CAMBRIDGE **CARES**

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

Biannual Research Report

October 2022 - March 2023

CAMBRIDGE CARES

CAMBRIDGE CENTRE
FOR ADVANCED RESEARCH AND
EDUCATION IN SINGAPORE LTD

Cover image

Trajectory of a human (yellow line), augmented with weather data and simulated ship emissions dispersion data.

Image by Mr Shin Zert PHUA (Software Developer, CARES, IRP JPS). *See more on page 77.*

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1 Create Way, #05-05 CREATE Tower
Singapore, 138602

enquiries@cares.cam.ac.uk
www.cares.cam.ac.uk

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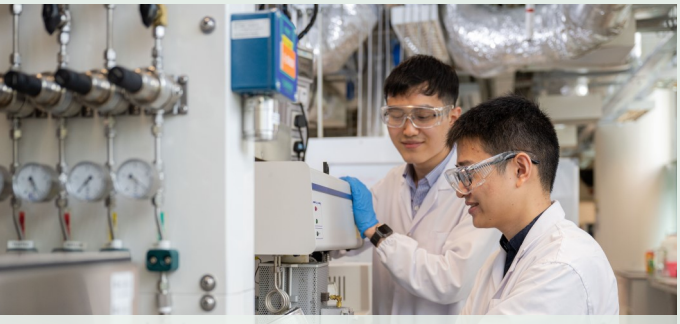
Focus on Fundamental Science



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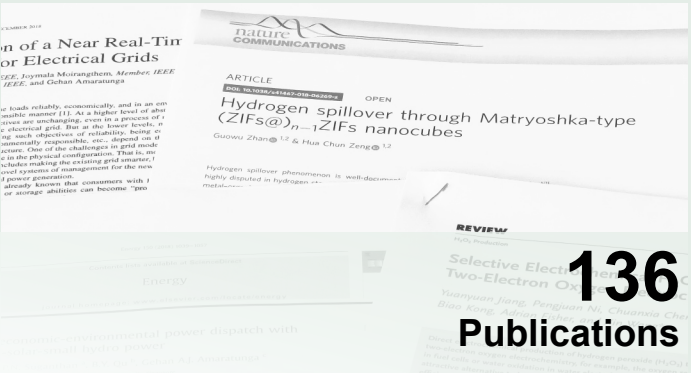

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FOREWORD

I am pleased to present the 18th Biannual Research Report for the Cambridge Centre for Advanced Research and Education in Singapore (CARES). The past six months have seen a strong relaunch of our C4T Visiting Scientists scheme with Prof Bassam Dally from KAUST delivering a talk on the future of alternative fuels in March. This was followed by Dr Molly Haugen's visit from the University of Cambridge in April. Dr Haugen presented her research (a collaboration with C4T Cambridge PI Prof Epaminondas Mastorakos and Co-I Prof Adam Boies) on using drones to measure emission plumes from ships, engagingly combining a talk and an outdoor drone demonstration. We were delighted to welcome colleagues from across the Singapore government for the drone demonstration, including representatives from the Maritime & Port Authority of Singapore, National Environment Agency and the National Climate Change Secretariat. I am thankful for the relationships we continue to forge with outstanding international researchers who are always welcome to our base in Singapore.

CLIC Expands Government Collaborations

CARES, University of Cambridge and Nanyang Technological University are celebrating the award of a further three years of funding for the Centre for Lifelong Learning and Individualised Cognition (CLIC) programme. The award will allow the team to continue their investigations into cognitive flexibility as a factor in learning throughout the human lifespan. As CLIC approaches this next phase, it is very encouraging that the group is already collaborating with the Singapore Examination & Assessment Board on a project to develop measures for inventive thinking. I am very pleased there is a strong demonstration of CARES work in real-world policy and decision-making among our diverse scientific programmes.

Online Calculator for Low-Carbon Fuels

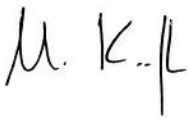
Our maritime decarbonisation group, C4T IRP4 collaborating with C4T IRP JPS have recently built an online calculator (https://lowcarbonship.com) to measure low-carbon fuels such as hydrogen and ammonia against shipping performance and design. This is a fantastic example highlighting the effective use of academic research as a tool to inform policy as we provide fact-based evidence on how ships of the future will change. The group have presented this calculator to maritime stakeholders in Singapore and will continue to incorporate their feedback to refine the tool.

A decade of CARES in Singapore

In tandem, 2023 marks ten years of my time as CARES Director and ten years of our operation in Singapore. We have plans for a public Scientific Showcase in December that will highlight a decade of achievements and past programme members. Please visit our LinkedIn Page or our website for more updates throughout the year.

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 2023



ABOUT US

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

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

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

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

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

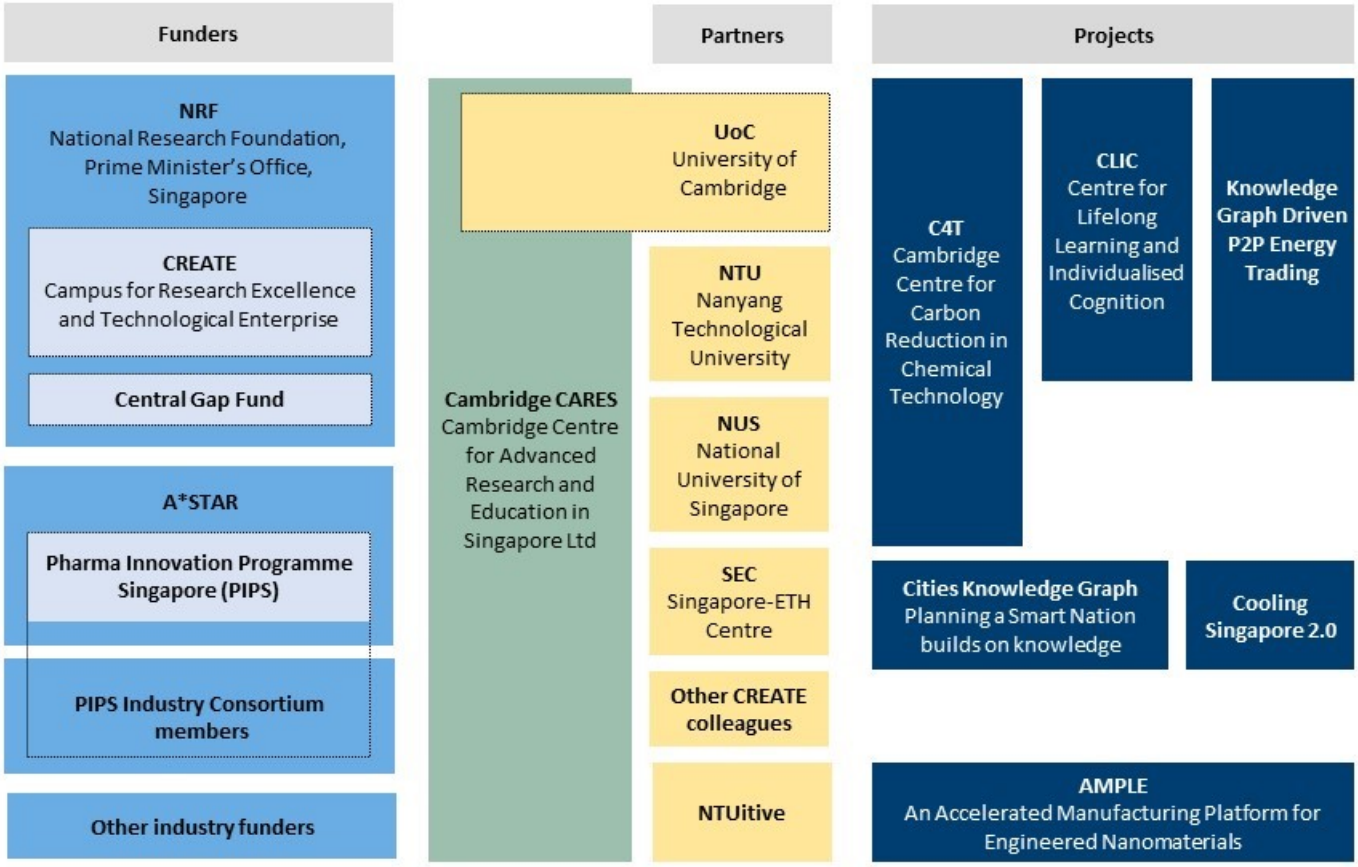
A second large CREATE-funded programme, the Centre for Lifelong Learning and Individualised Cognition (CLIC), began in October 2020. CLIC is a collaboration between University of Cambridge and NTU and focuses on the neuroscience of learning, a new research area for CARES. CLIC has recently received confirmation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

In April 2020, CARES was awarded a further Intra-CREATE large grant for Cities Knowledge Graph, which brings together researchers from University of Cambridge and ETH Zürich to

harness rapidly growing and diversifying data streams to improve the planning and design of cities. 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 this large Intra-CREATE grant, CARES is hosting AMPLE (An Accelerated Manufacturing Platform for Engineered Nanomaterials), funded by the Central Gap Fund. There are several smaller projects and spin-offs ongoing: The Intra-CREATE seed funded Knowledge Graph Driven P2P Energy Trading and Real-time Network Operation for High Renewables, and currently one ongoing stream under the Pharmaceutical Innovation Programme Singapore (PIPS) that involves 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 119.

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



HIGHLIGHTS

OUTSTANDING WORK FROM THE LAST SIX MONTHS OF CAMBRIDGE CARES RESEARCH

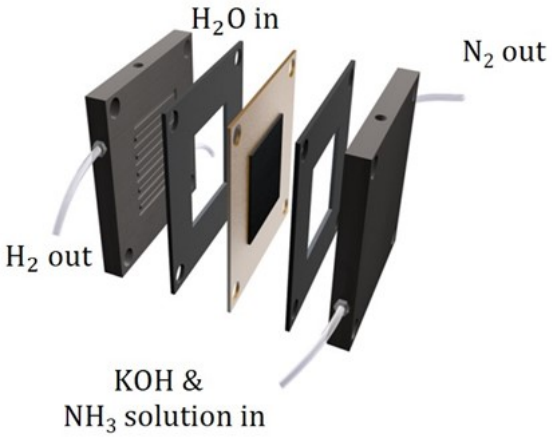
Electrochemical Approaches to Prepare Green Hydrogen

Dr Chencheng DAI, Research Fellow, C4T IRP 2

Hydrogen is an environmentally friendly and renewable chemical fuel with high energy density and zero carbon emission. It is a promising alternative to the fossil fuel and an ideal solution to the global warming issues. To date, 96% of global hydrogen is produced by petrochemical processes, including methane steam reforming and coal gasification. The increasing concerns for the depletion of fossil fuels, and the environmental issues caused by carbon emissions, have made the petrochemical processes undesirable in the long-term. Seeking a sustainable hydrogen production approach is, therefore, in urgently need.

Among various technologies for producing hydrogen, water electrolysis using electricity from renewable power sources shows great potential with near-zero greenhouse gas emission. In a conventional water electrolyser, the hydrogen is produced at the anode via hydrogen evolution reaction (HER, $2H_2O + 2e^- \rightarrow H_2 + 2OH^-$) at the cathode while the oxygen is generated through the oxygen evolution reaction (OER, $2OH^- \rightarrow 1/2O_2 + H_2O + 2e^-$) at the anode. Compared with the HER, the OER is a relatively more complicated four-electron-transfer process with intrinsically sluggish reaction kinetics and a high theoretical potential (1.23 V vs. RHE), which leads to a large overpotential to drive it and greatly reduces the energy conversion efficiency of water electrolysis. To improve the efficiency and reduce the cost of hydrogen generation through water electrolysis, we have proposed two approaches.

Firstly, we have developed a highly active OER catalyst made by spinel oxide with nickel, iron and chromium. This catalyst are earth-abundant non-noble metal oxides, with facile synthesis producing no pollutant. The surface of the transition metal oxide catalyst can be easily



An illustration of the MEA electrolyser for ammonia oxidation reaction-assisted hydrogen production.

converted to highly efficient (oxy)hydroxide, and the chromium leaching can further increase the surface area and further improve the OER performance. After loading the catalyst in a membrane electrolyte assembly, it shows better performance than most of the benchmark catalyst.

Another solution is to replace the OER with thermodynamically more favorable small molecule oxidation reactions, and one of the candidates is ammonia, of which the standard potential is only 0.06 V. In addition, it is the second largest commodity chemical worldwide with easy accessibility. We have investigated the possibility of coupling ammonia oxidation reaction (AOR) with HER, where AOR occurs at the anode to produce nitrogen as anode, and overall ammonia is electrochemically cracked into nitrogen and hydrogen. At an industrial-level current density of 200 mA cm^{-2}, the electricity consumption has reduced by ca. 60% for hydrogen generation from ammonia e-cracking compared with from water electrolysis in our first work.

In conclusion, these two inventions developed two environmentally friendly electrochemical hydrogen production methods that are highly active, energy-efficient, with zero GHG emission, and without the need of high temperature, pressure, and complicated equipment. These advantages perfectly suit the requirement for decentralised and on-demand hydrogen production, and can provide solutions to the global climate and energy crisis.

More information on Chencheng Dai's work can be found on page 42 of the report.

Dr Chencheng Dai obtained his bachelor's degree from the Department of Polymer Materials and Engineering at the Beijing University of Chemical Technology (BUCT) in 2011. He received his PhD investigating the electrochemical sensors from the Department of Chemical Engineering and Biotechnology at the University of Cambridge under the supervision of Prof Adrian Fisher in 2016. He is now a Research Fellow at CARES, through Nanyang Technological University in the group of Prof Jason Zhichuan Xu.

Keeping it cool in smart cities: Optimising a district heating system with artificial intelligence

Mr Markus HOFMEISTER, PhD student, IRP JPS

Energy prices for district heating are currently on the rise in Germany as with many places around the world. However, a municipal utility company is sparing its customers from this thanks to its adoption of an AI-supported heat generation system. The town of Pirmasens in Germany became the test site for Computational Modelling Pirmasens GmbH (CMPG) to develop AI-driven solutions to streamline citywide processes.

CMPG started collaboration with CARES in 2022 to optimise both cost and resource efficiency for a district heating system of a mid-size German town. The aim was to implement a software to describe district heating in Pirmasens within the dynamic knowledge graph framework known as the World Avatar (TWA) which IRP JPS researchers are currently developing. The success of this optimisation could provide the proof-of-concept for knowledge graph-based control problems using TWA and other AI-driven implementation in different markets.

Given the complexity of interoperability in smart cities, intelligent autonomous software agents are key to foster fact-based decision making and automation in an ecosystem of ever-growing data. The way the system works is that heat generation is optimised hierarchically based on merit-order principle. Electricity generators are ranked according to their marginal costs with low-cost generators being dispatched first. Data-driven models and AI enabled day-ahead forecasts are used to predict future energy demand and simulate system behaviour. These processes are embedded in a predictive framework to allow the system to incorporate recent information and react promptly to disturbances.

The city of Pirmasens in Germany provides district heating to hundreds of customers by sourcing heat from a combined-heat-and-power gas turbine, conventional heat boilers, and a waste incineration plant.

The effectiveness of these AI solutions resulted in a 45% reduction in gas usage, a 23% decrease in heat generation costs, and a reduction of 3,500 tonnes of CO_2 emissions annually. According to Christoph Dörr, Managing Director of the municipal utilities of Pirmasens, the calculations made by Professor Kraft and his team can predict how to produce the cheapest district heating 24 hours in advance. The cost savings made by this optimisation will be passed on to Pirmasens' customers in the form of stable tariffs.

This work has won a Smart 50 Award from the Smart Cities Connect Conference and Expo which honours the most innovative and influential global projects for smart cities. TWA offers great potential in the context of disaster management as it connects a variety of heterogeneous sources and cascades the potential consequences of imminent environmental hazards. CARES is currently developing a use case for flooding scenarios for a mid-size city in the UK..

Based on open protocols and standards, AI-driven solutions can easily be applied to other towns and cities to improve resource efficiency, lower carbon emissions and significantly reduce time to market. Optimising infrastructure in Pirmasens is only the beginning for CMPG, which already works on other smart city projects in both Germany and abroad.

While district heating is not of major interest in a tropical city like Singapore, district cooling or integrated building management could offer promising application areas.

CMPG is a technology company based in Pirmasens, Germany that aims to develop artificial intelligence solutions to monitor processes and solve challenges posed to cities around the world. This work is a joint effort between CMPG, its parent company Computational Modelling Cambridge Ltd. (CMCL) in the UK, and Cambridge CARES. More information on the IRP JPS research can be found on page 74 of the report.

Mr Markus Hofmeister (pictured right) is a PhD student in the Computational Modelling group at the University of Cambridge and a member of Clare Hall College. He completed a Bachelor of Science in Process Engineering at TU Freiberg (Germany) followed by a Dipl.-Ing. in Reservoir Engineering at Montanuniversität Leoben (Austria). Before starting his PhD, Mr Hofmeister worked as a management consultant focusing primarily on the chemical and energy sector. His PhD is funded by the Cambridge CARES Studentship Scheme (C4T) and by CMCL Ltd. CMCL began over a decade ago as a spin-out from the University of Cambridge's Department of Chemical Engineering and Biotechnology and is now a fully independent entity. CARES Director, Prof Markus Kraft, is a member of CMCL's board.

Highlighted research outputs from October 2022 - March 2023

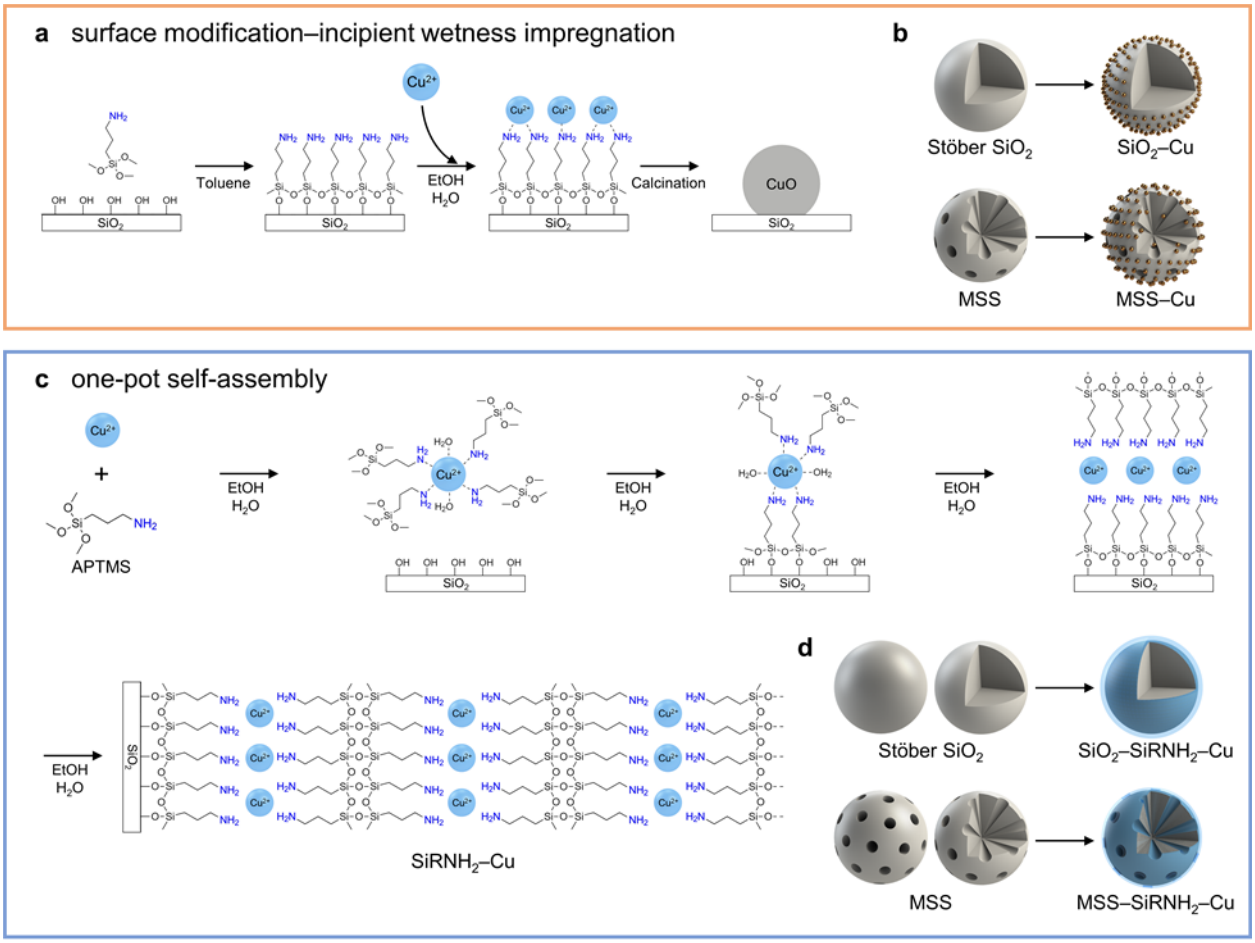
A selection of publications from across our programmes.

C4T IRP 1: Self-assembly of metal–organosilicate on porous silica substrates for efficient CO_2 hydrogenation to methanol

Yu Shao and Hua Chun Zeng, *Journal of Materials Chemistry A*

DOI: 10.1039/D2TA08830D

Abstract: CuZn-based nanocatalysts for the application of MeOH synthesis from the hydrogenation of CO_2 have been well-studied in the past few decades. However, many research endeavours have focused on individual aspects of the catalyst design such as the engineering of the support structure alone. In this study, we demonstrate the multiplying effect of an integrated design of both the active phase and support architecture. An active phase consisting of Cu–ZnO nanoparticles embedded inside a microporous silica matrix was derived from a self-assembled copper–organosilicate shell coated on a porous spherical silica support. The surface-silanol-induced self-assembly was carried out *via* simple one-pot synthesis. The obtained catalyst achieved a specific MeOH yield of 1634 mg MeOH per g Cu per h at 260 °C, 30 barg, as well as long-term stability over a 200 h on-stream operation. These results are attributed to the small Cu–ZnO nanoparticle dimensions with their decent dispersion and blending facilitating the strong metal–support interaction (SMSI) and the spatial confinement effect of the microporous silica matrix. Moreover, the appropriate silica substrate not only promoted self-assembly during the catalyst synthesis but also enhanced the fluid dynamics inside the packed bed. As a result, a higher single-pass CO_2 conversion was attained by the porous silica-supported active phase.

