on Jurong Island.

Dr Vishvak KANNAN

concept, the cross-domain query agent executes a federated query to retrieve entities with cost greater than $30,000 within a bounding box on Jurong Island as shown in Figure 9.9. Dr Kannan is in the process of developing the cross-domain query agent to allow retrieval of estimated heat emissions data and their corresponding geo-spatial locations which can subsequently be fed into the Digital Urban Climate Twin.

Dr Kannan together with **Ms Srishti GANGULY (Project Engineer, CARES)** collated and instantiated information about over 100 industries on Jurong Island in the knowledge graph. This information includes geo-spatial data such as the centroid coordinates, addresses, unique land lot numbers, and so forth; business activity data such as the Singapore Standard Industrial Classification (SSIC) codes, reactants and products, production technology, design capacity, year of construction, CO_2 emissions, and so forth; and economic performance data such as annual revenue and number of employees. This information can be utilised to estimate heat emissions and to identify their locations and nature.

C4T Emerging Opportunities Fund

1) Brown carbon laser characterisation and light-absorbing property

Prof. Markus KRAFT and Dr Yichen ZONG

The purpose of this research is to investigate brown carbon (BrC, light-absorbing organic carbonaceous species) from combustion emissions. BrC is a major air pollution source in Southeast Asia and a cause of climate change. The project's experimental work is carried out in partnership with researchers from CARES and the Department of Environmental Engineering, NUS. In the last round of experiments, PODE4, DMC, and DMM fuel blends were combusted in a compression ignition engine. The soot samples from the exhaust were collected to be characterised by Raman spectroscopy (RS), thermogravimetric (TG), Fourier-transform infrared (FTIR) and UV–visible spectrophotometry (UV-Vis). The characterisation results will distinguish the volatile compounds from the black carbon.

2) Chemical farming

Assoc Prof YAN Ning, Prof Alexei LAPKIN

We are working on the identification of nanoalloy catalysts for amination reactions. The aim is to find a catalyst that has a similar binding energy of NH_3 on its surface as the benchmark Ru catalyst. We are also exploring single-metal catalysts for the same reaction that have not been extensively investigated before. That includes Co-based and Ir-based catalysts.

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

Prof. Markus KRAFT, Ms Mei Qi LIM

The initial motivation of this work is to evaluate the impact of emissions from shipping activities on air quality in Singapore and to demonstrate the knowledge graph technology in handling a cross-domain application. The data required to simulate the dispersion of pollutants are highly heterogeneous as they are collected from different sources. Using knowledge graphs, data from different domains are stored semantically, eliminating data silos. Over the past six months, we have continued to work on the knowledge graph infrastructure, in particular investigating how to

represent morphology data in the knowledge graph. Morphological factors affect urban air quality. Specifically, street geometries, urban layout and landforms affect the ventilation and contaminant accumulation, which are ultimately reflected in urban air quality indicators. Additionally, amongst the many meteorological factors, urban thermodynamic circulation whose trajectories are determined by morphological factors are critical as it is the main way pollutants are dispersed. Morphology data is also an important component of the physical-based and data-driven models for urban air quality estimation.

We are investigating the extraction of morphology data from GeoTiff (a metadata standard) and storing the data in a relational database. Upon establishing a mapping based on an R2RML scheme, it becomes easier to access the non-RDF morphology data directly from geographic relational databases through the knowledge graph using the RDF query language. The use of R2RML provides both the ability to utilise existing functionalities in relational databases such as PostGIS and to view existing relational data in the RDF data model.