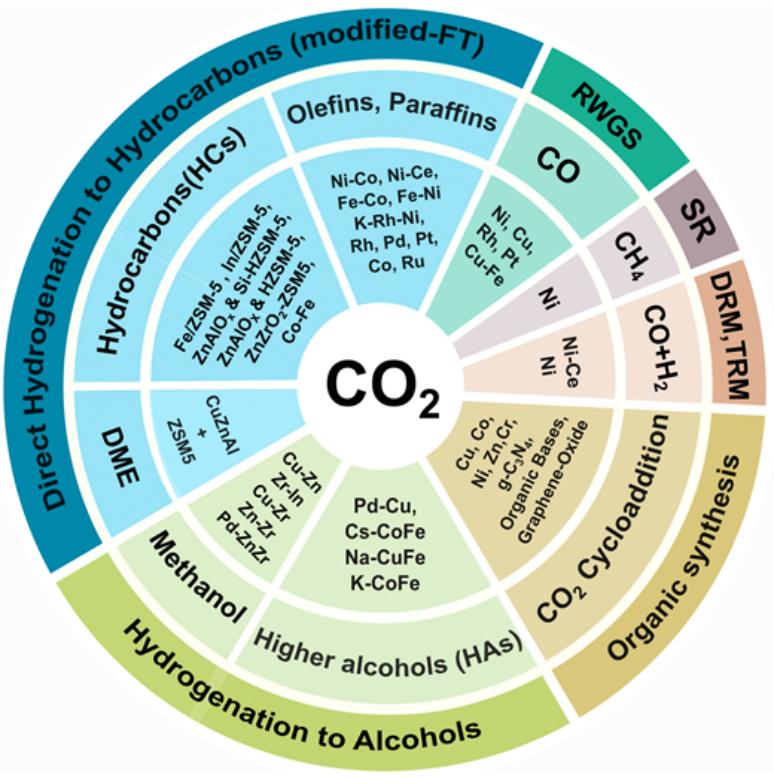


C4T IRP 1: Thermocatalytic CO_2 conversion by siliceous matter: a review

Mohammadreza Kosari, Alvin M. H. Lim, Yu Shao, Bowen Li, Kelvin M. Kwok, Abdul Majeed Seayad, Armando Borgna, and Hua Chun Zeng, *Journal of Materials Chemistry A*

DOI: 10.1039/D2TA07613F

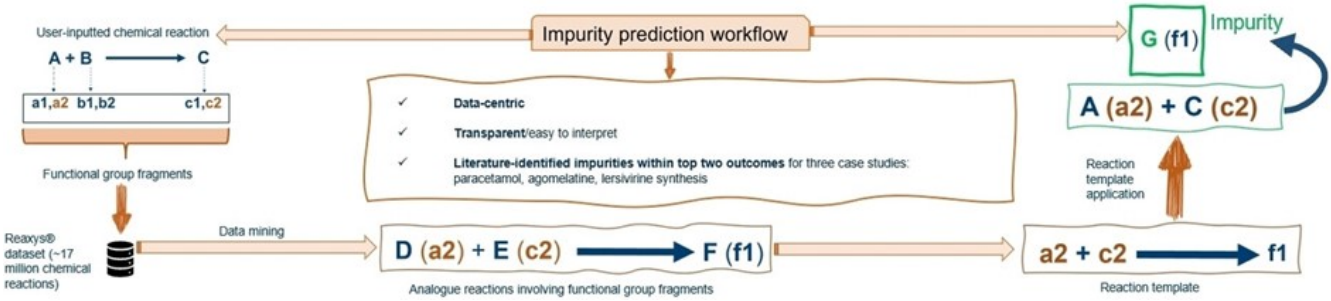
Abstract: Solid siliceous (silica/silicate) materials can substantially contribute to the strategic decarbonization and defossilization efforts based on carbon capture and utilization (CCU), where CO_2 footprint is mitigated by its capture and conversion into a wide variety of value-added chemical commodities. Targeting CO_2 utilization in particular, siliceous catalysts are widely utilized for thermal conversion of CO_2 due to their tunable porosity and morphology, ideal physiochemical properties such as high thermal resistivity, and ease of preparation by green protocols. In terms of catalytic performance and reactivity (activity, selectivity, and stability), thermocatalytic CO_2 conversion using siliceous-based catalysts is comparable to that with non-precious and precious pure metal–metal oxide catalysts, considering the inert nature of siliceous materials. Hence, in the current review, we focus on the recent advances in CO_2 conversion facilitated by conventional and advanced silica/silicate-based catalysts by reviewing and comparing proof-of-principle experiments on catalyst activity and stability for thermocatalytic CO_2 transformations. From this perspective, initially, we summarize the gas-phase thermocatalytic CO_2 reduction pathways (mainly reforming and hydrogenation) to produce C_1 and C_{2+} chemicals. Thereafter, we specifically outline the advanced design and synthesis techniques for silica/silicate-based catalysts having diverse focal, compositional, and structural features for these reactions. The categorized CO_2 reactions are then examined with respect to different subdivisions including conventional, morphology-defined, structurally-defined, and atomically-defined siliceous-based catalysts. Furthermore, after highlighting their hierarchical and porosity merits for CO_2 transformations, three important routes including CO_2 conversion to hydrocarbons, alcohols, and fine/specialty organic substances using siliceous-based catalysts are exclusively emphasized. Finally, based on our personal perspective, potential areas for improvement and further research opportunities will be proposed.



C4T IRP 1: Reaction Impurity Prediction using a Data Mining Approach

Adarsh Arun, Zhen Guo, Simon Sung, and Alexei Lapkin, *Chemistry Methods*
DOI: 10.1002/cmtd.202200062

Abstract: Automated prediction of reaction impurities is useful in early-stage reaction development, synthesis planning and optimization. Existing reaction predictors are catered towards *main* product prediction, and are often black-box, making it difficult to troubleshoot erroneous outcomes. This work aims to present an automated, interpretable impurity prediction workflow based on data mining large chemical reaction databases. A 14-step workflow was implemented in Python and RDKit using Reaxys® data. Evaluation of potential chemical reactions between functional groups present in the same reaction environment in the user-supplied query species can be accurately performed by directly mining the Reaxys® database for similar or 'analogue' reactions involving these functional groups. Reaction templates can then be extracted from analogue reactions and applied to the relevant species in the original query to return impurities and transformations of interest. Three proof-of-concept case studies (paracetamol, agomelatine and lersivirine) were conducted, with the workflow correctly suggesting impurities within the top two outcomes. At all stages, suggested impurities can be traced back to the originating template and analogue reaction in the literature, allowing for closer inspection and user validation. Ultimately, this work could be useful as a benchmark for more sophisticated algorithms or models since it is interpretable, as opposed to purely black-box solutions.

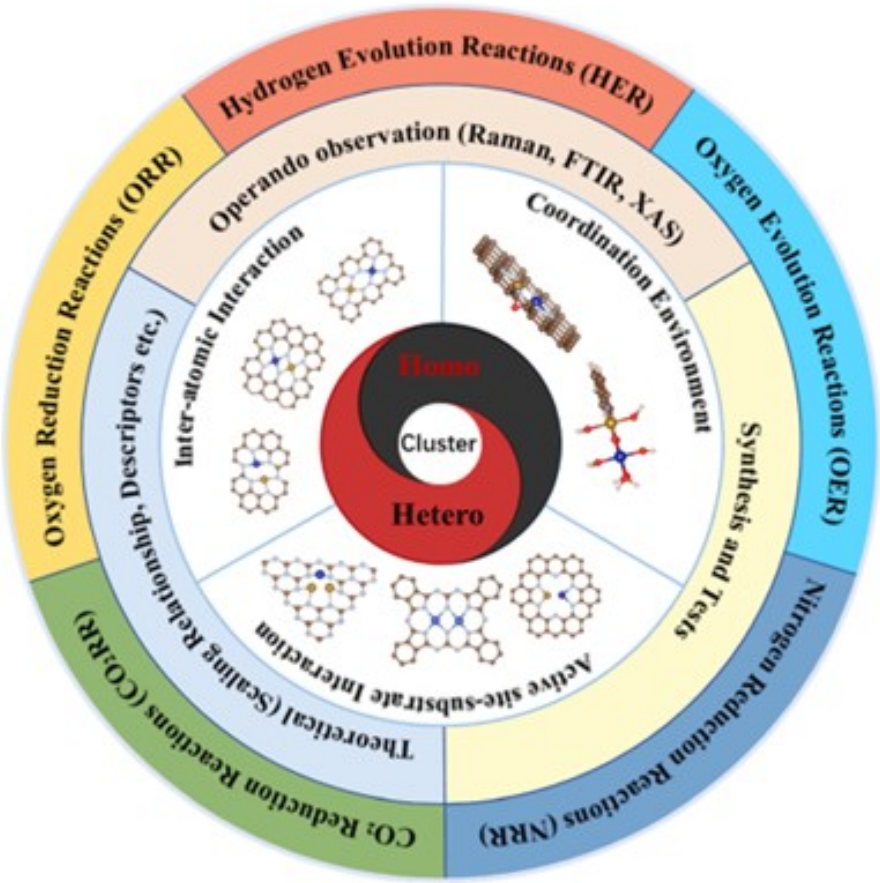


C4T IRP 2: Multi-atom cluster catalysts for efficient electrocatalysis

Libo Sun, Vikas Reddu, and Xin Wang, *Chemical Society Reviews*

DOI: 10.1039/D2CS00233G

Abstract: Multi-atom cluster catalysts have turned out to be novel heterogeneous catalysts with atomic dispersion for electrochemical energy applications. Beyond a simple combination of single-atom catalysts, they could offer boosted activity as a result of the synergistic effects between adjacent atoms. Meanwhile, the multiple active sites in the catalytic center may render them versatile binding modes toward adsorbates and provide an opportunity for catalyzing complex reactions with diverse products. Herein, a comprehensive review of the recent development of multi-atom cluster catalysts for electrochemical energy applications is provided. Specifically, the origin of synergistic effects in multi-atom cluster catalysts and related modulation methods are illustrated and summarized. The introduction of multi-atom cluster catalysts to circumvent the scaling relationships as well as their potential for developing new descriptors is then discussed. Subsequently, the methods for fabricating multi-atom cluster catalysts and related characterization techniques are reviewed. This is followed by the discussion of their application in key electrochemical reactions such as water splitting, oxygen reduction, and carbon dioxide/monoxide reduction, as well as the real-time techniques for their mechanistic study. Finally, the future challenges and opportunities concerning the improvement of multi-atom cluster catalysts are outlined, which are essential to make such electrocatalysts viable for electrochemical energy conversion.

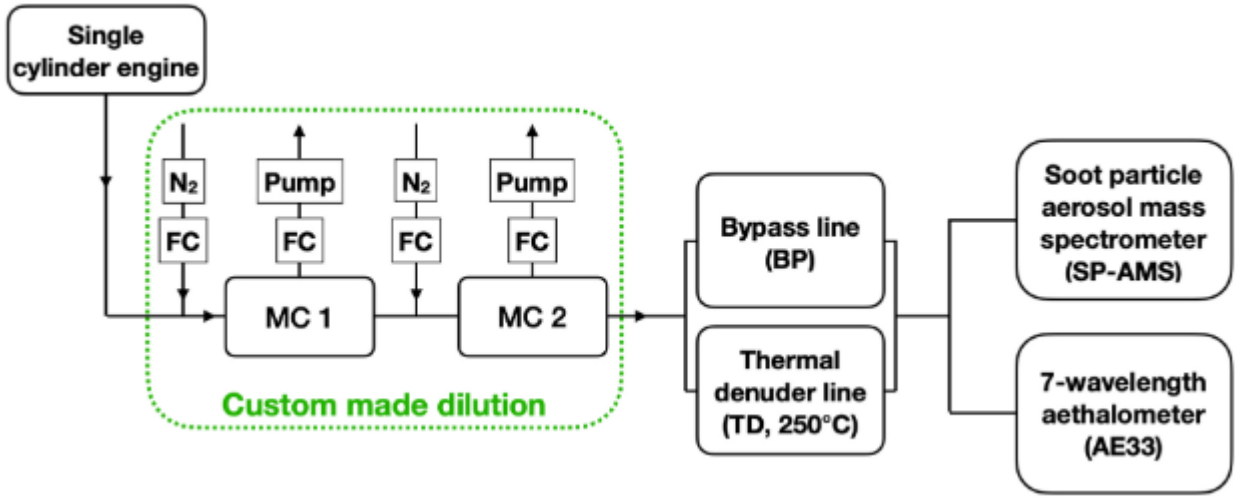


C4T IRP 3: Effects of polyoxymethylene dimethyl ether (PODEn) blended fuel on diesel engine emission: Insight from soot-particle aerosol mass spectrometry and aethalometer measurements

Mutian Ma, Laura-Hélèna Rivellini, Nethmi Kasthuriarachchi, Qiren Zhu, Yichen Zong, Wenbin Yu, Wenming Yang, Markus Kraft, and Alex Lee, *Atmospheric Environment: X*

DOI: 10.1016/j.aeaoa.2023.100216

Abstract: Polyoxymethylene Dimethyl Ether ($PODE_n$) is a promising diesel additive that can reduce particulate matter (PM) emission effectively, yet the changes in chemical and physical characteristics of PM emissions due to the application of $PODE_n$-diesel blended fuel remain largely unexplored. This laboratory study investigates the effects of $PODE_3$–diesel blended fuels (10, 20, and 30 vol% of $PODE_3$ mixed with diesel, denoted as P10, P20, and P30, respectively) on diesel engine emissions at 30% and 60% engine loads. Black carbon (BC) and organic aerosol (OA) were characterized in real time by a combination of a soot-particle aerosol mass spectrometer (SP-AMS) and a seven-wavelength aethalometer. Our results show that $PODE_3$ can significantly reduce both OA and BC emissions at both engine loads, with P20 producing the largest total PM mass reductions (>84%). The changes in the contribution of refractory oxygenated fragments to BC mass (i.e., $C_3O_2^+/C_3^+$ and C_3O^+/C_3^+) indicate that $PODE_3$ can reduce the functionality of soot surface/nanostructure. This is the first work showing that $PODE_3$ can affect the mixing state of BC and OA in diesel engine exhaust. Increasing $PODE_3$ blended volume can reduce the total fraction contribution of particle types that were composed of notably amounts of BC by mass. Furthermore, clustering analysis of single-particle data can identify two OA-dominated particle classes that were dominated by hydrocarbon fragments ($C_xH_y^+$), and one of them had higher signal contribution from high molecular weight compounds. Lastly, the absorption Ångström exponent of BC (AAE_{BC}) can be enhanced with $PODE_3$ blended volume for both engine loads, and brown carbon (i.e., a light absorbing fraction of OA) can contribute up to ~5% to the total aerosol absorption at the wavelength of 370 nm. Overall, this work provides insights into the potential impacts of $PODE_n$ blended fuel application on the chemical and optical properties of BC and OA emitted from diesel engine combustion.

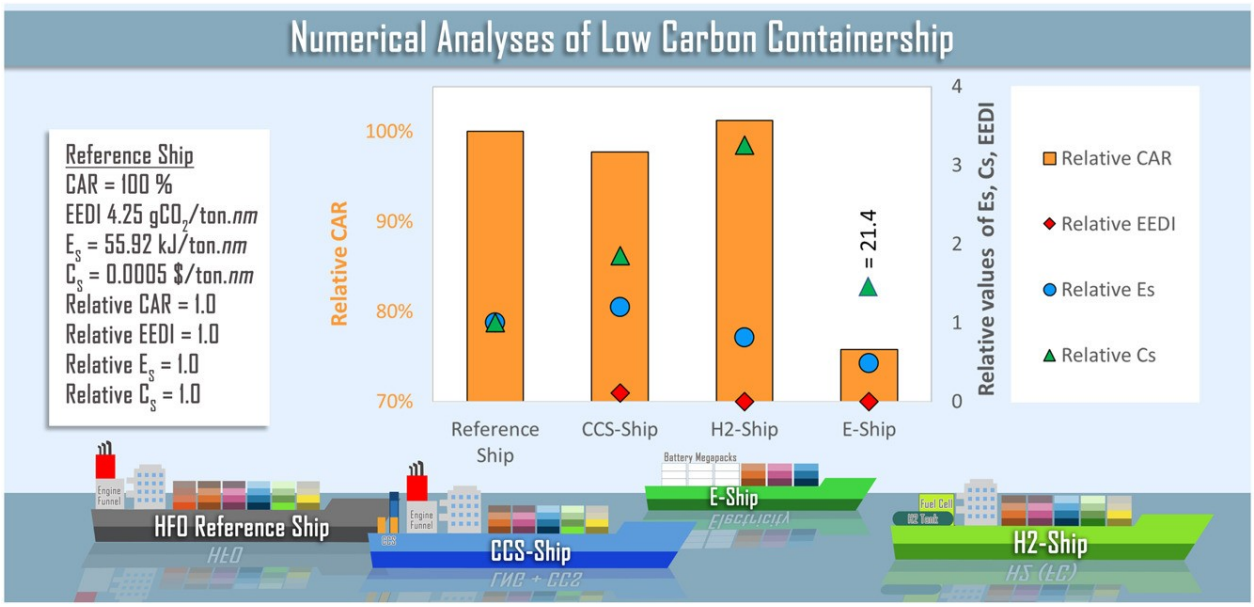


C4T IRP 4: Numerical analyses on performance of low carbon containership

Li Chin Law, Mohd Roslee Othman, and Epaminondas Mastorakos, *Energy Reports*

DOI: 10.1016/j.egyr.2023.02.035

Abstract: Onboard Carbon Capture and Storage (OCCS) was found to be a potential approach for maritime decarbonization. By using the optimized OCCS, 90% carbon capture rate was achieved with a lower regeneration duty of 3,637 MJ/ton CO_2. It was also found that with integration of waste heat recovery (WHR), the regeneration duty of CCS can be further reduced by 58.5% to 1,510 MJ/ton CO_2. Detailed numerical analyses on CCS-Ship showed that the OCCS installation onboard of the reference ship used less than 15% of the total ship length. In contrast, the E-Ship would occupy 80% of deck area for battery installation. In addition, the CSS-Ship was found to retain 97.73% of cargo, consume 66.94 kJ/ton.nm of ES, incur \$0.00093/ton.nm of CS, and improve the attained EEDI to 0.49 gCO $_2$/ton.nm, which improved the ship EEDI by 88% as compared to the ship built in year 2000-2010. Numerical analyses between various alternative fuelled-ships showed that the ship with CCS installation (CCS-Ship) was at least 1 time and 12 times more economical than hydrogen fuelled-ship (H2-Ship) and electrically propelled-ship (E-Ship) respectively. The data obtained from this research suggest that OCCS is a promising decarbonization alternative for shipping industry with relatively low cost, less than 3% capacity loss and that it achieved 88% of EEDI improvement.

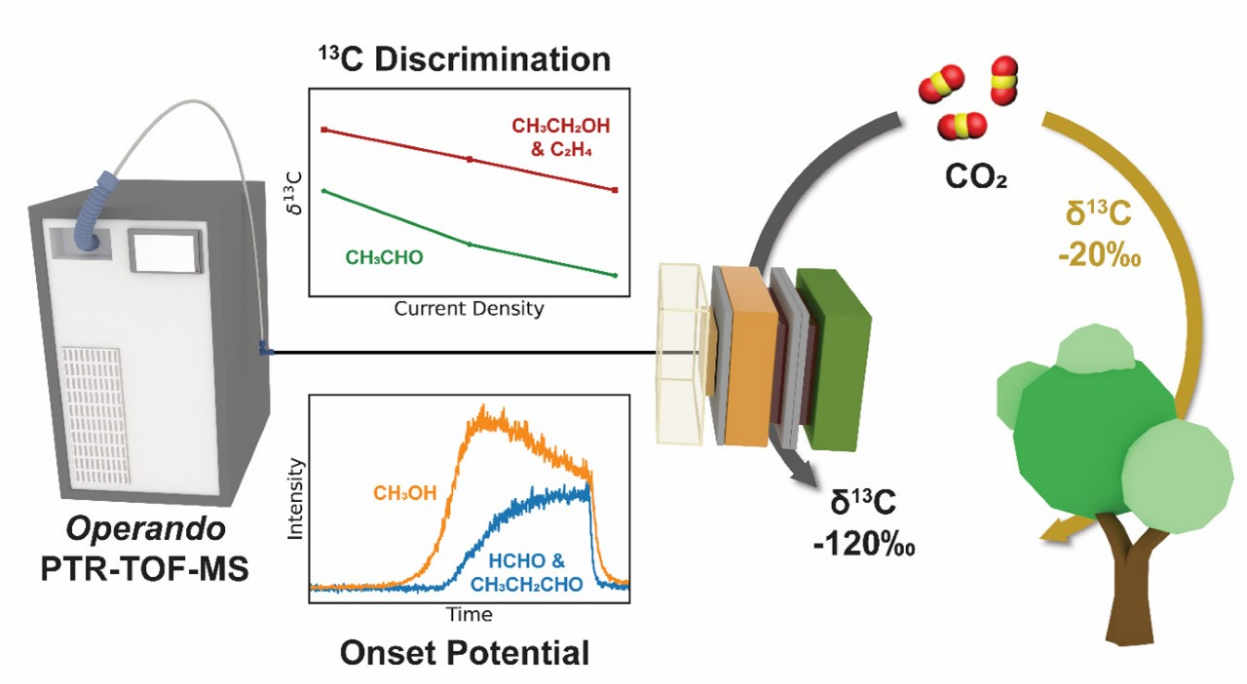


C4T IRP 1, IRP 2, IRP 3, and eCO$_2$EP: Operando proton-transfer-reaction time-of-flight mass spectrometry of carbon dioxide reduction electrocatalysis

Hangjuan Ren, Mikhail Kovalev, Zhaoyue Weng, Marsha Zakir Muhamad, Hongyang Ma, Yuan Sheng, Libo Sun, Jingjing Wang, Simon Rihm, Wanfeng Yang, Alexei Lapkin, and Joel Ager, *Nature Catalysis*

DOI: 10.1038/s41929-022-00891-3

Abstract: Electrochemical carbon dioxide reduction is a potential pathway for sustainable production of fuels and chemicals. However, the detailed catalytic mechanism in cells using high-current gas diffusion electrodes remains uncertain. Here we use proton-transfer-reaction time-of-flight mass spectrometry (PTR–TOF–MS) to perform operando analysis of intermediates and products generated by electrochemical carbon dioxide reduction in gas-diffusion-electrode-based flow cells with copper-based electrocatalysts. PTR–TOF–MS allows for sensitive detection of C_1–C_4 minor and major intermediates and products, measurement of their ^{13}C isotope composition and precise identification of onset potentials. We find that formaldehyde and acetaldehyde are not the major intermediates for formation of methanol and ethanol/ethylene, respectively, and that propionaldehyde reduction is on the major pathway for 1-propanol formation. Interestingly, the discrimination against ^{13}C in the reaction products is substantially larger than for biological CO_2 fixation in photosynthesis and Fischer–Tropsch synthesis of hydrocarbons.