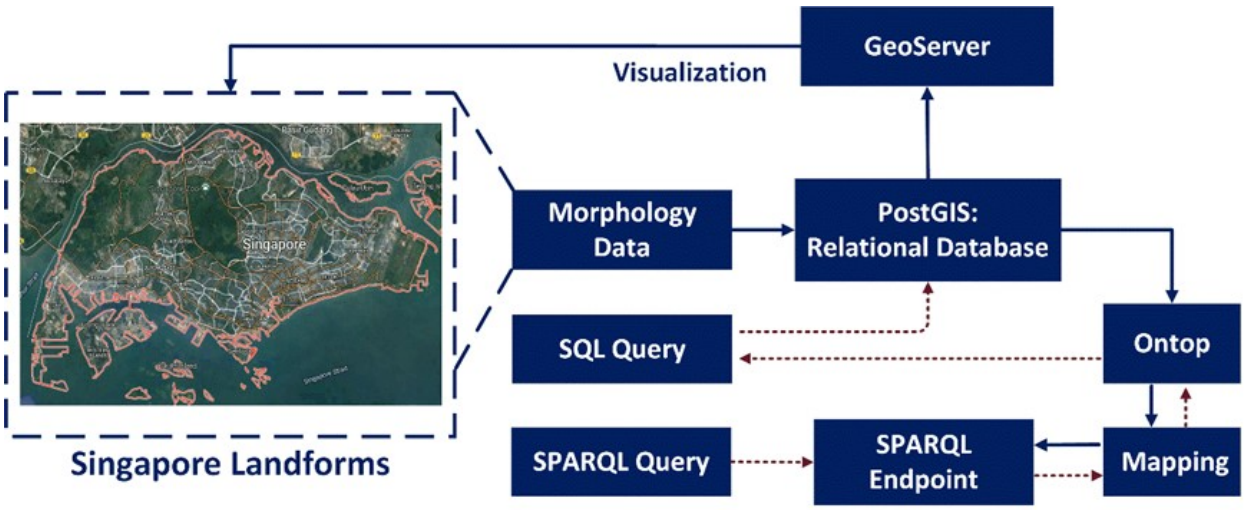


Figure 9.10: An illustration of the interaction framework between relational databases of morphology data and RDF query. Map data source: Google Maps.

4) Ignition systems for natural gas engines

Prof. Epaminondas MASTORAKOS, Dr B HARIKRISHNAN

Dr B HARIKRISHNAN (Research Fellow, CARES) has been working on turbulent reacting flows and improving the 0D – CMC (Conditional Moment Closure) code since his appointment on 9th Feb 2021.

He is also working on turbulent jet ignition (TJI) with methane-air mixture using CONVERGE CFD, intending to see the influence of the flow and the geometrical parameters on its performance. Setup involves a constant volume adiabatic combustion chamber with the prechamber (PC) (~12 cm^3) and the main chamber (MC) (~176 cm^3). The unsteady Reynolds-averaged Navier-Stokes (URANS) is used to model the turbulent mixing. Turbulent flame interaction is resolved with complete chemistry using the GRI-Mech 3.0 reaction mechanism for methane combustion in air. The combustion chamber is operating at P = 1atm, T = 300K and equivalence ratio phi = 1. The results show three phases in flow behaviour as observed in the 2D DNS simulation by *Benekos et al. 2021* – entry of unburned fuel from PC to MC (phase 1), burned gases from PC to MC (phase 2), and flow reversal from MC to PC (phase 3). The heat release rate shows rapid combustion of main chamber fuel after being injected with the hot turbulent jet. The total heat release value is ap-

proximately 486 J (total added heat ~ 514 J). The pressure evolution also corroborates with the qualitative results. The future direction of this work will be to test with varying nozzle diameters, turbulence levels, and equivalence ratios, and see its effect on flame quenching.

Additionally, Dr Harikrishnan is developing a massively parallel chemistry solver that can exploit the GPUs for faster computation in reacting flows.