C4T IRP 1 and IRP 2: Molecule Confined Isolated Metal Sites Enable the Electrocatalytic Synthesis of Hydrogen Peroxide

Xiaogang Li, Shasha Tang, Shuo Duo, Hong Jin Fan, Tej Choksi, and Wang Xin, *Advanced Materials*

DOI: 10.1002/adma.202104891

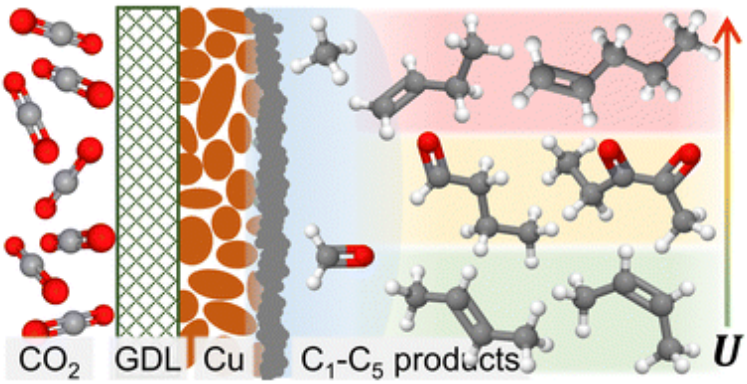
Abstract: The direct synthesis of hydrogen peroxide (H_2O_2) through the two-electron oxygen reduction reaction is a promising alternative to the industrial anthraquinone oxidation process. Selectivity to H_2O_2 is however limited by the four-electron pathway during oxygen reduction. Herein, it is reported that aminoanthraquinone confined isolated metal sites on carbon supports selectively steer oxygen reduction to H_2O_2 through the two-electron pathway. Confining isolated NiN_x sites under aminoanthraquinone increases the selectivity to H_2O_2 from below 55% to above 80% over a wide potential range. Spectroscopy characterization and density functional theory calculations indicate that isolated NiN_x sites are confined within a nanochannel formed between the molecule and the carbon support. The confinement reduces the thermodynamic barrier for OOH* desorption versus further dissociation, thus increasing the selectivity to H_2O_2. It is revealed how tailoring noncovalent interactions beyond the binding site can empower electrocatalysts for the direct synthesis of H_2O_2 through oxygen reduction.

C4T IRP 3, IRP JPS, and eCO_2EP: On the role of C_4 and C_5 products in electrochemical CO_2 reduction *via* copper-based catalysts

Simon Rihm, Mikhail Kovalev, Alexei Lapkin, Joel Ager, and Markus Kraft, *Energy & Environmental Science*

DOI: 10.1039/D2EE03752A

Abstract: Utilising carbon dioxide by synthesising commodity chemicals *via* electrocatalysis shows potential for long-term energy storage and industry decarbonisation. The latest copper-based gas-diffusion electrodes can operate at high currents, enabling large conversion rates. However, our incomplete understanding of active reaction paths in this system hinders us from designing catalysts with improved selectivities and reduced poisoning. Here, we identify and analyse ten previously unknown minor products of electrochemical CO_2 reduction. Using an ultra-sensitive GC-MS setup, we report more than 20 products, including C_5 species for the first time. From the trends in selectivity, we hypothesise two distinct reaction paths: while the coupling of oxygenated intermediates begins at very small potentials and favours double bond formation in the middle of carbon chains, coupling of highly-reduced methane precursors requires a large potential and leads to double bond formation at the chain end. This contribution represents a significant step towards the holistic comprehension of the mechanism for electrocatalytic CO_2 reduction and calls for further mechanistic exploration *via* minor products and investigation of favourable reaction conditions.



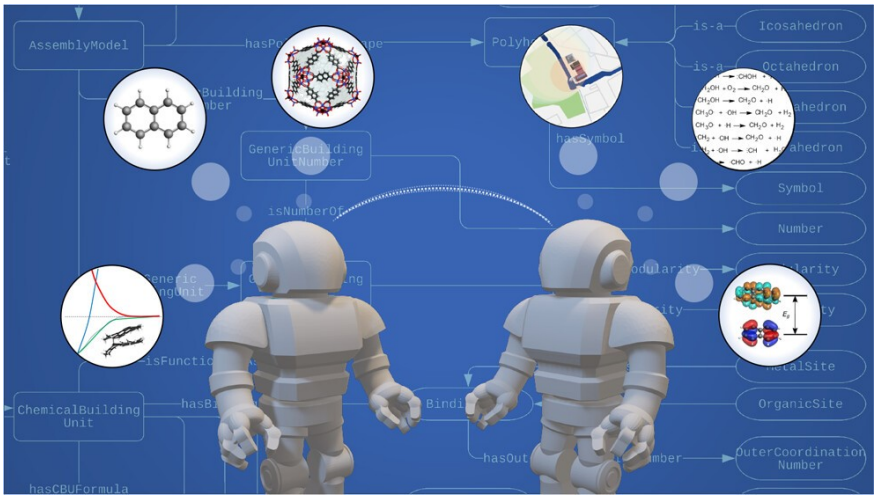
C4T IRP 3 and IRP JPS: Knowledge Engineering in Chemistry: From Expert Systems to Agents of Creation

Aleksandar Kondinski , Jiaru Bai, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft, *Accounts of Chemical Research*

DOI: 10.1021/acs.accounts.2c00617

Abstract: Passing knowledge from human to human is a natural process that has continued since the beginning of humankind. Over the past few decades, we have witnessed that knowledge is no longer passed only between humans but also from humans to machines. The latter form of knowledge transfer represents a cornerstone in artificial intelligence (AI) and lays the foundation for knowledge engineering (KE). To pass knowledge to machines, humans need to structure, formalize, and make knowledge machine-readable. Subsequently, humans also need to develop software that emulates their decision-making process. To engineer chemical knowledge, chemists are often required to challenge their understanding of chemistry and thinking processes, which may help improve the structure of chemical knowledge. Knowledge engineering in chemistry dates from the development of expert systems that emulated the thinking process of analytical and organic chemists. Since then, many different expert systems employing rather limited knowledge bases have been developed, solving problems in retrosynthesis, analytical chemistry, chemical risk assessment, etc. However, toward the end of the 20th century, the AI winters slowed down the development of expert systems for chemistry. At the same time, the increasing complexity of chemical research, alongside the limitations of the available computing tools, made it difficult for many chemistry expert systems to keep pace. In the past two decades, the semantic web, the popularization of object-oriented programming, and the increase in computational power have revitalized knowledge engineering. Knowledge formalization through ontologies has become commonplace, triggering the subsequent development of knowledge graphs and cognitive software agents. These tools enable the possibility of interoperability, enabling the representation of more complex systems, inference capabilities, and the synthesis of new knowledge.

This Account introduces the history, the core principles of KE, and its applications within the broad realm of chemical research and engineering. We first discuss how chemical knowledge is formalized and how a chemist's cognition can be emulated with the help of reasoning algorithms. Following this, we discuss various applications of knowledge graph and agent technology used to solve problems in chemistry related to molecular engineering, chemical mechanisms, multiscale modeling, automation of calculations and experiments, and chemist–machine interactions. These developments are discussed in the context of a universal and dynamic knowledge ecosystem, referred to as The World Avatar (TWA).

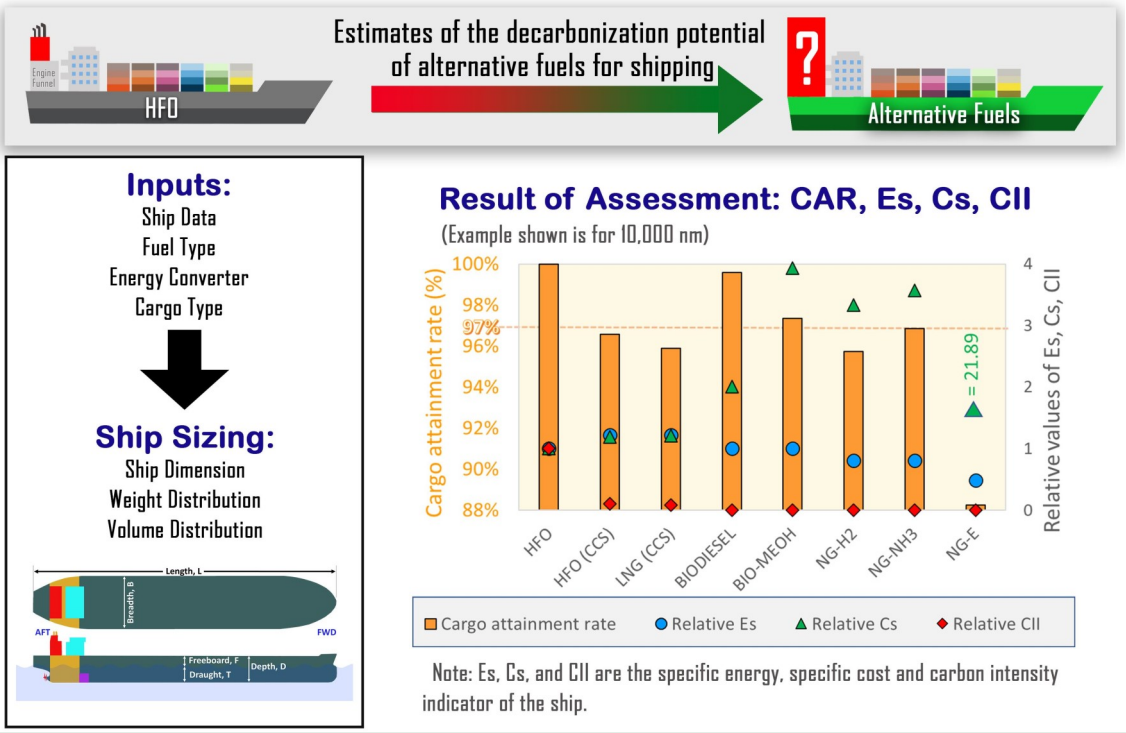


C4T IRP 4 and IRP BB: Estimates of the Decarbonization Potential of Alternative Fuels for Shipping as a Function of Vessel Type, Cargo, and Voyage

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

DOI: 10.3390/en15207468

Abstract: In this paper, HFO with CCS, LNG with CCS, hydrogen, ammonia, bio-methanol, biodiesel, and electricity were studied using empirical ship design models from a fleet-level perspective and at the Tank-To-Wake level, to assist operators, technology developers, and policy makers. The cargo attainment rate CAR, the E_S (i.e., TTW energy needed per ton*n.m.), the C_S (economic cost per ton*n.m.), and the carbon intensity index CII (gCO_2 per ton*n.m.) were calculated so that the potential of the various alternatives can be compared quantitatively as a function of different criteria. The sensitivity of CAR towards ship type, fuel type, cargo type, and voyage distance were investigated. All ship types had similar CAR estimates, which implies that considerations concerning fuel transition apply equally to all ships (cargo, containership, tankers). Cargo type was the most sensitive factor that made a ship either weight or volume critical, indirectly impacting on the CAR of different fuels; for example, a hydrogen ship is weight-critical and has 2.3% higher CAR than the reference HFO ship at 20,000 nm. Voyage distance and fuel type could result in up to 48.51% and 11.75% of CAR reduction. In addition to CAR, the E_S, C_S, and CII for a typical mission were calculated and it was found that HFO and LNG with CCS gave about 20% higher E_S and C_S than HFO, and biodiesel had twice the cost, while ammonia, methanol, and hydrogen had 3–4 times the C_S of HFO and electricity about 20 times, suggesting that decarbonisation of the world's fleet will come at a large cost. As an example of including all factors in an effort to create a normalized scoring system, an equal weight was allocated to each index (CAR, E_S, C_S, and CII). Biodiesel achieved the highest score (80%) and was identified as the alternative with the highest potential for a deep-seagoing containership, followed by ammonia, hydrogen, bio-methanol, and CCS. Electricity has the lowest normalized score of 33%. A total of 100% CAR is achievable by all alternative fuels, but with compromises in voyage distance or with refuelling. The results can guide decarbonization strategies at the fleet level and optimise emissions as a function of specific missions.



CLIC: Learning at your brain's rhythm: individualized entrainment boosts learning for perceptual decisions

Elizabeth Michael, Lorena Santamaria Covarrubias, Victoria Leong, and Zoe Kourtzi, *Cerebral Cortex*
DOI: 10.1093/cercor/bhac426

Abstract: Training is known to improve our ability to make decisions when interacting in complex environments. However, individuals vary in their ability to learn new tasks and acquire new skills in different settings. Here, we test whether this variability in learning ability relates to individual brain oscillatory states. We use a visual flicker paradigm to entrain individuals at their own brain rhythm (i.e. peak alpha frequency) as measured by resting-state electroencephalography (EEG). We demonstrate that this individual frequency-matched brain entrainment results in faster learning in a visual identification task (i.e. detecting targets embedded in background clutter) compared to entrainment that does not match an individual's alpha frequency. Further, we show that learning is specific to the phase relationship between the entraining flicker and the visual target stimulus. EEG during entrainment showed that individualized alpha entrainment boosts alpha power, induces phase alignment in the pre-stimulus period, and results in shorter latency of early visual evoked potentials, suggesting that brain entrainment facilitates early visual processing to support improved perceptual decisions. These findings suggest that individualized brain entrainment may boost perceptual learning by altering gain control mechanisms in the visual cortex, indicating a key role for individual neural oscillatory states in learning and brain plasticity.

CITIES: The conundrum in smart city governance: Interoperability and compatibility in an ever-growing ecosystem of digital twins

Hou Yee Quek, Franziska Sielker, Jethro Akroyd, Amit N Bhave, Aurel von Richthofen, Pieter Herthogs, Claudia van der Laag Yamu, Li Wan, Timea Nochta, Gemma Burgess, Mei Qi Lim, Sebastian Mosbach, and Markus Kraft, *Data & Policy*
DOI: 10.1017/dap.2023.1

Abstract: Today, technological developments are ever-growing yet fragmented. Alongside inconsistent digital approaches and attitudes across city administrations, such developments have made it difficult to reap the benefits of city digital twins. Bringing together experiences from five research projects, this paper discusses these digital twins based on two digital integration methodologies—systems and semantic integration. We revisit the nature of the underlying technologies, and their implications for interoperability and compatibility in the context of planning processes and smart urbanism. Semantic approaches present a new opportunity for bidirectional data flows that can inform both governance processes and technological systems to co-create, cross-pollinate, and support optimal outcomes. Building on this opportunity, we suggest that considering the technological dimension as a new addition to the trifecta of economic, environmental, and social sustainability goals that guide planning processes, can aid governments to address this conundrum of fragmentation, interoperability, and compatibility.

IRP 1

SUSTAINABLE REACTION ENGINEERING FOR CARBON NEUTRAL INDUSTRY

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

IRP 1 Principal Investigators:

Professor Alexei LAPKIN
University of Cambridge

Asst Professor Paul LIU Wen
Nanyang Technological University

Assoc Professor YAN Ning
National University of Singapore

OVERVIEW

IRP1 continues to work on new catalytic materials for activation of CO_2. This is done in a large collaboration on inverse catalysts design that involves the groups of Tej Choksi and Alexei Lapkin, as well as our collaborators in Canada and India. In this theme the groups of NTU and NUS are actively working on exploring reactivities towards CO_2 hydrogenation and have also started to work on ammonia cracking. In the bio-based technologies, work is continuing on creating a unique dataset of bio-based raw materials linked with their processing technologies. This will later be linked with development of bio-based overall routes to functional molecules. We have also made significant progress in creating a dataset of formulations that is needed to develop a machine learning model of formulations design. This task is creating a pathway to faster substitution of ingredients in design of formulations with their bio-based analogues.

Professor Alexei Lapkin, PI
University of Cambridge

Update on work package 1.1

Design of nano-structured catalysts

Dr Quan ZHANG (Research Fellow, NUS) has continued synthesising new catalysts for conversion of renewable resources. Very recently, he discovered an interesting catalyst with outstanding catalytic performance for ammonia cracking. The ammonia conversion can reach above 90% at 450 °C with a gas hourly space velocity of 6,000 mL/g_{cat} h, which is one of the best-reported catalysts at present. Furthermore, the structure of the catalyst was clearly revealed by using XRD, STEM-EDX and XPS analysis. The results demonstrated that the catalyst shows a novel solid-solution oxide supported metal nanoparticle structure. To clarify the mechanism of the outstanding catalytic performance, several comparison experiments were designed and performed. With the results of the controlled experiments, the catalytic activity enhancement was attributed to the novel structure of the solid-solution oxide support. His recent discovery may provide a new strategy to design highly efficient catalysts for ammonia cracking.

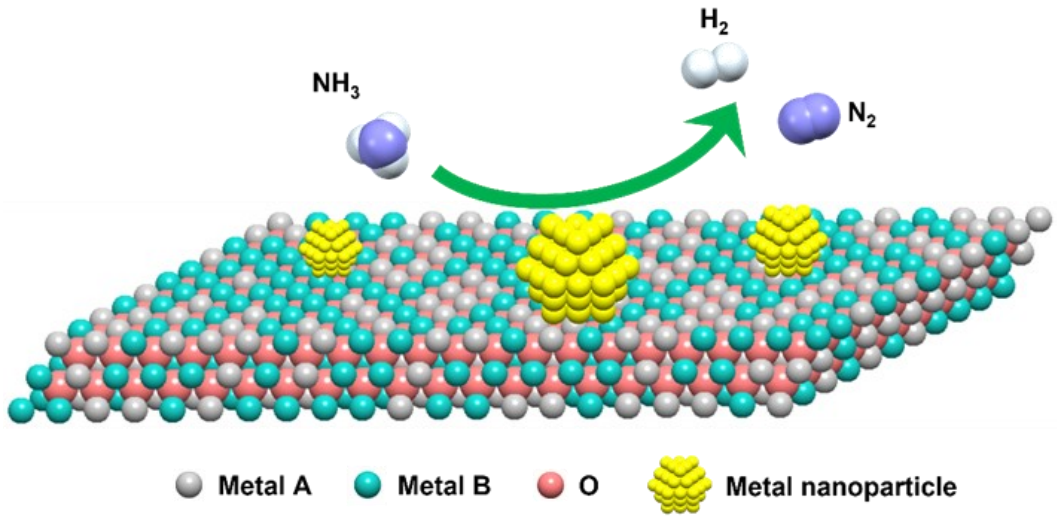


Figure 1.1: Schematic diagram of solid-solution oxide supported metal nanoparticle catalyst for highly efficient ammonia cracking

Dr Quan ZHANG

Update on work package 1.2

Novel reactions and functional molecules

Guided by **Prof Alexei LAPKIN (PI, CAM)**, **Dr Zhen GUO (Senior Research Fellow, CARES)** focused on the development of a tool for chemical route searching. Tasks have been conducted include:

1. Developed new Application Programming Interfaces (APIs) to facilitate the searching process.

2. Continue testing, building and deployment of the tool as an application.

3. Develop architectures for production version of the tool.

4. Complete the development of a reaction condition recommendation system (RCRS), which will be an additional function of the existing tool.

In addition, Dr Guo has also been working on reaction balancing and extraction of reaction templates, which is highly relevant to carbon flow along chemical transformations. Part of this work, in collaboration with **Mr Adarsh ARUN (PhD student, CAM)** has recently been published in *Chemistry Methods*.

Dr Guo will continue improving the tool for searching of chemical routes, by implementing new features that are relevant to sustainability.

Mr Aniket CHITRE'S (PhD student, CAM) has developed a semi-automated high-throughput formulations workflow, integrating different technologies and sub-domains of machine learning, such as Bayesian optimisation and computer vision, to make liquid formulations. This workflow includes the previously highlighted (in the 17th Biannual Report) self-driving titration robot, as well as a customised Opentrons OT-2 robot. After a year's work developing the hardware and software, the platforms are now being used to generate a valuable formulations dataset in collaboration with the project's industry partner (BASF). The ultimate goal is to use this dataset to develop hybrid property prediction models, which in conjunction with the demonstrated lab automation will facilitate the acceleration of formulations' R&D. So far 250+ samples have been prepared and characterised, with the goal to prepare up to 1000 samples. Mr Chitre has developed a new Design of Experiments (DoE) methodology to drive the suggested experiments towards regions of phase stability, whilst also optimising the space-filling properties of the generated dataset. The DoE strategy continues to be actively developed whilst the data-generation campaign remains underway.