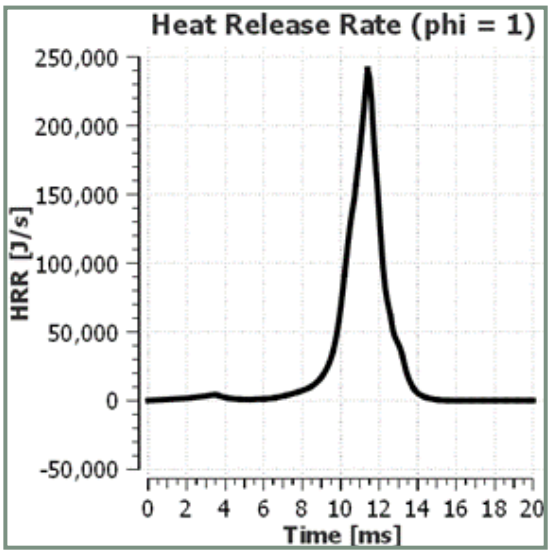


Figure 9.11: Instantaneous heat release from the constant volume chamber

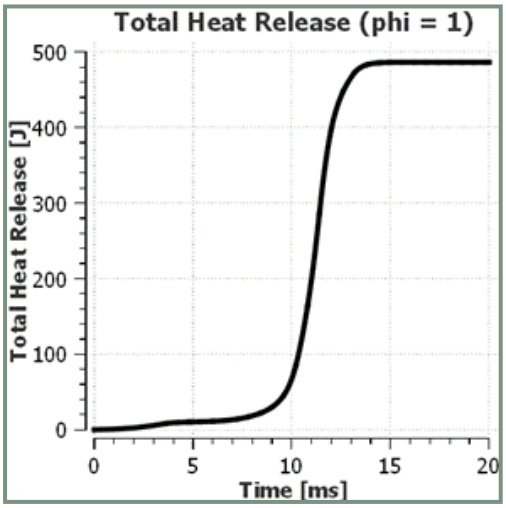


Figure 9.12: Cumulative heat release

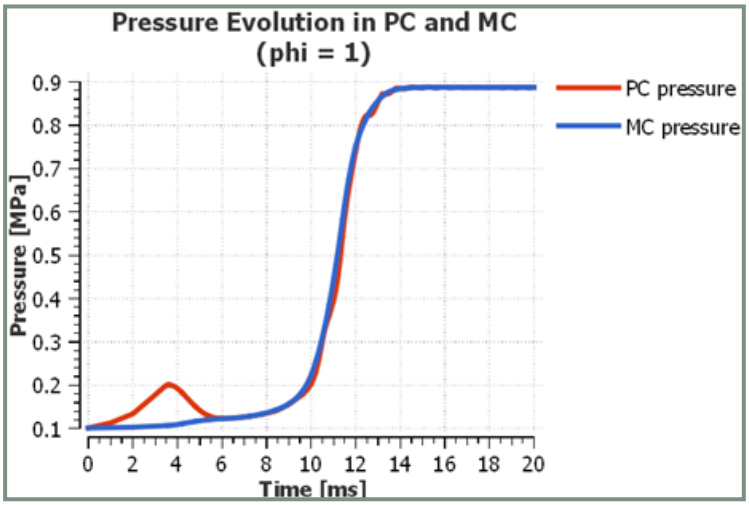


Figure 9.13: Pressure evolution in PC and MC

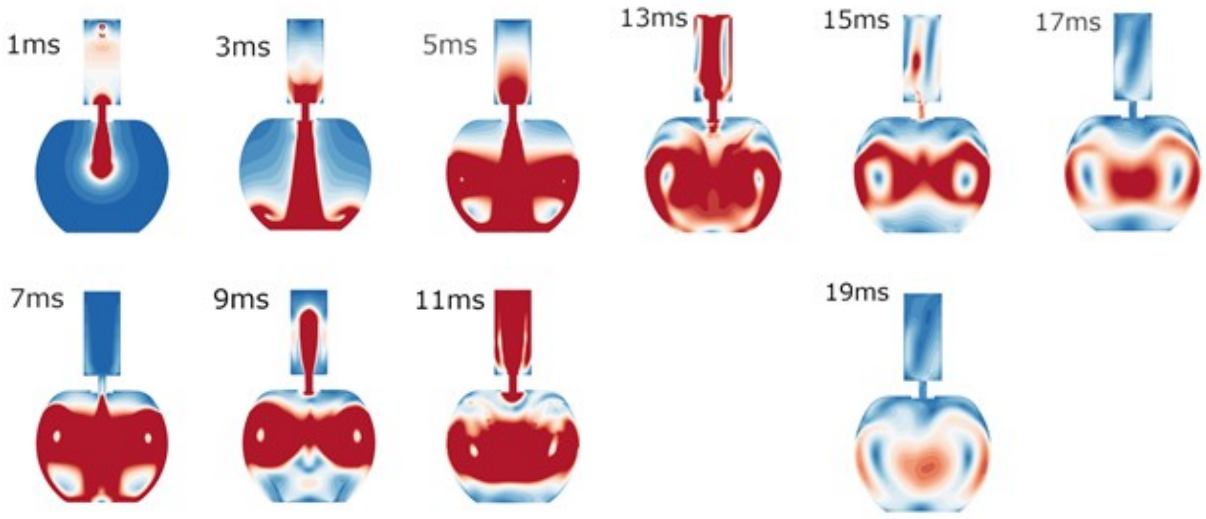


Figure 9.14: Snapshot of the velocity magnitude displaying three phases during the combustion process.