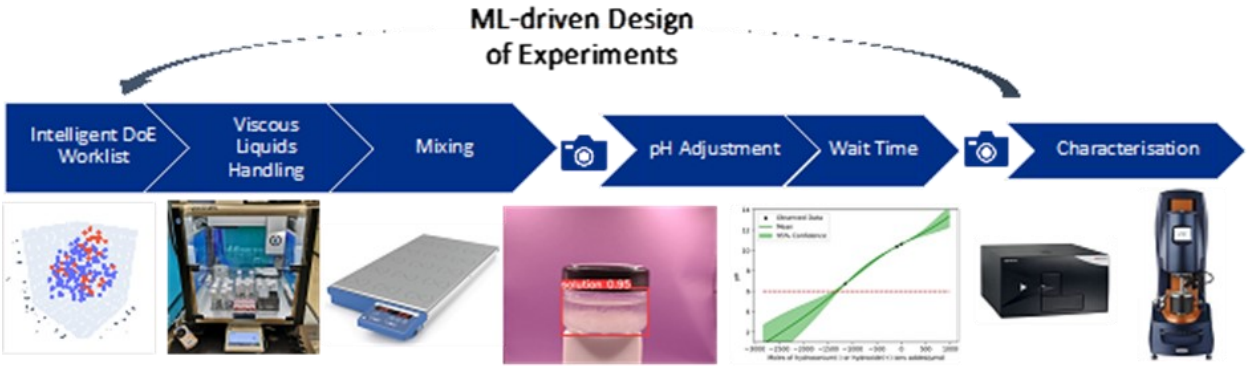


*Figure 1.2: Semi-automated high-throughput formulations workflow developed in collaboration @ IMRE, A*STAR*

Mr Aniket CHITRE

Mr Adarsh ARUN (PhD student, CAM) commenced his PhD in January 2021, and focuses mainly on identifying sustainable routes from biowaste to chemicals using networks and knowledge graphs. He has completed the development of an early-stage ontology/schema to represent the required data, integrating a variety of existing ontologies and data sources from a variety of domains (location, agronomy, reactions, processes). Over the past several months, he has been populating a preliminary knowledge graph based on the literature on common biowaste sources in Asia, including pre-treatment processes to isolate key feedstocks from biowaste. Mr Arun is now investigating thermodynamic metrics to assess the sustainability of pathways. He has also completed his work on enriching reaction networks by data mining large chemical databases such as Reaxys to predict impurities and by-products in chemical reactions. The paper has now been published in the journal *Chemistry Method* and he is continuing to liaise with potential pharmaceutical collaborators to improve the adoption of the work.

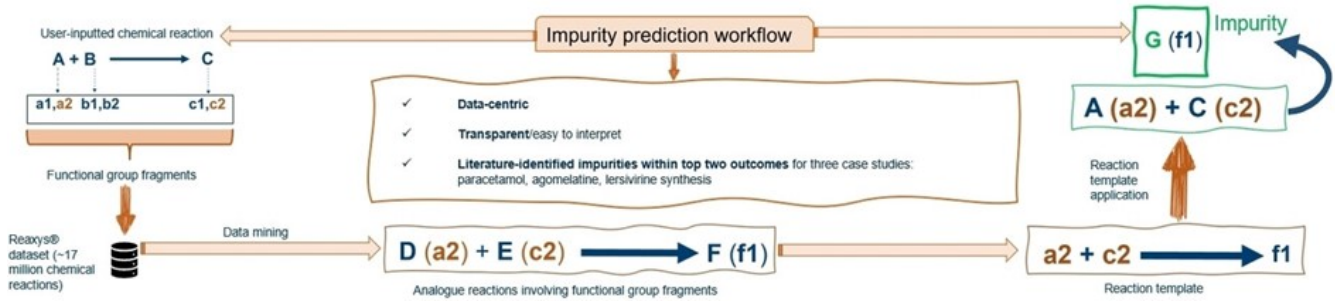


Figure 1.3: A graphical abstract of the published paper. An automated chemical reaction impurity prediction workflow is proposed, based on data mining chemical reaction databases (Reaxys®). The workflow aims to be data-centric, transparent, and interpretable. It was applied to three case studies: paracetamol, agomelatine, and lersivirine synthesis. In all cases, the literature-identified impurities were suggested within the top two outcomes.

Mr Adarsh ARUN

Update on work package 1.3

Novel reactors and process technology

Guided by **Asst Prof Wen LIU (PI, NTU)**, **Ms Xianyue WU (CARES Visitor, NTU)** has been actively working on the development of CO_2 capture and in-situ hydrogenation process using Ni/alkaline earth metal carbonate dual-function materials (DFMs). She has conducted a series of characterisation work to investigate the surface intermediate species during the hydrogenation on Ni/$CaCO_3$ and Ni/$MgCO_3$ DFMs (Figure 1.4). Therefore, she proposed that the reaction pathways on Ni/$CaCO_3$ and Ni/$MgCO_3$ DFMs are different during this scheme of CO_2 hydrogenation: the former undergoes a formate reaction pathway while the latter undergoes a reverse-water-gas-shift pathway (Figure 1.5). She also proposed that there could be two reactions: the Ni metal nanoparticles are mostly surrounded by CaO after hydrogenation, whereas the $CaCO_3$ far away from the Ni particles still remains undecomposed (Figure 1.6). Currently, she is working on the particle size and dispersion effects of Ni-based DFMs on their CO_2 capture and in-situ hydrogenation performance.

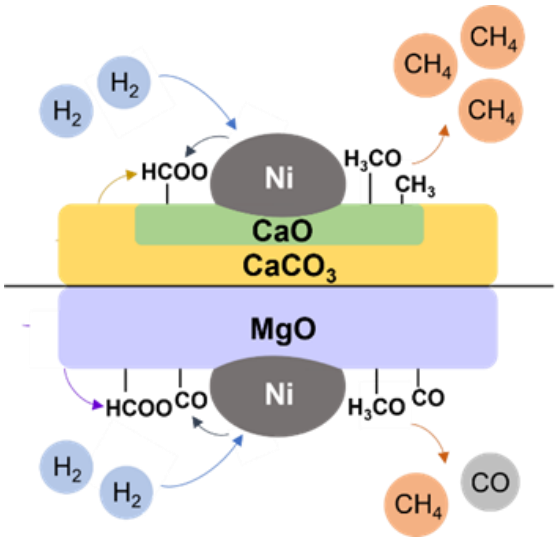


Figure 1.4: Graphical abstract of the surface intermediate species during the hydrogenation on Ni/$CaCO_3$ and Ni/$MgCO_3$ dual functional materials.

Ms Xianyue WU

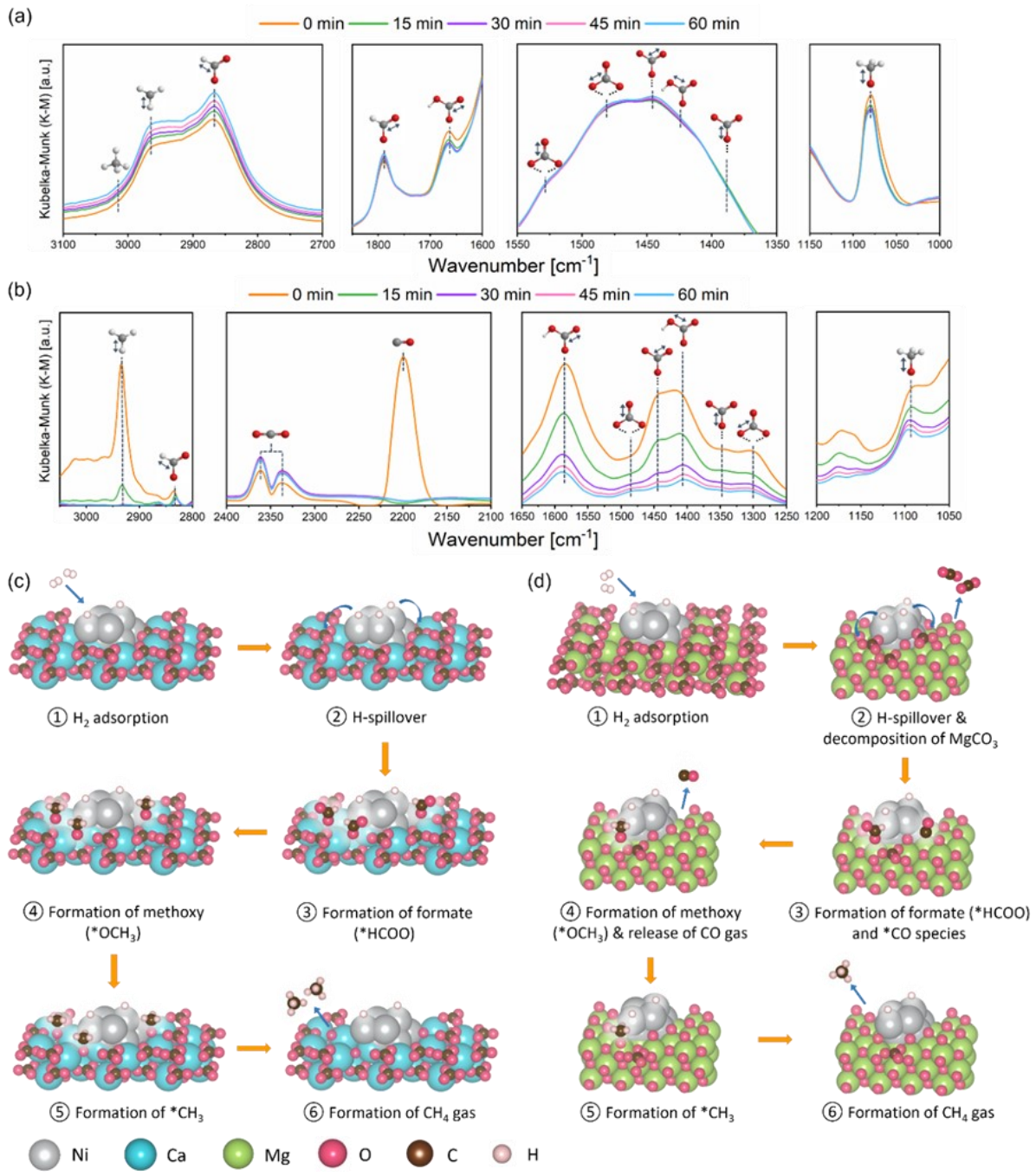


Figure 1.5: in situ DRIFTS measurements on Ni/Ca (a) and Ni/Mg (b) at 400 °C under direct hydrogenation conditions. (c) and (d) schematically illustrates the proposed reaction mechanism of direct hydrogenation on Ni/Ca and Ni/Mg, respectively.

Ms Xianyue WU

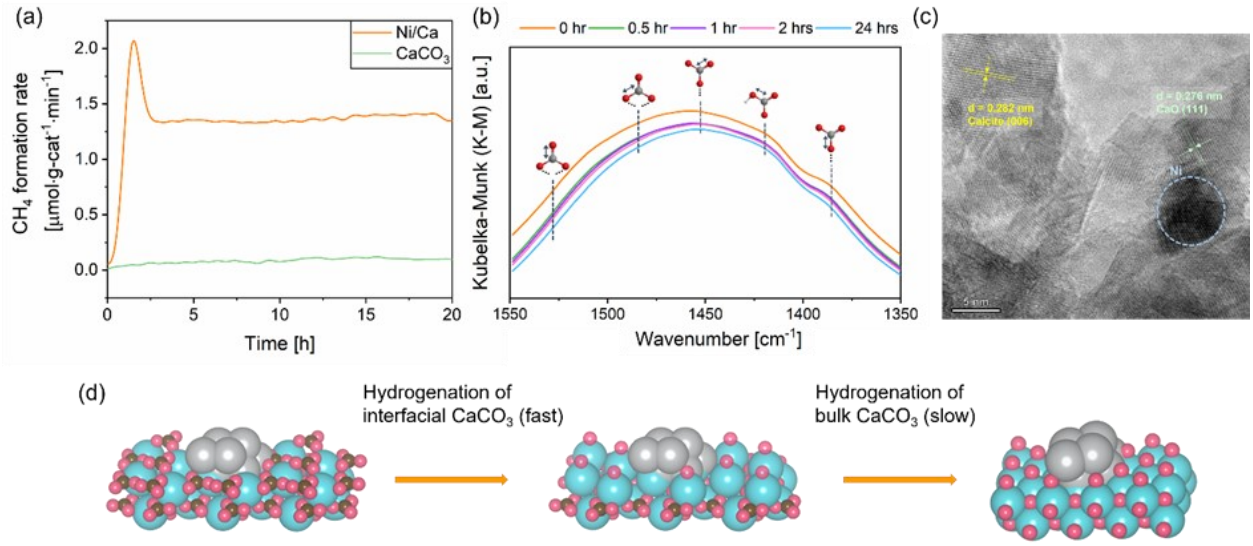


Figure 1.6: (a) Gas profile of rate of CH_4 formation and (b) in situ DRIFTS spectra of surface carbonate species during a 24-hour hydrogenation experiment on Ni/Ca. (c) TEM image of a hydrogenated Ni/$CaCO_3$ sample; the blue circle indicates a Ni particle. (d) Schematic illustration of the progressive hydrogenation of Ni/$CaCO_3$ over time.

Ms Xianyue WU

Asst Prof Tej CHOKSI's (Co-PI, NTU) group is part of IRP1 and is funded by an Emerging Opportunities Fund grant. The objective of this grant is to design supported metal catalysts that enable CO_2 conversion using first principles methods. In the last six months, this group has made progress with two of the project's aims: (1) predicting catalytic stability, and (2) understanding the selectivity trends among CO_2 reduction catalysts. The group tested a generalised model to determine the stability of gold nanoparticles across a range of 2D and 3D carbide, nitride, supports. The goal is to determine the selectivity of CO_2 reduction on these gold/support systems using first principles methods. The group observed inherent correlations between the reaction energies of various CO_2 reduction intermediates (e.g., adsorption free energies of CO* vs OH*). These linear scaling relations can be exploited to rapidly determine which product a supported gold system is selective towards. The group has also started constructing a machine learning model to expeditiously estimate the adsorption free energy of CO* on supported gold sites, using the properties of the binding sites as inputs.

Asst Prof Choksi's group has also finished up a collaboration with an experimentalist, Prof Lydia Wong (Non-C4T PI, NTU) on determining selectivity differences for CO_2 reduction to sun-gas or HCOOH as Cu_xSb_y catalysts are modified with sulphur.

Dr Shenghui ZHOU (Research Fellow, NUS) and **Prof Hua Chun ZENG's (Co-PI, NUS)** work investigates in-plane sulfur vacancies in MoS_2. While edge sulfur vacancies facilitate methane formation, in-plane sulfur vacancies were newly unveiled as efficient active sites for selective hydrogenation of CO_2 to methanol. Thus, selective exposure and activation of basal plane in MoS_2 nanosheets, although extremely challenging, is crucial for boosting methanol synthesis. In this project, they developed a mesoporous silica-encapsulated few-layer MoS_2 catalyst with a fullerene-like hollow structure (Figure 1.7). The main approach was based on a physically constrained epitaxial conversion of MoO_2 to MoS_2 within the central space of mesoporous silica. The spherical curvature enabled the generation of strain and sulfur vacancies in the inert MoS_2 basal plane. More importantly, fullerene-like structure of MoS_2 can selectively expose in-plane sulfur vacancies and reduce the exposure of edge sulfur vacancies. They are currently applying the designed catalyst to the hydrogenation of carbon dioxide to methanol and expect to achieve good performance.

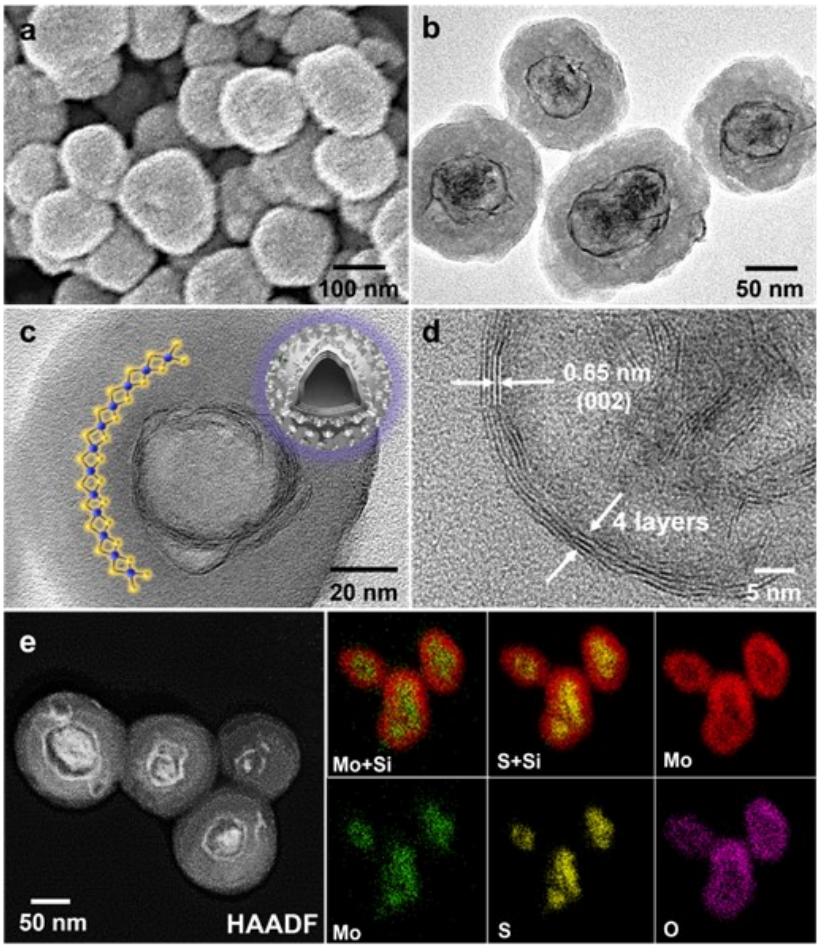


Figure. 1.7. FESEM (a), TEM images (b-d), HAADF-STEM image and corresponding elemental mappings (e) of $MoS_2@SiO_2$.

Dr Shenghui ZHOU

Mr Chao WANG (Non C4T-PhD student, NUS) and **Prof Hua Chun ZENG's (Co-PI, NUS)** work focused on Cu/ZrO_2 as a catalyst for CO_2 hydrogenation to methanol. Cu/ZrO_2 system with high catalytic efficiency and great application potential has attracted substantial interest from researchers; works have been carried out to study this binary catalyst system in terms of crystal structures of ZrO_2, reaction mechanism, structure-activity relationship, and surface properties. From the aspect of catalyst structure, it is desirable to design a stable structure of Cu/ZrO_2 catalyst to thus enable a longer catalytic lifetime of it under harsh reaction condition. Over the past months, they have fabricated an amorphous ZrO_2 -containing host material by directly substituting organic ligands of UiO-66 with oligomeric silica units (Figure 1.8). This engineering of host matrix not only creates a moderate surface area and a concrete structure but also boosts a considerable catalytic activity towards methanol synthesis from CO_2/H_2 after loading Cu. As a result, the aggregation of catalyst host has been effectively prevented during the preparation and reaction. Moreover, the CuO/s-UiO-66 catalyst exhibited a high space-time yield to methanol because Cu component is uniformly dispersed and confined in the host material. After a prolonged stability test, no sintering of Cu or ZrO_2 phase was detected in the spent catalyst. Additionally, they have studied the Cu component and key surface intermediates under in situ condition, confirming that copper mainly presents in its metallic form and it is responsible for H_2 dissociation to activated hydrogen (which further reduces carbonate species to carbonyl and formate).

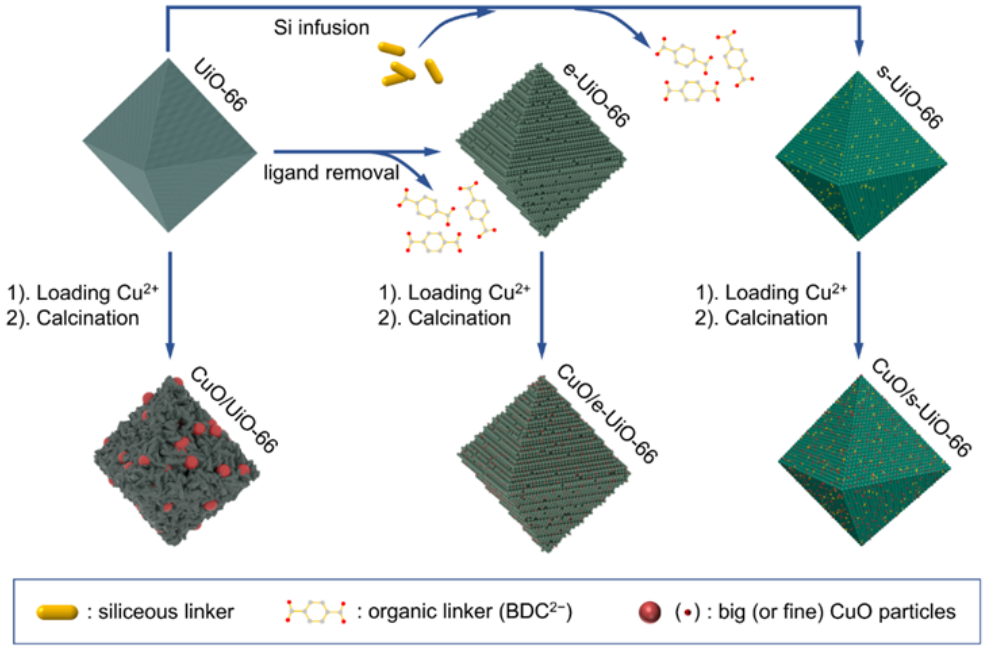


Figure 1.8: Schematic illustration of post-synthetic modifications of UiO-66 via two different strategies (etching ligands and infusing Si) and following fabrication steps of corresponding Cu catalysts (BDC^{2-}: 1,4-benzenedicarboxylate anions; e-UiO-66: etched UiO-66; s-UiO-66: Si-infused UiO-66; siliceous linker: oligomeric siliceous species).