5) Future marine economy

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

A paper titled "A Comparison of Alternative Fuels for Shipping in Terms of Lifecycle Energy and Cost" has been published on December 2021 summarising the progress of this project. In this paper, 22 fuel pathways were compared in terms of quantifiable parameters including (i) fuel mass, (ii) fuel volume, (iii) life cycle (Well-To-Wake—WTW) energy intensity, (iv) WTW cost, (v) WTW greenhouse gas (GHG) emission, and (vi) non-GHG emissions. Based on the result of comparison, 9 fuel pathways were selected for fleet-level analysis whereby the selection was based on the score of the fuel, refer to Figure 9.15 for the score of various alternative pathways. The selected fuels are heavy fuel oil (HFO) as reference fuel, liquefied natural gas (LNG), HFO and LNG with on-board carbon capture (CCS), biodiesel, bio-methanol, natural gas-based hydrogen, ammonia, and electricity. In the next stage of study, fleet-level analysis will be carried out to study the potential of the selected fuels as marine fuel for tankers, cargo ships, and container ships.

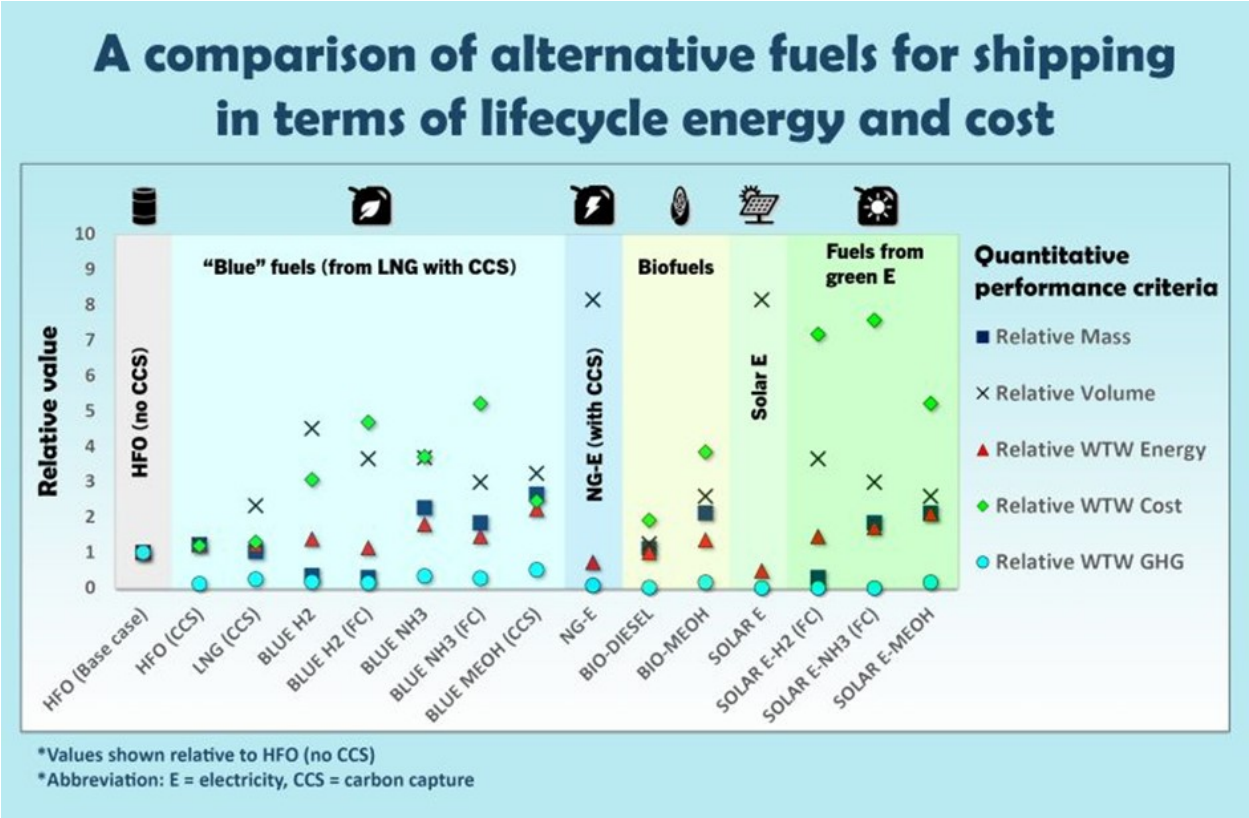


Figure 9.15: A comparison of alternative fuels for shipping in terms of lifecycle energy and cost.

6) Carbon reduction strategies of top chemical companies

Prof. S. VISWANATHAN, Dr Abhiruchi GADGIL

The team are analysing three hard-to-abate sectors based on the S&P global datasets they procured in November 2021. The comparison is being made based on emissions, carbon earnings at risk considering different carbon tax scenarios, and status in or out of alignment with the Paris Agreement goals of 1.5 degrees and 2 degrees.

They are also analysing different technological advancements toward GHG reduction in oil and gas, cement, and the steel industry. Energy efficiency improvements are one of the immediate goals for companies working toward decarbonisation. The variation in technological advancements across the sector is a good source of insight into their decarbonisation pathways. A manuscript for the same is in the works and will be submitted in the next few months.

7) Decarbonisation of Singapore by 2050

Asst Prof. Paul LIU, Prof. Markus KRAFT, Dr Erika LORENZ-CALDERON

Dr Erika LORENZ-CALDERON's (Senior Research Fellow, NTU) main research lies in reducing carbon emissions by developing a 2050 roadmap towards achieving, at least partially, a carbon-circular economy in Singapore. Dr Lorenz -Calderon's work aims to project and develop solutions to decarbonise Singapore, especially, in the chemical sector in Jurong Island, as well as in the power, transport, buildings, and household sectors. For the purpose to understand the Singapore CO_2 emission landscape, she and her team will use a digitalised tool of the real world developed by CARES called knowledge-graph.

For developing the roadmap until 2050, she has recently started analysing the chemical sector until 2030 and found that the main subsectors that highly emit CO_2 are: chemical, petroleum refining, and semiconductor subsectors. Additionally, she has found that by using basic and emerging technologies in the chemical subsector, 12.9% of energy use can be reduced by 2030. From that 12.9%, 49% comes from furnaces and 21% from steam boilers and steam systems. Similarly, in the petroleum refining subsector, 22.6% of energy use can be reduced by 2030. From that 22.6%, 67% comes from furnaces and 16% from steam boilers and steam systems. Lastly, in the semiconductor subsector, 33.1% of energy use can be reduced by 2030. From that 33.1%, 33% comes from air-conditioning and mechanical ventilation (ACMV) and 29% from industry-specific processes. Finally, an initial projection until 2050 on the estimation of CO_2 values at constant CAGR (2016 -2050) (2.69%) showed a tendency to increase within 49.2 $MtCO_2e$ in 2016 and 121.6 $MtCO_2e$ in 2050.

The one-hectare floating solar PV test bed on Tengeh Reservoir.

Source: Solar Energy Research Institute of Singapore.

8) Reaction Pathways of Formic Acid Conversion

Asst Prof. Paul LIU, Dr Mingwu TAN

Dr Mingwu TAN's (Research Fellow, NTU) main research interest lies in the study of formic acid dehydrogenation reaction. Recently, he has been focusing on exploring the reaction pathway of formic acid conversion in both aqueous and gas phases. His results show that the prepared TiB_2 catalyst has a certain activity during formic acid conversion. The catalyst activity significantly increased with loading Pd. His investigations demonstrated that formic acid conversion over TiB_2 or Pd/TiB_2 in aqueous phase was achieved through dehydrogenation reaction. However, formic acid conversion in gas phase over TiB_2 can be achieved through dehydrogenation and dehydration reaction. With supported Pd, Pd/TiB_2 could significantly enhance H_2 production rate due to improvements in dehydrogenation. His research provides a fundamental understanding of hydrogen production from formic acid dehydrogenation reaction.