Mr Chao WANG

Ms Ziyu GAO (Non-C4T PhD student, NUS) and **Prof Hua Chun ZENG's (Co-PI, NUS)** work focused on improving catalytic performance. Catalysts with large cavities, mesoporous and 1D nanostructure can accelerate the diffusion of reacting substrates during catalytic reactions. Thus, a compound *m*SiO_2@ZnO/Cu with anchored Cu on the surface of mesoporous silica (*m*SiO_2) was designed and developed by Ms Gao and Prof Zeng. In Figure 1.9(a), it is clear that the *m*SiO_2 layer (ca. 20 nm) formed a hollow cylinder through using CNTs as a template, resulting in the 1D nanostructure (ca. 7 nm) channel. Then the ZIF-8 layer was synthesised on the surface of *m*SiO_2 and 3-amino-1,2,4-trizole (Atz) was introduced in ZIF-8 through post-synthesis modification (PSM) method, leading to the formation of solid precursor *m*SiO_2@ZIF-8-A. The amino groups in the structure of *m*SiO_2@ZIF-8-A can anchor Cu^{2+}, and the *m*SiO_2@ZnO/Cu catalyst was obtained by simple calcination. The resultant *m*SiO_2@ZnO/Cu was applied to catalyse the hydrogenation of CO_2 to methanol and performed well. The MeOH yield can reach 1230 $mg_{MeOH} \cdot g_{Cu}^{-1} \cdot h^{-1}$ with a 100% selectivity for MeOH at 260°C. Additionally, the Cu can be dispersed uniformly on the surface of *m*SiO_2 support, maintaining the initial morphology and size after prolonged reactions.

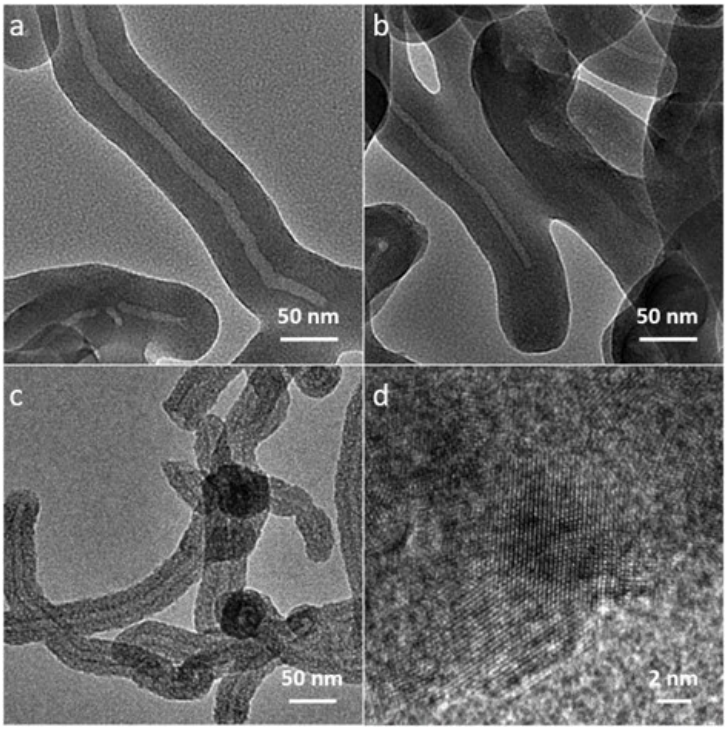


Figure 1.9: Representative TEM images of (a) SiO_2@ZIF-8, (b) SiO_2@ZIF-8-A, (c) mSiO_2@ZnO/Cu, and (d) mSiO_2@ZnO/Cu observed with high magnification.

Ms Ziyu GAO

Dr Nicholas JOSE (Research Fellow, CARES) has been developing the third iteration of FLAB, an open-source Python platform for automating laboratories, which is intended to decrease the time and cost of digitising laboratories. Dr Jose has also been working on several case studies, including automated flow chemistry, batch chemistry and analytical devices. He plans to publish these papers describing FLAB 3.0 this year, which will include retrospectives from all case studies done since 2021.

Scientific output

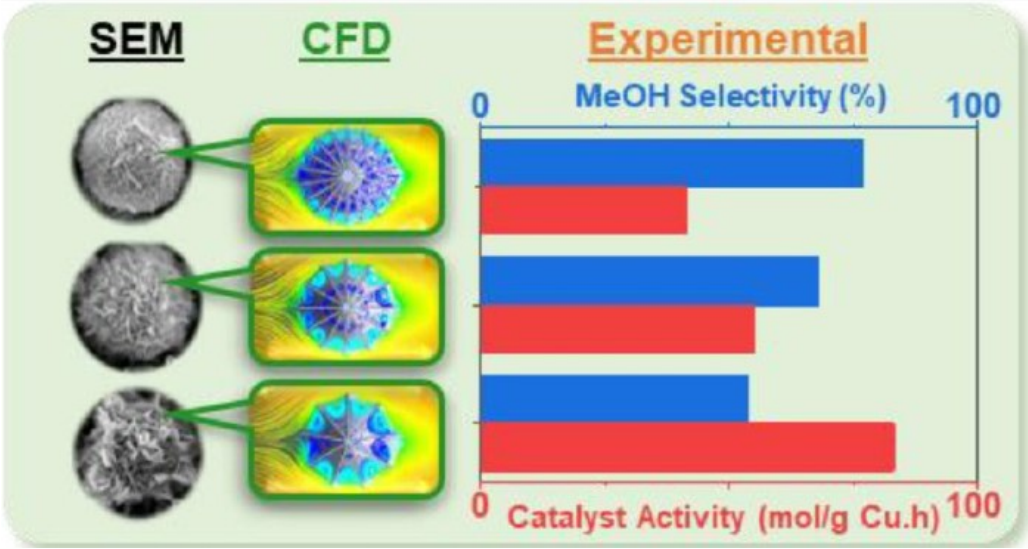
The following are the CREATE-acknowledged publications generated by IRP 1 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Controlling Nanosheet Spacing of ZnAl-Layered Double Hydroxide Assemblages for High-Efficiency Hydrogenation of CO_2 to Methanol

Alvin M. H. Lim and Hua Chun Zeng, *Industrial & Engineering Chemistry Research*

DOI: 10.1021/acs.iecr.2c03583

Abstract: Three different morphological variations of monodispersed Zn-Al-containing layered double hydroxide (ZnAl-LDH) microspheres were synthesized, with varying degrees of spacing between the nanosheets. The ZnAl-LDH materials were calcined into Zn-Al-containing layered double oxide (ZnAl-LDO) microspheres and loaded with Cu to be used as catalyst candidates for CO_2 hydrogenation to methanol under high pressure and constant flow. Two different low-cost facile Cu loading methods were also employed, namely, wet impregnation and ion exchange. The different morphological variations were then evaluated and compared by computational fluid dynamics (CFD) simulation (ANSYS Fluent) as well as the hydrogenation reaction of CO_2 to methanol with the purpose of exploring the effect of nanosheet spacing on catalyst performance in terms of the overall catalytic activity and methanol selectivity. The different metal loading methods have also led to different stability results, where there is a slight drop in performance of the incipient wet-impregnated catalyst, while the ion-exchanged catalyst retains much better performance over the same period of 40 h. Based on our simple CFD modeling, an increase in the nanosheet spacing improves convection-driven vortices within the wider channels of the LDH assemblage, with the vortices reaching deeper into the interior core of the microsphere. The simulated vortex phenomena explain the higher catalytic activities observed in our experimental results. This work indicates that catalysts with intricate morphological structure engineering would significantly enhance their catalytic activities.

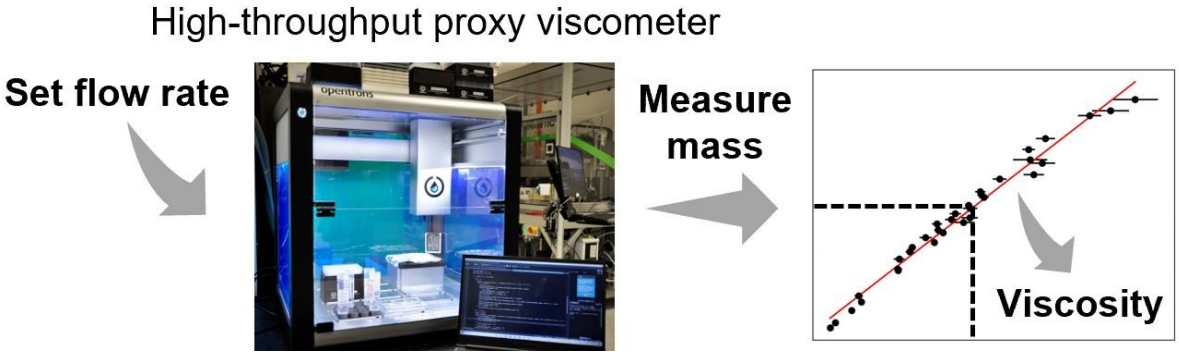


Automated pipetting robot for proxy high-throughput viscometry of Newtonian fluids

Beatrice W. Soh, Aniket Chitre, Wen Yang Lee, Daniil Bash, Jatin N. Kumara, and Kedar Hippalgaonkar, *Digital Discovery*

DOI: 10.1039/D2DD00126H

Abstract: In this work, we develop a high-throughput viscometer for Newtonian fluids with viscosities between 1500 and 12 000 cP. The viscometer is developed based on an automated pipetting robot Opentrons (OT-2), with a commercial wide bore tip. The measurement protocol exploits the known characteristics of air-displacement pipettes in dispensing and gravimetrically measuring fluids of different viscosities. Specifically, by measuring the actual dispense flow rate of fluids with varying viscosities under fixed dispense conditions, we construct a calibration curve and propose a scaling analysis based on flow through an idealized pipette tip geometry. Our model can predict the viscosity of Newtonian fluids with an error of 6.5%. We also showcase the flexibility of our platform by integrating a custom-design tip for a different viscosity range.



Shear and Solvent-Mediated Fabrication of Layered Double-Hydroxide Superstructures for High-Rate Supercapacitor Cathodes

Nicholas Jose, Mikhail Kovalev, and Alexei Lapkin, *Energy Technology*

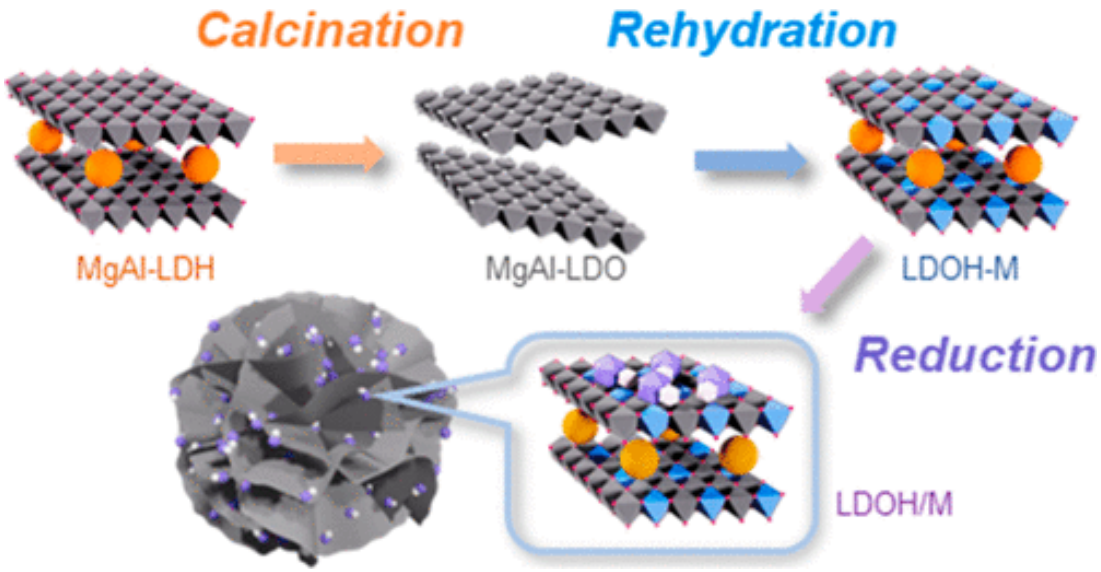
DOI: 10.1002/ente.202200633

Abstract: The development of sustainable energy economies is blocked by the lack of stable electrical energy sources with high power and energy densities. Next-generation supercapacitors utilizing 2D layered double hydroxides (LDHs) promise to fill this need in hybrid and standalone architectures; however, despite their high power and energy densities, LDH supercapacitors have poor stability. New methods for creating robust LDH electrodes are necessary to prevent this degradation. Herein, the recently developed annular microreactor is used to synthesize defect-rich NiCoLDH nanocrystals. A simple, solvent-based method is used to rationally generate binder-free, superstructured thin films on Ni foam electrodes. Control over crystallite size, thinness, and orientation improves contact with the conductive substrate, increases reactivity, and improves structural stability. Optimized electrodes are fabricated with specific capacitances from 3000 to 5000 F g^{-1} at charging rates as high as 1000 A g^{-1}, a performance that is retained after 20 000 cycles. This is twice as stable at 5000 times the current density of the most stable reported Ni-based supercapacitor. Ultimately, this study addresses key concerns in electrode development, introduces new approaches through reactor technology and solvent-mediated assembly, and opens new ground for more fundamental inquiries into the mechanisms of electron transport in 2D systems.

Preparation of CuZn-Doped MgAl-Layered Double Hydroxide Catalysts through the Memory Effect of Hydrotalcite for Effective Hydrogenation of CO_2 to Methanol

Alvin Ming Hao Lim, Jun Wen Yao, and Hua Chun Zeng, *ACS Applied Energy Materials*
DOI: 10.1021/acsaem.2c03045

Abstract:: In this work, a synthesis procedure was developed to introduce transition metal ions into a MgAl-layered double hydroxide (MgAl-LDH, or hydrotalcite) by utilizing the unique "memory effect" property of calcined LDH. This technique allows our MgAl-LDH to retain its pristine flower-like morphology, which prevents stacking of nanosheets and is fully accessible for reactants. Briefly, calcined MgAl-LDH (or MgAl-layered double oxide, MgAl-LDO) was submerged in dilute monometal or mixed transition metal nitrate solutions, allowing ion exchange of M^{2+} cations and the rehydration of MgAl-LDO back into LDH through the memory effect. The product was centrifuged and dried, allowing preselected transition metals (e.g., Cu, Zn, Ni, and Co) to occupy some of the octahedral sites of the LDH phase in which Mg^{2+} ions were previously located. A CuZn-doped MgAl-LDH was then carefully reduced under a hydrogen atmosphere, precipitating tiny Cu nanoparticles out of the reformed LDH nanosheets, and was subsequently used in a series of CO_2 hydrogenation experiments. The bifunctional material, which comprises a CO_2-sorbent LDH support with active metal cocatalysts, has achieved high specific activity per copper loading and high methanol selectivity, while maintaining a stable performance with over 70% methanol selectivity over 40 h at 280 °C. The excellent performance of this catalyst is attributed to the easily accessible active sites (Cu^0 nanoparticles) located on the surface of nanostructured petals for the gaseous reactants. The performance was found to be remarkably better than that of a well-established commercial Cu-based catalyst for methanol synthesis. Future potential development could entail the functionalization of other transition metals for the utilization of CO_2.



Predicting the work function of 2D MXenes using machine-learning methods

Roy Pranav, Laie Rekhi, See Wee Koh, Hong Li, and Tej Choksi, *Journal of Physics: Energy*

DOI: 10.1088/2515-7655/acb2f8

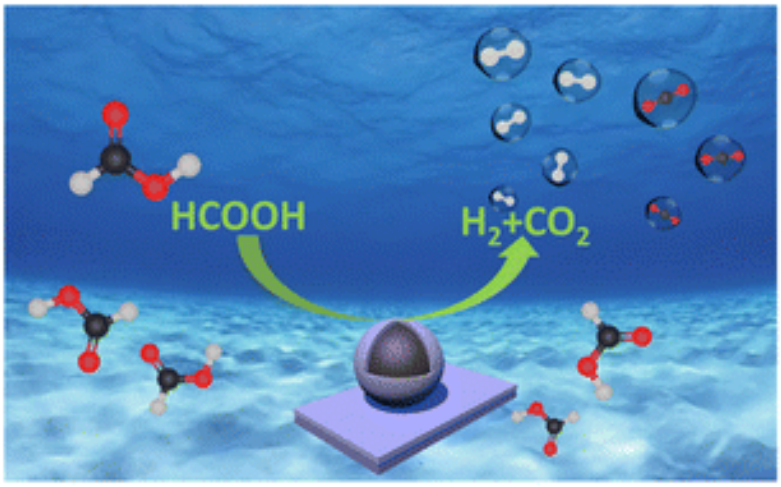
Abstract: MXenes, which are graphene-like two-dimensional transition metal carbides and nitrides, have tuneable compositions and exhibit rich surface chemistry. This compositional flexibility has resulted in exquisitely tuneable electronic, optical, and mechanical properties leading to the applications of MXenes in catalysis, electronics, and energy storage. The work function of MXenes is an important fundamental property that dictates the suitability of MXenes for these applications. We present a series of machine learning models to predict the work function of MXenes having generic compositions and containing surfaces terminated by O*, OH*, F*, and bare metal atoms. Our model uses the basic chemical properties of the elements constituting the MXene as features, and is trained on 275 data points from the Computational 2D Materials Database (C2DB). Using 15 different features of the MXene as inputs, the neural network model predicts the work function of MXenes with a mean absolute error (MAE) of 0.12 eV on the training data and 0.25 eV on the testing data. Our feature importance analysis indicates that properties of atoms terminating the MXene surface like their electronegativity, most strongly influence the work function. This sensitivity of the work function to the surface termination is also elucidated through experimental measurements on Ti3C2. We also introduce reduced-order models comprising of 10-, 8-, and 5-features to predict the work function. These reduced-order models exhibit easier transferability to new materials, while maintaining their accuracy. We demonstrate the transferability of these reduced order models to new materials, by predicting the work function of MXenes having surface terminations beyond the original training set, like Br*, Cl*, S*, N*, and NH*. Predicting electronic properties like the work function from the basic chemical properties of elements, paves the way towards rapidly identifying tailored MXenes having a targeted range of properties that are required for a specific application.

Synergistic effect of PtNi alloy loading on TiB_2 to construct SMSI catalysing formic acid dehydrogenation

Hongliang Zhu, Roong Jien Wong, Xiangbowen Du, Leilei Du, Zhikang Jin, KaiCheng Qian, Junjie Song, Renhong Li, and Wen Liu, *Sustainable Energy & Fuels*

DOI: 10.1039/D2SE01048H

Abstract:: Low-cost and highly active catalysts are attractive for catalysing formic acid (FA) dehydrogenation at room temperature. The PtNi alloy nanoparticles with the characteristic of lattice contraction and synergy effects were loaded on two-dimensional TiB_2 by incipient-wetness impregnation. Compared to Pt/TiB_2, the substitution of Ni reduces the amount of noble metal required, with the added advantage of significantly improving the catalyst activity by sixteen times. By investigating the various PtNi ratios, the Pt_3Ni_8/TiB_2 (total metal loading = 2.0 wt%) catalyst was found to provide a low activation energy of 27.7 kJ mol^{-1} in 10.0 M FA aqueous solution at room temperature. This is the first example of using the alloy supported on TiB_2 to achieve strong metal–support interaction (SMSI) to catalyse formic acid dehydrogenation at ambient temperature. XPS and TEM characterisation studies show that higher temperatures induced TiB_2 to encapsulate the PtNi NPs, with the TiB_2 surfaces serving as the active site for catalysing FA dehydrogenation. The catalytic activity of the obtained Pt_3Ni_8/TiB_2 catalyst for the dehydrogenation of FA was much higher than those of its monometallic counterparts (Pt/TiB_2 and Ni/TiB_2) prepared by the same method, while demonstrating higher stability against agglomeration and CO poisoning. The excellent catalytic activity and stability of Pt_3Ni_8/TiB_2 were mainly attributed to the presence of the SMSI effect of the catalyst. Additionally, the lattice distortion and local interactions within the ferromagnetic clusters of Pt_3Ni_8 alloy NPs created a synergistic effect, which resulted in an enhanced SMSI effect throughout the catalyst. This study introduces a new concept that magnetic Ni metal partially replacing noble metals can improve thermal stability and catalytic performance, while enabling facile catalyst recovery. Moreover, this research demonstrates that the controlled synthesis and rational design of 2D reticular crystal structure TiB_2-supported alloy NPs may provide new opportunities to enhance the catalytic activity and improve the SMSI effect of noble metal-based nanostructures.



Other activities and achievements

Asst Prof Tej CHOKSI's (Co-PI, NTU) group gave in-person presentations at the conferences below:

- AIChE Annual Meeting in Phoenix, Arizona from 13 –18 November 2022, presenting "Establishing Structure-Function Relationships in Low Dimensional MXenes using Machine Learning".
- 265th American Chemical Society Meeting in Indianapolis from 26 – 30 March 2023, presenting "On the Stability and Morphology of Metal Nanoparticles Supported on two-dimensional MXenes: Insights from First Principles Calculations" and "Microkinetic Study of How Strong Metal Support Interaction Phenomena Influences Reaction Rates and Selectivity".

Asst Prof Choksi was also the recipient of the 2022 Nanyang Education Award (School) for excellence in teaching presented by NTU. He also joined the early career editorial board of the *Journal of Catalysis* and the early career advisory board of *ChemSusChem*.

Two CARES Professors were recognised as Highly Cited Researcher by Clarivate in 2022:

- **Prof Ning YAN (PI, NUS)** in the Cross-Field category, indicating strong multidisciplinary influence by contributing to highly cited papers across several different fields.
- **Prof Manish CHHOWALLA (Co-PI, CAM)** in the field of Materials Science.