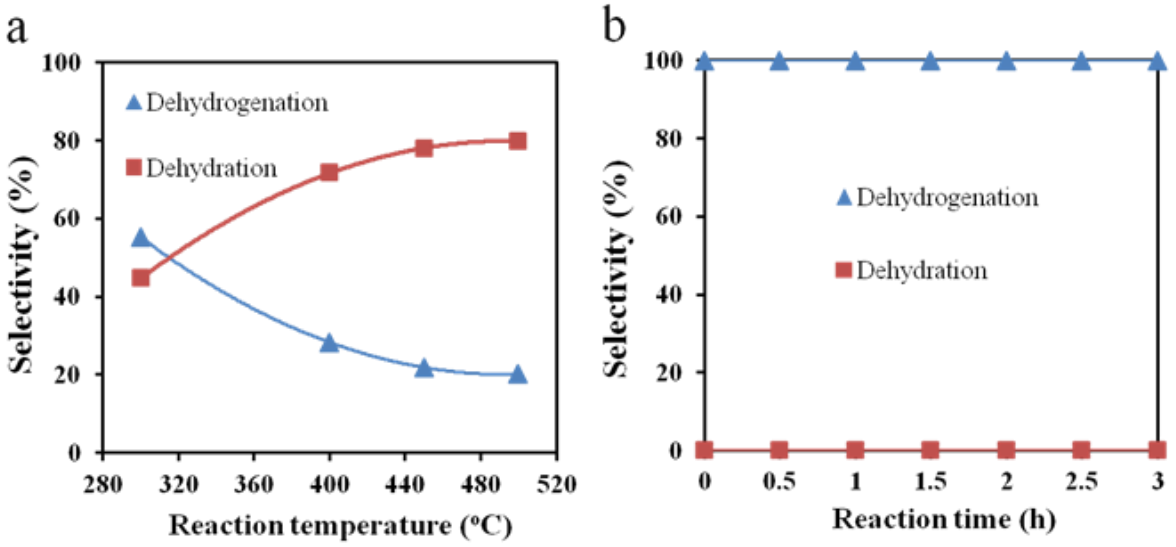


Figure 9.16: Reaction pathway of formic acid conversion over Pd/TiB_2 in (a) gas phase and (b) aqueous phase.

9) Electrified Chemical Production

Prof. Jason XU Zhichuan, Dr Adrian FISHER, Dr CHEN Yubo

Metal leaching during water oxidation has been typically observed in conjunction with surface reconstruction on perovskite oxide catalysts, but the role of metal leaching at each geometric site has not been distinguished. Here, we manipulate the occurrence and process of surface reconstruction in two model ABO_3 perovskites, i.e., $SrSc_{0.5}Ir_{0.5}O_3$ and $SrCo_{0.5}Ir_{0.5}O_3$, which allow us to evaluate the structure and activity evolution step by step. The occurrence and order of leaching of Sr (A-site) and Sc/Co (B-site) were controlled by tailoring the thermodynamic stability of B-site. Sr leaching from A-site mainly generates more electrochemical surface area for the reaction, and additional leaching of Sc/Co from B-site triggers the formation of a honeycomb-like IrO_xH_y phase with a notable increase in intrinsic activity. A thorough surface reconstruction with dual-site metal leaching induces an activity improvement by approximately two orders of magnitude, which makes the reconstructed $SrCo_{0.5}Ir_{0.5}O_3$ among the best for water oxidation in acid.