Mr Aniket CHITRE (PhD student, CAM) presented a short talk online titled "Automating and Accelerating Formulations R&D" for the University of Cambridge's Innovation Centre in Digital Molecular Technologies (iDMT) Digitalising Chemistry Workshop from 29 – 30 March 2023.

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

IRP 2

ELECTROSYNTHETIC PATHWAYS FOR ADVANCED LOW-CARBON CHEMICAL MANUFACTURING

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

IRP 2 Principal Investigators:

Professor Adrian FISHER
University of Cambridge

Professor WANG Xin
Nanyang Technological University

Asst Prof ZHANG Sui
National University of Singapore

OVERVIEW

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

Dr Chencheng Dai and Dr Libo Sun's research is focused on electrode architectures and synthesis reactors. In this reporting period they have been exploring future energy vectors including ammonia and new approaches for electrochemical generation of disinfectants.

Nitrate conversion electrochemically to ammonia is a potentially exciting opportunity to offer an alternative synthetic pathway to the high energy Haber-Bosch process for generating ammonia. They have explored strategies that promote the generation of ammonia, such as modulating adsorption, impeding N-N coupling, and the hetero -atomic synergistic effect can be satisfied simultaneously. The work has led to a recent technology disclosure.

In addition, exploration of electrochemical generation of reactive oxygen species has been extended with new reports for the industrially important electrocatalytic production of H_2O_2. This catalytic route is important as it can be performed at environmentally friendly ambient temperature and pressure, with higher catalyst activity and product selectivity. Considering that the activity and selectivity of an electrocatalyst are greatly affected by the intrinsic properties of the active site configuration, molecular catalysts are under investigation.

Asst Prof Sui Zhang's research is focused on the development of (re)active membrane structures, including targets such as self cleaning, disinfection and gas separation (e.g., H_2). In this reporting period new characterisation and separation performance of robust CMPs membrane fabricated via electropolymerisation of tris (4-carbazoyl-9 -ylphenyl) amine (TCTA) on the surface of the carbon nanotubes (CNTs) support have been explored.

IRP 2 Singapore-based start-up company Datum ElectroniX, which was launched by Dr Kamal Elouarzaki and Prof Adrian Fisher, has continued to develop and has seen progress with the recent award of a MIT SMART innovation awarded exploring opportunities for localised, on-site synthetic production of economy critical chemicals.

Professor Adrian Fisher, PI
University of Cambridge

Update on work package 2.1

Advanced electrode architectures

Dr Chencheng DAI (Research Fellow, NTU) studied spin-related Cu-Co pair to increase ammonia generation on high entropy oxides. The electrochemical conversion from nitrate to ammonia is a way to eliminate nitrate pollutants in water, as well as a potential alternative to the Haber-Bosch process for generating ammonia. Current strategies that promote the generation of ammonia, such as modulating adsorption, impeding N-N coupling, and the hetero-atomic synergistic effect can be satisfied simultaneously by the high-entropy oxide $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ due to its multi-fraction and paired Cu-Co active sites. Herein, Dr Dai studied the ammonia generation via nitrate reduction reaction (NO_3RR) on $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ with six-coordinated cations, which has a maximum ammonia Faradaic efficiency of 99.3% and a yield rate up to 26.6 mg mg_{cat}^{-1} h^{-1}.

In contrast, $Mg_{0.25}Co_{0.25}Ni_{0.25}Zn_{0.25}O$ and $Li_{0.20}Mg_{0.16}Co_{0.16}Ni_{0.16}Cu_{0.16}Zn_{0.16}O$, which have similar coordination environments, exhibit inferior NO3RR performance. By correlating the electronic structure, we find that the synergistic effect of Cu-Co pair, together with Co spin and valence state are crucial for ammonia generation. The Cu-Co pair in $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ can facilitate the performance of ammonia generation while a lower spin state and higher valence state in Co induced by the Li in $Li_{0.20}Mg_{0.16}Co_{0.16}Ni_{0.16}Zn_{0.16}O$ decrease the Cu-Co synergistic effect on ammonia generation. These findings offer important insights into utilising high-entropy oxides to disperse the homo-cation well to provide relatively isolated active sites and to employ the synergistic effect and spin states inside, for the selective generation of specific targets in catalysis more efficiently.

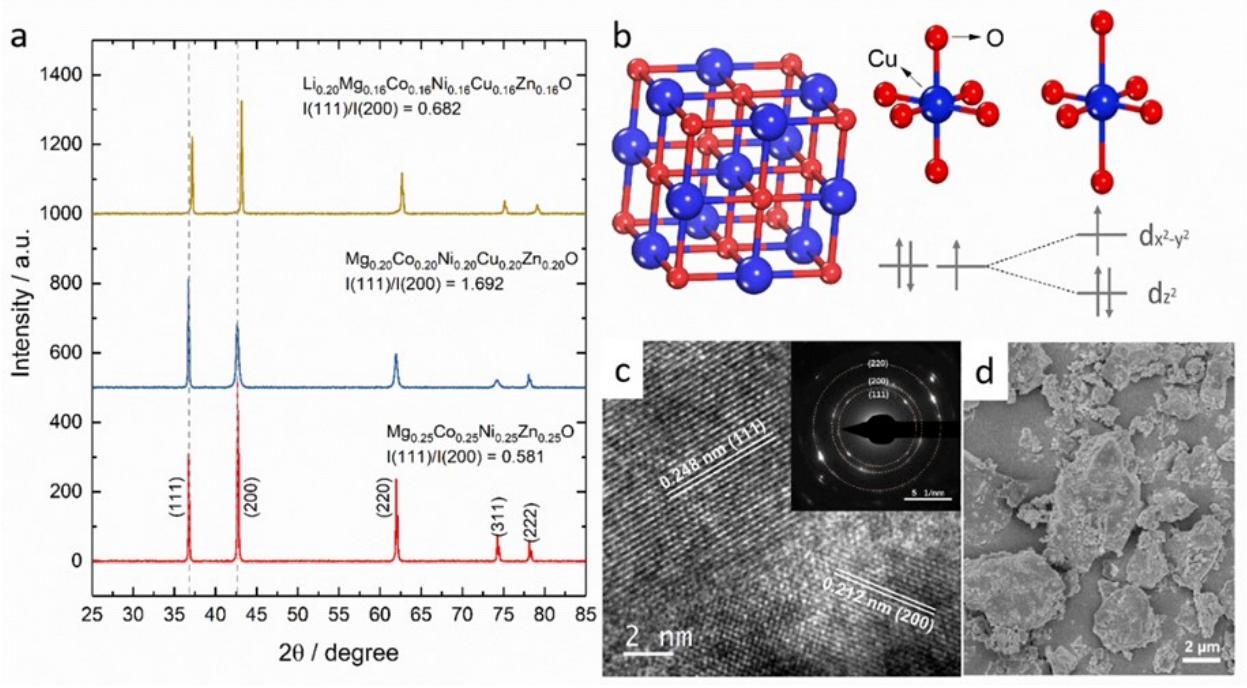


Figure 2.1: (a) XRD patterns of $Mg_{0.25}Co_{0.25}Ni_{0.25}Zn_{0.25}O$ (RS-0), $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ (RS-20), and $Li_{0.20}Mg_{0.16}Co_{0.16}Ni_{0.16}Cu_{0.16}Zn_{0.16}O$ (Li-RS-16); (b) schematic of the rock-salt structure and Jahn-Teller distortion caused by Cu^{2+}; (c) the TEM image and SAED pattern and (d) SEM image of RS-20

Dr Chencheng DAI

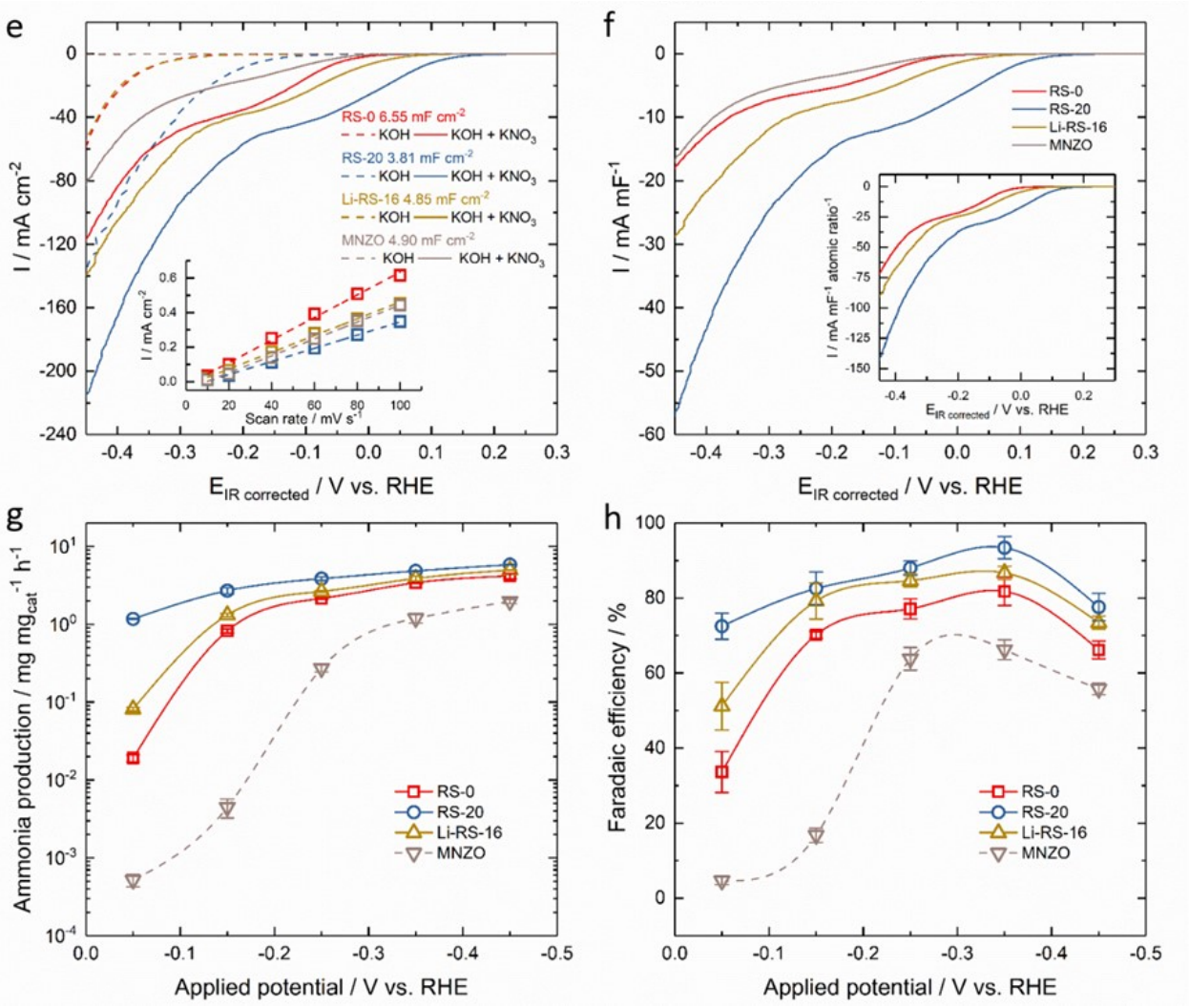


Figure 2.1 (cont.): (e) LSV curves of nitrate reduction on RS-0, RS-20, and Li-RS-16 and their double-layer capacitance (inset); (f) capacitance-normalized LSV curves, and atomic ratio (Cu and Co) and capacitance-normalized LSV curves (inset) derived from (e); (g) ammonia production rate and (h) faradaic efficiency on RS-0, RS-20, Li-RS-16, and MNZO at different applied potentials.

Dr Chencheng DAI

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

Herein, the group's main research focuses on the study of fabrication of CMPs by electrochemical polymerisation for challenge separation applications. They have been focusing on the characterisation and separation performance of robust CMPs membrane fabricated via electropolymerisation of tris (4-carbazoyl-9-ylphenyl) amine (TCTA) on the surface of the carbon nanotubes (CNTs) support. TCTA which has three carbazole groups and triphenylamine was chosen as the monomer due to its good thermal properties. Multiple carbazole functional groups on the TCTA can easily form a microporous polymer network. The impact of electrochemical conditions on membrane properties was studied, and the permeance and rejection of TCTA membrane were evaluated against a wide range of organic solvents, dyes and pharmaceutical molecules. Following efforts in the last report, they continue to explore the transport across the CMP membranes, and have found the high dimethylformamide permeance, in particular the impressive size - and shape-based separation. They have also obtained preliminary results on the potential of membranes for CO_2 separation.

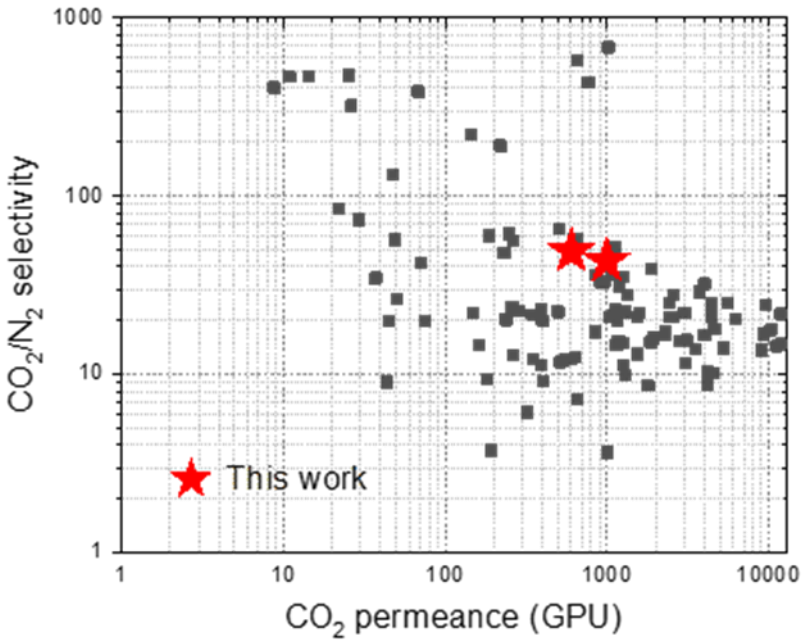


Figure 2.2: A comparison of the permeance and selectivity of our membranes with literature work.

Asst Prof Sui ZHANG

Update on work package 2.2

Co-generation and electrolytic synthesis reactor engineering

Dr Libo SUN (Research Fellow, NTU) reports that electrocatalytic H_2O_2 production has emerged as a promising alternative to the commercially used chemical method. This is because the electrocatalytic process is usually accompanied with an environmentally friendly ambient temperature and pressure, with higher catalyst activity and product selectivity. Considering that the activity and selectivity of an electrocatalyst are greatly affected by the intrinsic properties of the active site configuration, molecular catalysts could be ideal when used in electrocatalytic H_2O_2 production. Molecular catalysts could be judiciously designed, modified and tailored with diverse functional groups, thus affecting activity and selectivity of the active sites. In this work, nickel phthalocyanines derivatives are identified as effective to be one kind of pH universal electrocatalyst in H_2O_2 production, wherein increased conjugation is beneficial to boosted selectivity. This is explained to be the regulated d-band center, which could optimise the binding energy of reaction intermediate, thus lowering the energy required for reduction of O_2, and leading to optimised product selectivity to H_2O_2. The best catalyst, NiPyCN/CN optimised in this work, exhibits a highly H_2O_2 electrosynthesis activity with ca. 95% of H_2O_2 faradic efficiency in alkaline, thus could be potentially promising for H_2O_2 production. The work is to be submitted.

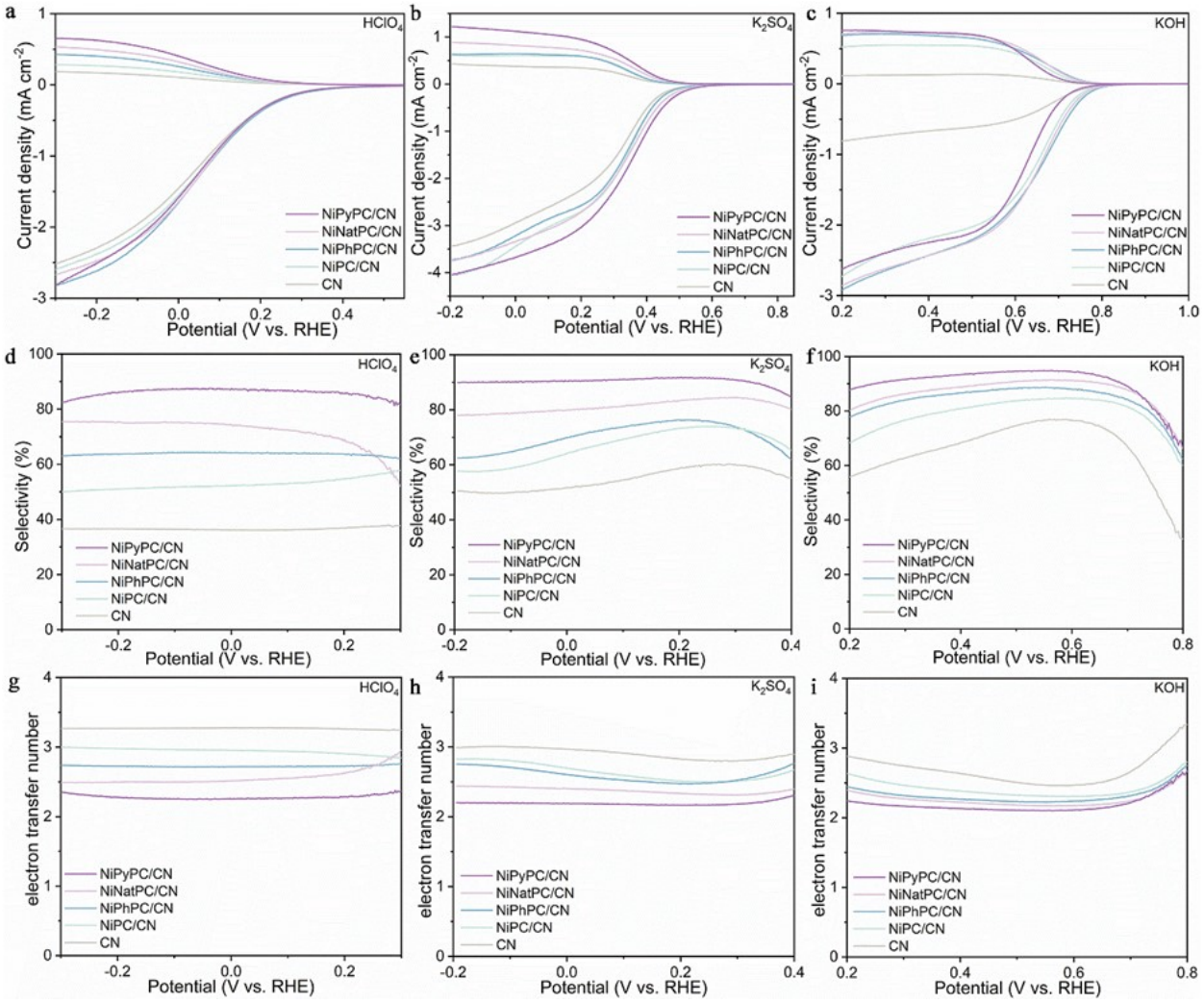


Figure 2.3: Electrocatalytic LSV curves at the ring-disk electrodes for electrocatalysts in a) 0.1 mol $HClO_4$, b) 0.1 mol K_2SO_4, and c) 0.1 mol KOH. Calculated selectivity of the electrocatalysts in d) 0.1 mol $HClO_4$, d) 0.1 mol K_2SO_4, and f) 0.1 mol KOH. Calculated electron transfer numbers of the electrocatalysts in g) 0.1 mol $HClO_4$, h) 0.1 mol K_2SO_4, and i) 0.1 mol KOH.

Dr Libo SUN

Update on work package 2.3

Micro-variable pressure and temperature electrosynthesis plant

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. She is currently writing her thesis on Electrochemical Systems which will be submitted in mid-2023.

Scientific output

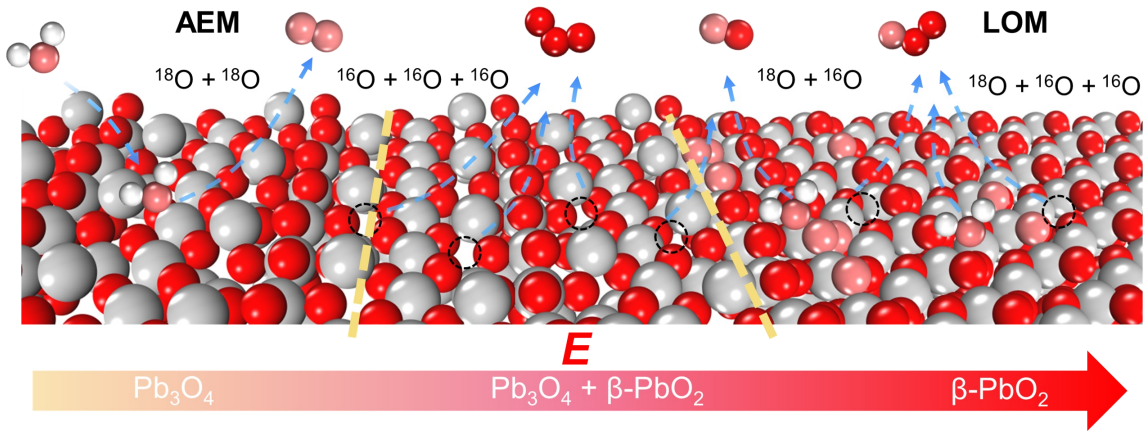
The following are the CREATE-acknowledged publications generated by IRP 2 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Phase shuttling-enhanced electrochemical ozone production

Jia Liu, Shibin Wang, Zhangnv Yang, Chencheng Dai, Ge Feng, Beibei Wu, Wenwen Li, Lu Shu, Kamal Elouarzaki, Xiao Hu, Xiaonian Li, Hui Wang, Zhen Wang, Xing Zhong, Zhichuan J. Xu, and Jianguo Wang, *EES Catalysis*

DOI: 10.1039/D3EY00015J

Abstract: Ozone can be produced by the electrochemical oxidation of water, which provides a technical solution to on-demand ozone production for disinfection and sterilization. Lead oxides have been found to be unique in catalyzing such a process. However, the fundamental understanding of these catalysts' mechanisms remains limited, hindering the development of high-performance catalysts for electrochemical ozone production (EOP). Herein, the effect of phase shuttling on the reactivity of Pb_3O_4 was systematically investigated during the EOP process by *in situ*/*ex situ* characterizations. It was found that Pb_3O_4 undergoes a phase shuttle towards β-PbO_2 *via* the lattice oxygen oxidation mechanism (LOM) pathway, and the reconstructed β-PbO_2 shows enhanced EOP activity and stability compared to commercial β-PbO_2. The *ex situ* characterization of materials combined with theoretical calculations reveals that the performance enhancement is mainly attributed to the stable presence of (101) and (110) surfaces in the reconstructed β-PbO_2 with undercoordinated Pb–O. Pourbaix diagrams of lead oxides calculated by DFT demonstrate that the phase shuttling to β-PbO_2 is thermodynamically favorable under EOP conditions. Surface Pourbaix diagrams of β-PbO_2 (101) and Pb_3O_4(110) further reveal the adsorption behavior of O*/OH* intermediates and explain the observed change of EOP kinetics at ~1.6 V *vs.* RHE. The catalyst is integrated and assembled in a membrane electrode assembly (MEA) electrolyzer, and the produced ozonated water successfully inactivated severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). This work provides a new insight into EOP catalysts and demonstrates the possibilities of further optimization of electrochemical approaches for on-demand ozone generation.

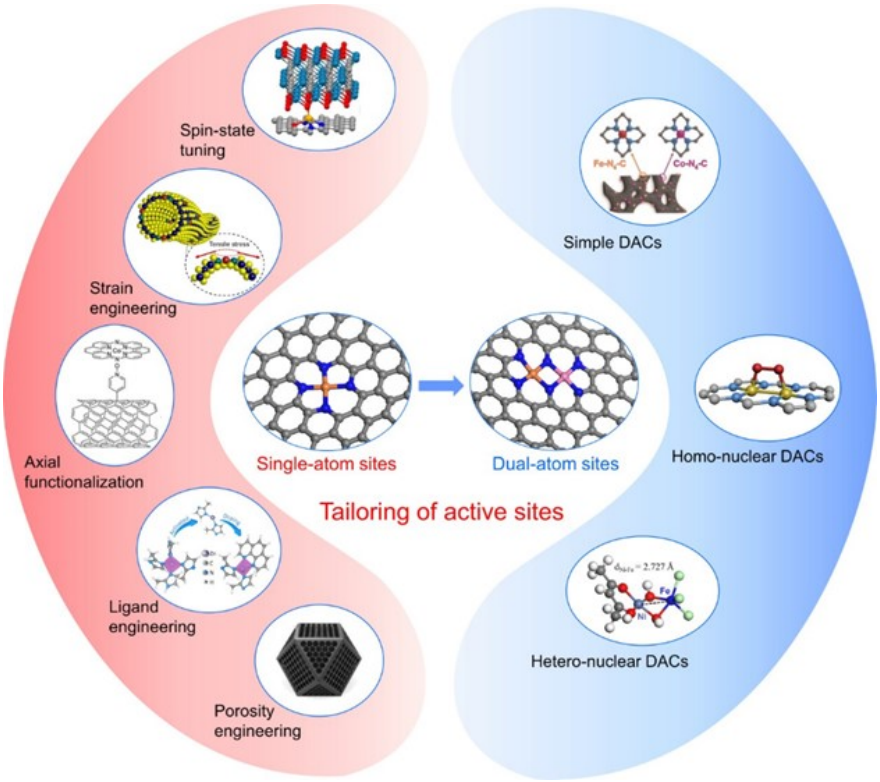


Tailoring of Active Sites from Single to Dual Atom Sites for Highly Efficient Electrocatalysis

Hongwei Zhang, Xindie Jin, Jong-Min Lee, and Wang Xin, *ACS Nano*

DOI: 10.1021/acsnano.2c06827

Abstract: Single atom catalysts (SACs) have been attracting extensive attention in electrocatalysis because of their unusual structure and extreme atom utilization, but the low metal loading and unified single site induced scaling relations may limit their activity and practical application. Tailoring of active sites at the atomic level is a sensible approach to break the existing limits in SACs. In this review, SACs were first discussed regarding carbon or non-carbon supports. Then, five tailoring strategies were elaborated toward improving the electrocatalytic activity of SACs, namely strain engineering, spin-state tuning engineering, axial functionalization engineering, ligand engineering, and porosity engineering, so as to optimize the electronic state of active sites, tune *d* orbitals of transition metals, adjust adsorption strength of intermediates, enhance electron transfer, and elevate mass transport efficiency. Afterward, from the angle of inducing electron redistribution and optimizing the adsorption nature of active centers, the synergistic effect from adjacent atoms and recent advances in tailoring strategies on active sites with binuclear configuration which include simple, homonuclear, and heteronuclear dual atom catalysts (DACs) were summarized. Finally, a summary and some perspectives for achieving efficient and sustainable electrocatalysis were presented based on tailoring strategies, design of active sites, and *in situ* characterization.



Reconstruction of Thiospinel to Active Sites and Spin Channels for Water Oxidation

Tianze Wu, Yuanmiao Sun, Xiao Ren, Jiarui Wang, Jiajia Song, Yangdan Pan, Yongbiao Mu, Jianshuo Zhang, Qiuzhen Cheng, Guoyu Xian, Shibo Xi, Chengmin Shen, et al, *Advanced Materials*

DOI: 10.1002/adma.202207041

Abstract: Water electrolysis is a promising technique for carbon neutral hydrogen production. A great challenge remains at developing robust and low-cost anode catalysts. Many pre-catalysts are found to undergo surface reconstruction to give high intrinsic activity in the oxygen evolution reaction (OER). The reconstructed oxyhydroxides on the surface are active species and most of them outperform directly synthesized oxyhydroxides. The reason for the high intrinsic activity remains to be explored. Here, a study is reported to showcase the unique reconstruction behaviors of a pre-catalyst, thiospinel $CoFe_2S_4$, and its reconstruction chemistry for a high OER activity. The reconstruction of $CoFe_2S_4$ gives a mixture with both Fe–S component and active oxyhydroxide ($Co(Fe)O_xH_y$) because Co is more inclined to reconstruct as oxyhydroxide, while the Fe is more stable in Fe–S component in a major form of Fe_3S_4. The interface spin channel is demonstrated in the reconstructed $CoFe_2S_4$, which optimizes the energetics of OER steps on $Co(Fe)O_xH_y$ species and facilitates the spin sensitive electron transfer to reduce the kinetic barrier of O–O coupling. The advantage is also demonstrated in a membrane electrode assembly (MEA) electrolyzer. This work introduces the feasibility of engineering the reconstruction chemistry of the precatalyst for high performance and durable MEA electrolyzers.

Other activities and achievements

Two CARES Professors were recognised as Highly Cited Researcher by Clarivate in 2022:

- **Prof Xin WANG (PI, NTU)** in the Cross-Field category, indicating strong multidisciplinary influence by contributing to highly cited papers across several different fields.
- **Prof Jason Zhichuan XU (Co-PI, NTU)** in the field of Materials Science.

Dr Yubo CHEN (Research Fellow, NTU) has submitted a technical disclosure for "A Unique Cation Leaching-Triggered Molecular Aggregate for Water Oxidation in Acidic Condition" which relates to the work on the preparation of high-performance IrO_xH_y catalyst from Sr_4IrO_6. The other inventors are Prof Xu and **Prof Adrian FISHER (PI, CAM).** See more of Dr Chen's work on page 134.

Dr Chencheng DAI (Research Fellow, NTU) has submitted two technical disclosures:

- An MEA electrolyzer for hydrogen production by electrochemical cracking of ammonia. The other inventors are Prof Xu, Prof Fisher, and **Dr Kamal ELOUARZAKI (Co-Founder of Datumelectronix, IRP2 spin-off)**.
- A highly active water oxidation catalyst made by spinel oxide with nickel, iron, and chromium. The other inventors are Prof Xu, Prof Fisher, and Mr Songzhu LUO (Non-C4T PhD student, NTU).

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

During the last six months, we have made further progress investigating the electrocatalytic CO_2 reduction (eCO_2R) mechanism as a process to turn carbon dioxide into fuels and other useful chemicals. Following on from our earlier work on the detailed microkinetics of this mechanism, we have now used gas-chromatography mass-spectrometry (GC-MS) to discover several previously unknown products of very small concentrations. We have managed to establish the identity and characterise more than 20 minor products, half of which have not been reported before, including for the first time species with five carbon atoms. We have studied trends in selectivity of all these products for industrially relevant conditions and found mechanistic differences for different isomers.

Additionally, in the field of cheminformatics, we have embarked on a new project to automate the rational design of Covalent Organic Frameworks (COFs), building upon previous successes for Metal-Organic Polyhedra. COFs are porous polymeric materials with exciting properties and great promise in applications such as printable electronics and the direct air capture of carbon dioxide and water. We have started to develop ontologies and autonomous software agents that imitate how human molecular engineers would approach the design process. The COF discovery agents make use of existing knowledge in the form of several hundred COFs and precursors that have been reported in the literature and apply general principles of chemical assembly modelling as well as chemical reactivity captured in inductive reasoning algorithms in order to construct new combinations of building blocks. The aim is not only to describe the new materials themselves, but also to include chemical synthesis routes for how they can be manufactured in the lab, and to predict some of their properties such as density and porosity.

Professor Markus Kraft, PI
University of Cambridge

Update on work package 3.1

Refinery, fuel and engine of the future — experimental

Properties of surrogate fuels, marine engine after-treatment

Dr Yichen ZONG (Research Fellow, NUS) is currently leading experimental research on future fuels aimed at reducing emissions and decarbonising the environment. This research is being conducted with researchers from NUS and the University of Cambridge. In the past two years, the engine study on blending fuels has yielded six research papers, which cover a broad range of potential fuel additives.

Dr Zong has now embarked on a new research project focused on plasma combustion. The objective of this study is to evaluate the effectiveness of non-equilibrium plasmas in achieving clean combustion using laser diagnostics.

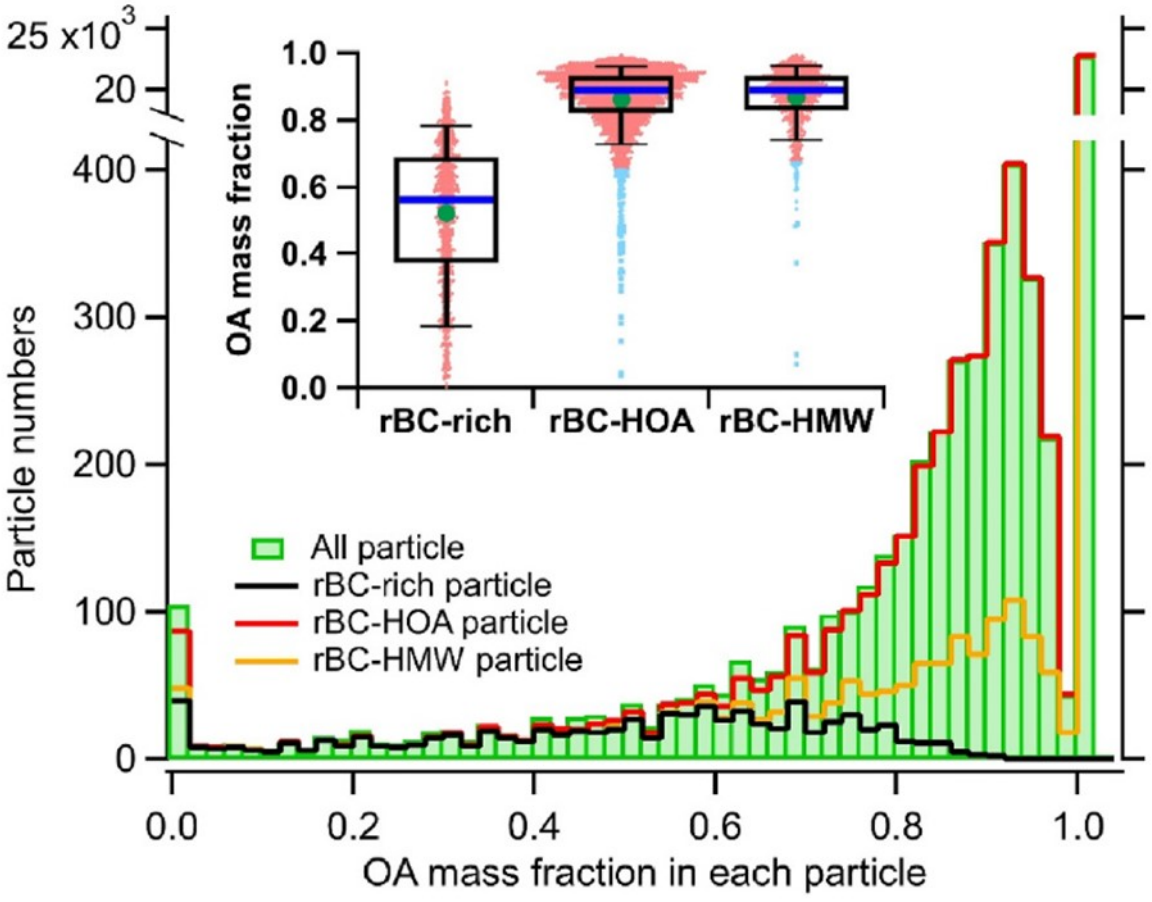


Figure 3.1: Detailed analysis of OA mass fraction in the particulate emissions from engine combustion.

Dr Yichen ZONG

Update on work package 3.2

Refinery, fuel and engine of the future — modelling

Chemical mechanisms, PAH chemistry, after-treatment

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

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

Update on work package 3.3

Better, cheaper, cleaner nanostructures — experimental

Flame synthesis of thin films of mixed metal oxide nanoparticles

Dr Yuan SHENG's (Senior Research Fellow, NTU) recent work focused on the construction of novel gas diffusion electrodes (GDEs). Regardless of whether the catalyst particles are obtained by flame or wet chemical synthesis, the lifespan of CO_2 reduction GDEs has been found severely limited by electrowetting. To alleviate the issue, Dr Sheng proposed the inverse GDE which is expected to bypass the negative effects of electrowetting. He has developed the methods for coating carbon papers with hydrophilic microporous layers and PTFE gas diffusion layers as the major steps in the fabrication of inverse GDEs. Prototype electrodes have been made and shown usable. Moreover, while studying alkaline water electrolysis in industrial conditions, he has found Cr-based additives in the electrolyte to be effective in controlling Fe migration and hence extending the stability of the anode.

Dr Sheng has recently left for an academic position in Zhejiang University of Technology, but maintained the collaboration with CARES on the CO_2 reduction technology and the flame synthesis of relevant catalysts. **Dr Morteza KOLAEI (Research Fellow, NTU)** is continuing his research in this direction. They have worked together to optimise the deposition conditions for flame synthesised CuO_x nanoparticles on carbon GDEs, and are now developing Cu-carbon composite substrates for inverse GDEs.

Update on work package 3.4

Better, cheaper, cleaner nanostructures — modelling

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

Mr Simon RIHM (PhD student, CARES) continued his work on advancing our understanding of electrocatalytic CO_2 reduction (eCO_2R) mechanism. He has been working on the characterisation of minor products in an eCO_2R flow reactor via gas-chromatography mass-spectrometry (GC-MS) measurements conducted by **Dr Mikhail KOVALEV (Product Development Manager, AMPLE)**. The mass-spectrometry method used is based on proton-transfer reactions (PTR) and can reveal previously unknown products of very small concentrations which are separated via the GC column as shown in Figure 3.2. Mr Rihm was able to identify more than 20 products, 10 of which were previously unknown, including C_5 species for the first time. Most notably, selectivity trends of all these products were analysed under commercially relevant conditions and revealed mechanistic differences in constitutional isomers as well as stereoisomers. Based on these findings, a few general hypotheses regarding the reaction mechanism for high-current systems were derived. The results were published in *Energy & Environmental Science*.

Mr Rihm is now working on the automation and integration of experimental analysis and computational modelling of such processes, which he outlined in a recently published perspective. To enable the creation of meaningful multi-scale models at the required speeds, full automation of many research activities are necessary – from experimental chemistry to data analysis and model generation. He is now working on a digital twin of the CARES laboratory as part of The World Avatar (a larger expansion of IRP JPS).

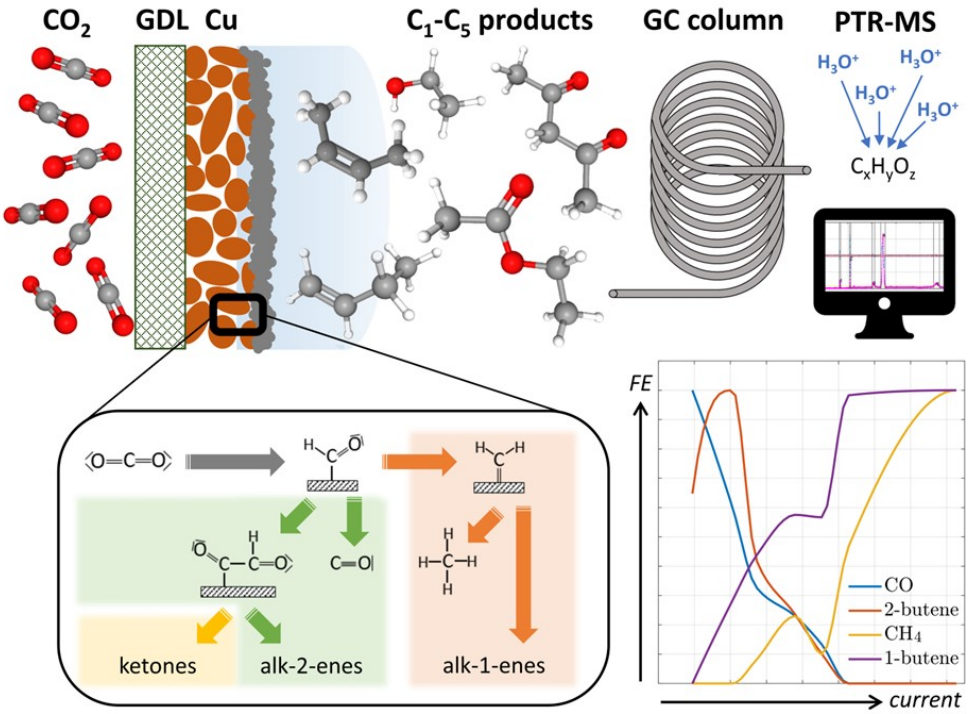


Figure 3.2: Illustration of the flow cell with gas-diffusion layer (GDL) and a copper catalyst (Cu), converting carbon dioxide to a variety of products that can be detected and analysed within a GC-MS setup. The sensitive PTR-MS used here allows for distinction of minor product isomers and detailed analysis of selectivity trends that unveil new insights into the general reaction mechanism of eCO_2R.

Mr Simon RIHM

Dr Aleksandar KONDINSKI's (Research Fellow, CARES) ongoing project focuses on developing explainable, knowledge-based AI technology that rationally designs covalent organic frameworks (COFs). COFs are a subclass of porous polymeric materials that show prominent properties and applications in various fields, including printable electronics and gas storage (CO_2 and water vapour capture from air).

To design new COFs automatically, Dr Kondinski is developing ontology and software agents that emulate the decision-making process of molecular engineers. In this regard, the ontology OntoCOFs takes into consideration aspects of chemical assembly modelling and chemical reactivity and builds upon existing knowledge of over 500 experimentally reported COF materials and ca. 400 available precursors. His COF discovery agents are based on inductive reasoning algorithms that conduct sets operations and derive the construction of new meaningful building block combinations, for which they are then able to print chemical synthesis useful for labs, construct the COF materials *in silico*, and to probe their properties (e.g., density, porosity, electronic structure, etc.).

Using this technology, Dr Kondinski intends to systematically explore the overall chemical space of rationally designed COFs, lab synthesis, and calculated properties. From this set of structures, the next target would be to allocate a subset of materials that have suitable properties and techno-economic parameters that make them applicable in real-world applications, namely printable electronics and gas capture.

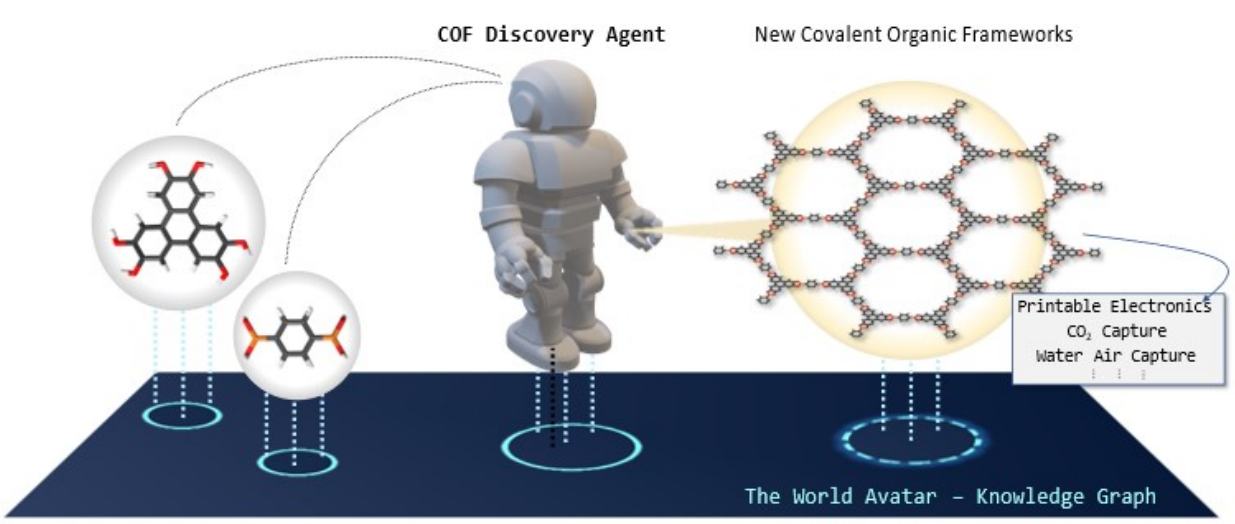


Figure 3.3: A COF discovery agent operates on the knowledge graph (dark blue surface), taking chemical building blocks information and deducing new rationally designed polymeric materials.