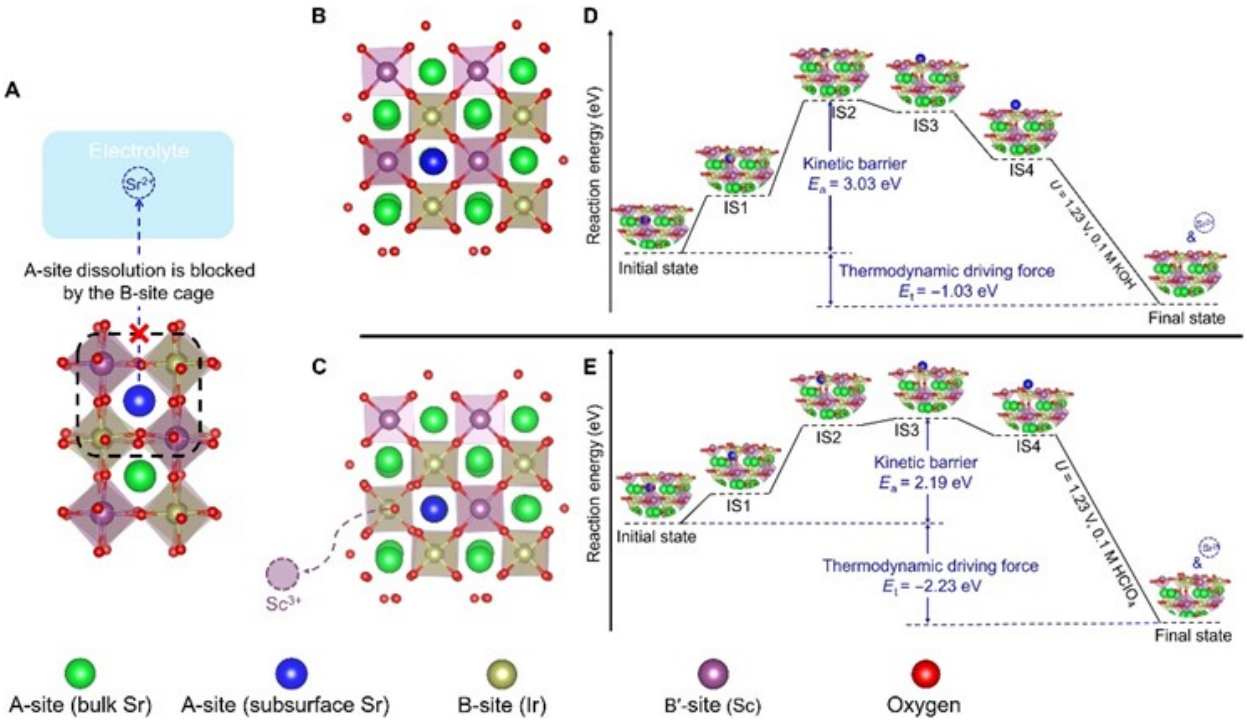


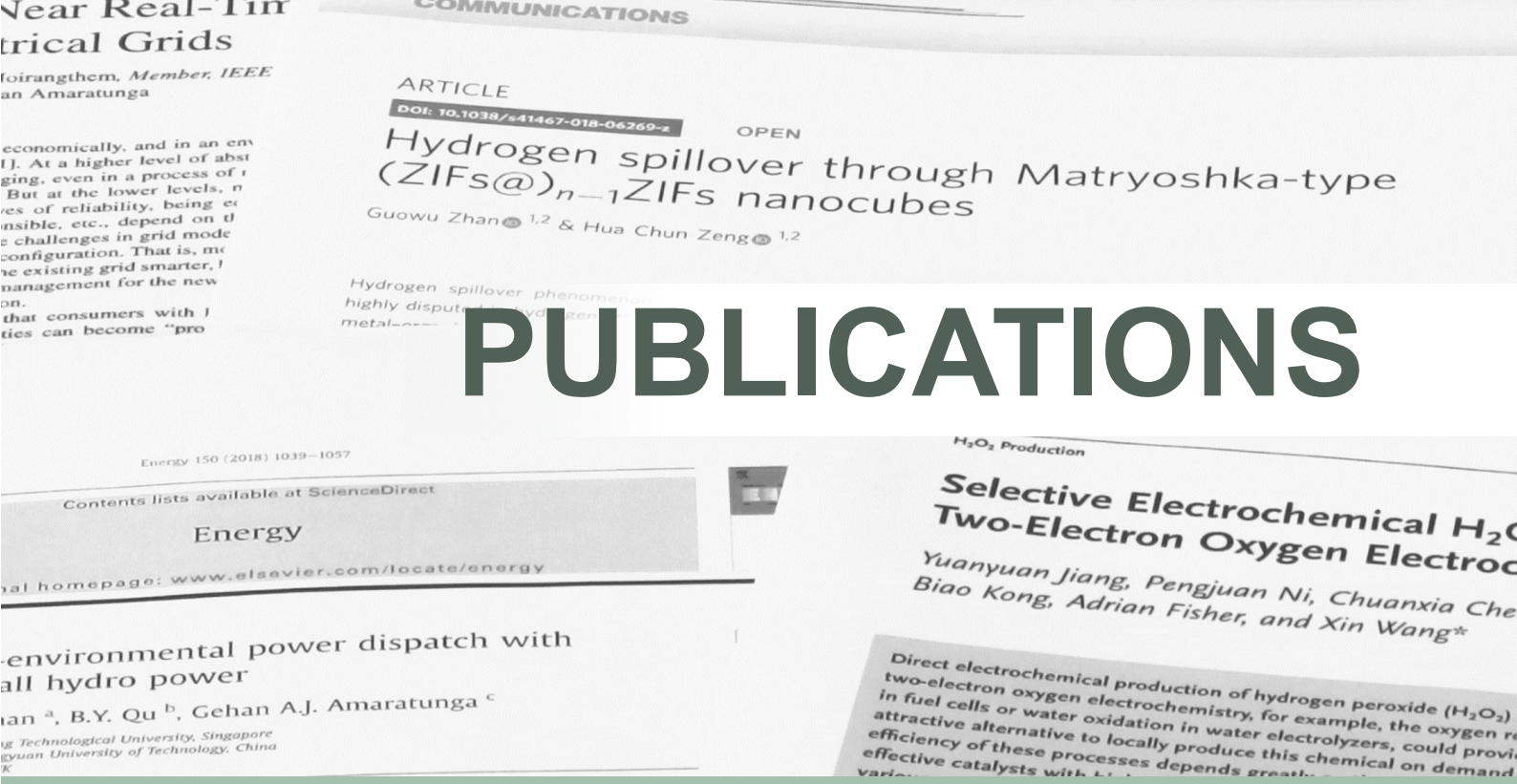
*Figure 9.17: Theoretical prediction of model perovskites' surface stability. (**A**) The schematic shows the dissolution of A-site Sr (the blue ball) from the subsurface layer of SSI to electrolyte which can be kinetically blocked by the cage composed of B-site (Ir/Sc) octahedra. The Sr atom away from the surface is considered as bulk Sr (the green ball). (**B** and **C**) Surface of SSI without (B) and with (C) a B-site (Sc) vacancy. (**D** and **E**) Energy diagrams that illustrate the dissolution of A-site (Sr) from the subsurface of SSI without (D) and with (E) a B-site (Sc) vacancy. In (B) to (E), for a better illustration, only the selected subsurface Sr atom, which migrates to the outer surface, is marked with blue colour. All the rest of subsurface Sr atoms are marked with green colour.*

10) Construction of isolated metal sites for selective electrocatalytic production of H_2O_2

Prof. WANG Xin and Dr ZHANG Hongwei

Dr ZHANG Hongwei (Research Fellow, NTU) has made great efforts to the development of novel electrocatalysis for renewable carbon utilisation. His recent focus has been on the design of excellent MOF based carbon electrodes with specially designed active sites. Thanks to versatile properties of various linkers in MOF, the structure and active sites can be finely controlled. The coordination and surrounding chemical environment of single atoms can be varied to achieve a significant performance for electrocatalysis CO_2 reduction to C1 or C2 fine chemicals. He has made progress on the design of special electrocatalysts with novel active sites. The characterisation and fundamental illustration are ongoing. Subsequently, CO_2 reduction performance will be carried out to examine its activity and stability. The breakthrough in catalyst design and application with special active sites will shine a light and inspire other scientists in the research field of electrocatalysis.

He also presented a poster (virtual) titled "Cascade Meerwein–Pondorf–Verley Reduction and Dehydration of 4'-Methoxypropiophenone to Anethole Over Zr-based catalysts" at the 4th Chemistry National Meeting (ChnmSG4) in Singapore on 15 September 2021.



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 2 and EOF

- **Li, Haiyan, Yubo Chen, Justin Zhu Yeow Seow, Chuntai Liu, Adrian C. Fisher, Joel W. Ager, and Zhichuan J. Xu. 2022. 'Surface Reconstruction of Perovskites for Water Oxidation: The Role of Initial Oxides' Bulk Chemistry'. Small Science 2 (1): 2100048. https://doi.org/10.1002/smsc.202100048.**

IRP 4 and IRP BB

- **Law, Li, Beatrice Foscoli, Epaminondas Mastorakos, and Stephen Evans. 2021. 'A Comparison of Alternative Fuels for Shipping in Terms of Lifecycle Energy and Cost'. Energies 14 (24): 8502. https://doi.org/10.3390/en14248502.**

IRP JPS and PIPS

- **Bai, Jiaru, Liwei Cao, Sebastian Mosbach, Jethro Akroyd, Alexei A. Lapkin, and Markus Kraft. 2022. 'From Platform to Knowledge Graph: Evolution of Laboratory Automation'. JACS Au 2 (2): 292–309. https://doi.org/10.1021/jacsau.1c00438.**

IRP JPS and CEUS

- **Savage, Thomas, Jethro Akroyd, Sebastian Mosbach, Michael Hillman, Franziska Sielker, and Markus Kraft. 2022. 'Universal Digital Twin – the Impact of Heat Pumps on Social Inequality'. Advances in Applied Energy 5 (February): 100079. https://doi.org/10.1016/j.adapen.2021.100079.**

IRP 1 and IRP 3

- **Liu, Guanyu, Parvathala Reddy Narangari, Quang Thang Trinh, Wenguang Tu, Markus Kraft, Hark Hoe Tan, Chennupati Jagadish, et al. 2021. 'Manipulating Intermediates at the Au–TiO2 Interface over InP Nanopillar Array for Photoelectrochemical CO_2 Reduction'. ACS Catalysis 11 (18): 11416–28. https://doi.org/10.1021/acscatal.1c02043.**

C4T IRP 1: Sustainable reaction engineering

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- **Kanwat, Anil, Biplab Ghosh, Si En Ng, Prem J. S. Rana, Yulia Lekina, Thomas J. N. Hooper, Natalia Yantara, et al. 2022. 'Reversible Photochromism in ⟨110⟩ Oriented Layered Halide Perovskite'. ACS Nano 16 (2): 2942–52. https://doi.org/10.1021/acsnano.1c10098.**
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C4T IRP 2: Electrosynthetic pathways

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