Dr Aleksandar KONDINSKI

Scientific output

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

The influence of alcohol, carbonate and polyethers as oxygenated fuels on the soot characteristics from a CI engine

Yong Ren Tan, Qiren Zhu, Yichen Zong, Jiawei Lai, Maurin Salamanca, Jethro Akroyd, Wenming Yang, and Markus Kraft, *Fuel*

DOI: 10.1016/j.fuel.2022.127296

Abstract: Dimethyl carbonate (DMC), ethanol (EtOH), polyoxymethylene dimethyl ether 1 (PODE1) and polyoxymethylene dimethyl ether 4 (PODE4) were blended with Jet A1 into fuel blends with 5 % oxygen content to investigate the effect of the oxygenated fuels on the soot produced by a compression ignition engine. Particle size distribution (PSD) was measured using a differential mobility spectrometer. Thermogravimetric analysis (TGA), Raman spectroscopy, ultraviolet–visible spectroscopy (UV–Vis) and Fourier transform infrared (FT-IR) spectroscopy were performed on the soot collected from the engine. The addition of EtOH, PODE1 improves brake thermal efficiency (BTE) by up to 4.5 %, while DMC reduces BTE by 0.9–1.5 % compared to Jet A1. EtOH fuel blends have the shortest combustion duration (10.0 deg), followed by PODE1, DMC and PODE4. EtOH blends also have the highest heat release rate peak (4–14 % higher than Jet A1). This, combined with improved premixing of EtOH fuel blend in the engine improves the combustion and reduces soot growth. PSD measurements showed that the addition of EtOH significantly reduces accumulation mode particle number concentrations by up to 70 % but promotes the formation of nucleation mode particles. Meanwhile, TGA revealed that the soot from oxygenated fuel blends oxidises at a lower temperature than Jet A1. Notably, PODE1 exhibited a reduction of 54 °C in the starting oxidation temperature, which is the largest reduction among the oxygenated fuel blends. Lastly, the conjugation length of the soot aromatic structure for the organic carbons (derived from the optical band gap of UV–Vis) is up to 11 % greater for the oxygenated fuel blends, indicating that oxygenated fuel blends promote organic carbon formation. The blending of oxygenated fuels in influencing the soot properties through the dilution effect, combustion condition effect and chemical effect is then critically assessed.

Fully Automated Kinetic Models Extend our Understanding of Complex Reaction Mechanisms

Simon Rihm, Jiaru Bai, Laura Pascazio, and Markus Kraft, *Chemie Ingenieur Technik*

DOI: 10.1002/cite.202200220

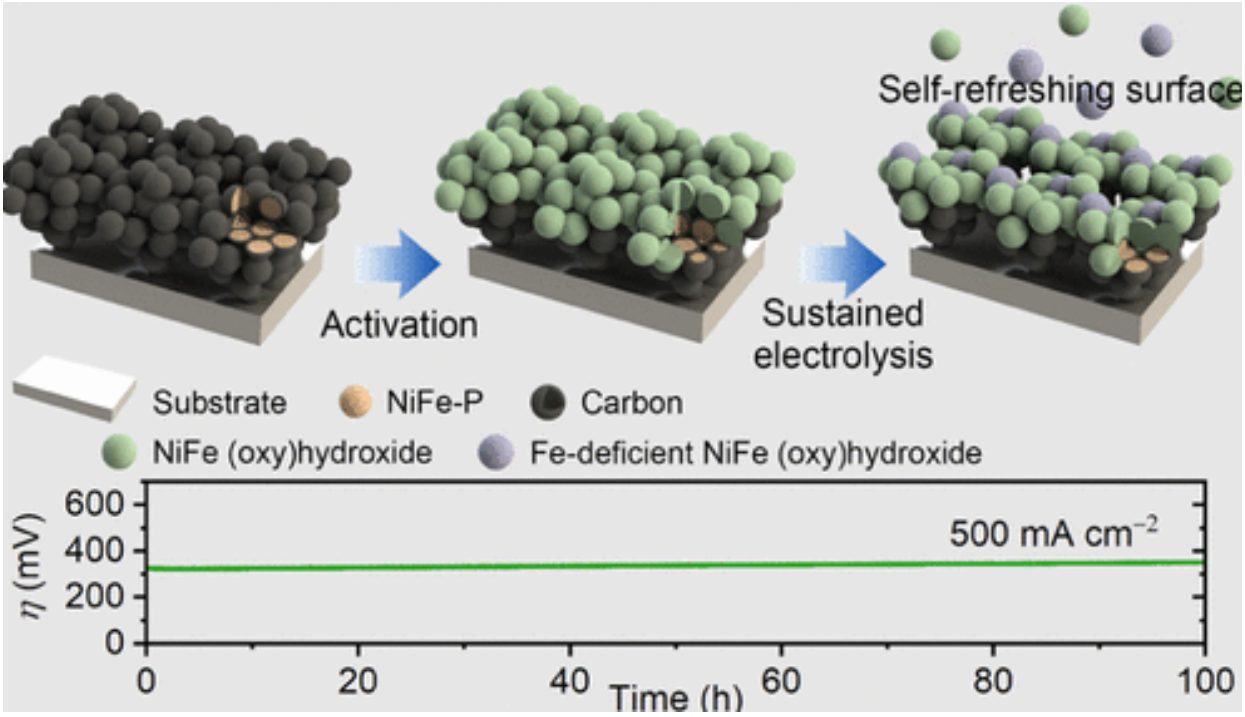
Abstract: Automating the creation and calibration of microkinetic models enables researchers to perform detailed analysis of reaction mechanisms as well as multi-scale modelling of reactors based on ab initio calculations. The example of electrochemical CO_2 reduction shows that this requires a structured and standardised representation of concepts across multiple scales. Massive progress has been made in this area through dynamic knowledge graphs, whereby the first partial successes can be reported in the area of mechanism generation, quantum mechanical calculations as well as calibration with experimental data.

Structural Evolution and Durability of Ultrafine NiFe Phosphide Nanoparticle/Carbon Composite Films in Water Oxidation at High Current Densities

Sheng Yuan, Manoel Manuputty, Markus Kraft, and Xu Rong, *ACS Applied Energy Materials*

DOI: 10.1021/acsaem.2c03514

NiFe phosphide (NiFe-P) is a highly active precatalyst for the oxygen evolution reaction (OER), but its compositional and structural changes during sustained electrolysis have not been thoroughly understood. Moreover, the size control of NiFe-P particles remains challenging yet desirable without multistep synthesis or surface capping agents. To realize this, flame aerosol synthesis (FAS) is a promising method due to its short particle residence time, tunable redox environment, and good scalability. Herein, the one-step FAS of NiFe-P is reported for the first time. With the controlled coformation of carbon, interlaced NiFe-P nanoplates and <5 nm NiFe-P nanoparticles are selectively synthesized on nickel foam in 10 min. At the anodic potential of OER, NiFe-P transforms into highly active (oxy) hydroxides in situ by surface oxidation and dephosphorylation. The overpotential of the optimal film at 500 mA cm^{-2} increases at only 0.28 mV h^{-1} over 100 h, making it among the most durable NiFe-based catalysts reported. Post-OER cyclic voltammetry, double-layer capacitance, and inductively coupled plasma mass spectrometry (ICP-MS) measurements indicate performance degradation to be mainly caused by the selective leaching of Fe from the (oxy)hydroxides. Counterintuitively, slight structural instability of the films induced by the electrochemical removal of carbon enhances durability by keeping a relatively stable surface Fe content through a self-refreshing mechanism.



Other activities and achievements

Mr Simon RIHM's (PhD student, CARES) article "Modelling a detailed kinetic mechanism for electrocatalytic reduction of CO_2" contributing to the 39th International Symposium on Combustion was selected as Distinguished Paper in the colloquium "Multi-Physics Phenomena". This paper, which was co-authored by **Dr Jethro AKROYD (Senior Research Fellow, CARES)** and **Prof Markus KRAFT (PI, CAM)** provides new insights into the voltage-dependent dimerisation reactions of *CHO and *CH_2 and potential mechanisms of deactivation, in the context of developing effective strategies for reducing greenhouse gas emissions.

Dr Aleksandar KONDINSKI (Research Fellow, CARES) was selected as a Young Star Editor for the journal *Polyoxometalates* published by Tsinghua University Press. This recognition highlights Dr Kondinski's expertise in the field and provides an opportunity to contribute to the advancement of polyoxometalate research through editorial work.

Dr Yichen ZONG (Research Fellow, NUS) has been forging connections with industrial partners, such as City Energy for hydrogen utilisation in Singapore, and PS Energy for the commercialisation of fuel additives.

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

Better energy efficiency, lower pollution, and decarbonisation in the marine sector is becoming of huge importance worldwide and for Singapore. This IRP addresses these significant problems by a series of research projects, including fundamental studies on particulate emissions from marine engines burning fossil or alternative fuels, waste heat utilisation methods such as the use of 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, some of the Tasks were not active due to shortage of personnel. Work Package 4.1 has shifted to ways of predicting jet ignition and dual-fuel combustion (such as that occurring in large marine engines). Dispersion simulations and measurement in Work Package 4.4 have focused on novel methods to include near-field mixing, measurements and apportionment of particulate emissions, and connection of the above with JPS.

There are two more researchers for this group, Dr B. Harikrishnan and Dr Law Li Chin whose work is reported under the C4T Emerging Opportunities Fund section. Their progress updates are on page 128 and 130 respectively but their external activities and achievements are listed here.

Professor Epaminondas Mastorakos, PI
University of Cambridge

Update on work package 4.1

Engine combustion — best fuel, best operating condition

In conjunction with C4T Emerging Opportunities Fund 04, **Dr B. HARIKRISHNAN (Research Fellow, CARES)** and Dr Savvas GKANTONAS (Research Associate, CAM) have further developed the Imperfectly Stirred Reactor Networking (ISRN) modelling approach. This method has already been used for large marine engines and was previously reported in the 17th Biannual Report. In this reporting period, the ISRN method has been used for mixing of hydrogen with hot air, studied as a preliminary canonical problem for hydrogen engines. The danger of autoignition must be assessed. The method has shown that it is capable of capturing correctly the autoignition locations. In the next 6 months, hydrogen and ammonia marine engines will be studied and the possibility of unwanted or wanted ignition will thus be captured properly.

Update on work package 4.2

Closed power cycles—selection and analysis

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

Update on work package 4.3

High-efficiency heat exchanger

Dr Mohamed Fadhel AYACHI (Senior Research Fellow, NTU), has recently joined the research group for this work package.

Update on work package 4.4

Process system model for the J-Park Simulator

Dr Ramesh KOLLURU (Research Fellow, CARES) carried out CFD simulations using Converge CFD to better understand the dispersion process of shipping emissions in the near field, and hence assist the development of atmospheric pollution calculations. The headwind case is shown in Figure 4.1. Three different grids have been studied to achieve grid independence of the CFD solution: a Coarse grid (46 Million Grid points), Medium grid (85 Million Points) and Fine grid (92 million points) and adaptive mesh refinement (AMR). Wind directions inclined to the ship's motion have also been carried out.

Figure 4.1 shows the computational domain used for the headwind case. Inlet profiles for velocity, turbulent intensity and turbulent length scales are prescribed at the inlet boundary (1). The bottom boundary (5) is the sea surface and is treated as a wall boundary with log-law velocity condition. The front and back boundaries (3 & 4) in the y direction are assigned symmetry boundary conditions. The outlet boundary (2) is imposed with outflow flow which simply says that there is no change in the flow. The top boundary of the domain is prescribed with the pressure and outflow boundary condition (i.e., Naumann boundary for all other variables).

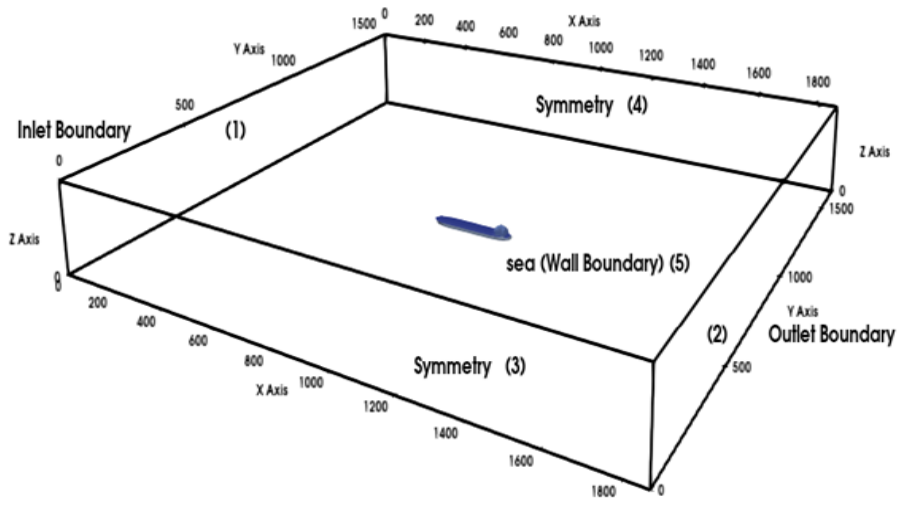


Figure 4.1: Computational domain used to study headwind. The spatial coordinates are in metres.

Dr Ramesh KOLLURU

The ship's engine exhaust is emitted at the top from a small pipe and diffuses in the turbulent wind. This is treated by following the evolution of a passive scalar, defined as 1 at the exhaust and 0 in the air. A typical grid generated by the adaptive mesh refinement process based on the passive scalar value is shown in Figure 4.2. Figure 4.3 shows the streamlines on the ship coloured based on the magnitude of the velocity. The recirculation zone in the wake region of the ship can clearly be seen. The plume disperses because of mixing by the turbulence and is also continuously reacting and generating other species. The evolution of the passive scalar 'ξ' from the exhaust of the main engine chimney at various planes is shown in Figure 4.4.

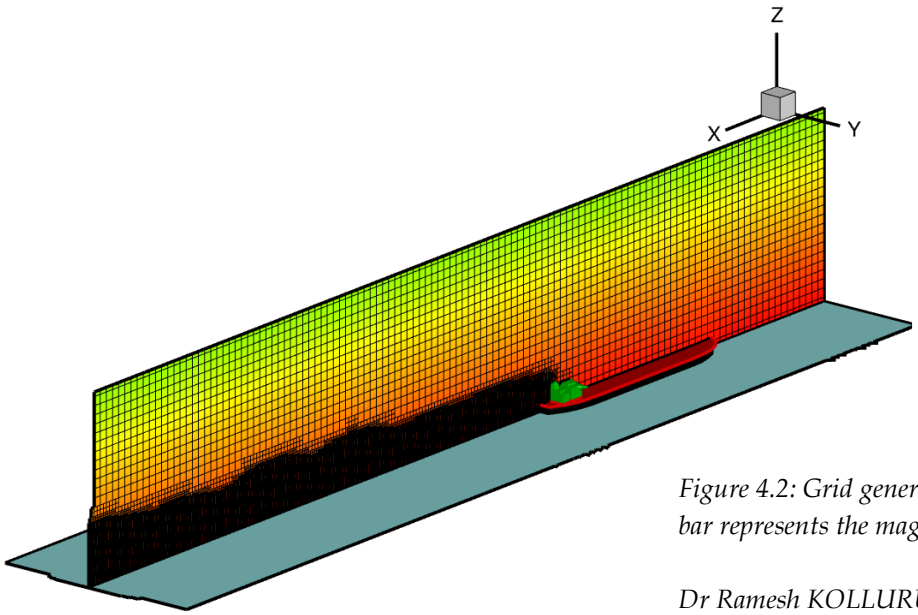


Figure 4.2: Grid generated by AMR. The colour bar represents the magnitude of the velocity.

Dr Ramesh KOLLURU

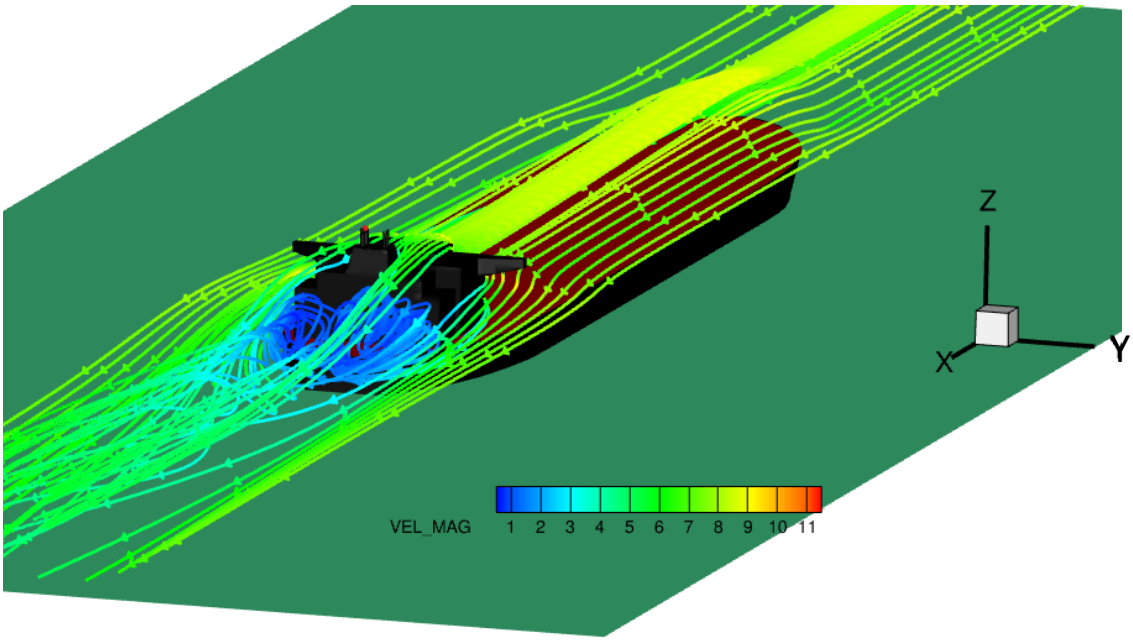


Figure 4.3: Streamlines coloured based on magnitude of the velocity. The model is generated in a 3D plane (X, Y, and Z).

Dr Ramesh KOLLURU

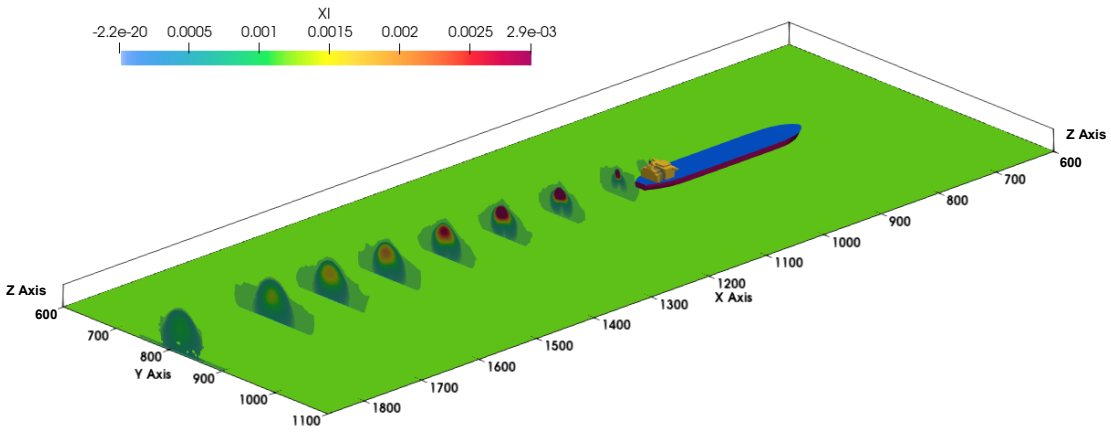


Figure 4.4: Evolution of the passive scalar Xi from the exhaust of the main engine chimney at various planes. The spatial coordinates are in metres.

Dr Ramesh KOLLURU

Figure 4.5 shows the distribution of passive scalar ξ between 0 and 1 on xz plane corresponding to the mid-section of the main chimney for the ship under consideration.

The chemical mechanism considered for this study is the Carbon Bond Mechanism IV (CBM – IV). This is a commonly used mechanism for studying atmospheric reactions and is typically used in studies of air pollution. This mechanism consists of 32 species which involves 70 thermal and 11 photolytic reactions. This is the mechanism which is designed for the numerical simulation of chemical process in urban and regional scale models. The input for the background concentrations for the species are taken from another study by Cao et al, "Sensitivity analysis of the dependence of the Carbon Bond Mechanism IV (CBM-IV) on the initial air composition under an urban condition". Typical emissions from the marine diesel engines commonly used in ships are CO, CO_2, NOx (NO, NO_2), SOx (SO_2), hydrocarbons, and smoke.

Incompletely stirred reacting network (ISRN) method which is a kinetic post processing technique is used here as a post-processing step of the CFD simulations. This method retains the turbulence-chemistry interactions and uses the conditional moment closure (CMC) of turbulent reacting flows (Gkantonas et al, 2020) to solve the chemical reactions in the plume as it is evolving. The ISRN equations are solved in mixture fraction space η which varies between 0 and 1.

The solution obtained from the ISRN equations are then transformed back to Figure 4.6, Figure 4.7 and Figure 4.8 to show the evolution of NO, NO_2 and O_3 respectively obtained after post processing with ISRN. It is clear that capturing simultaneously dilution and chemical reaction is important for capturing the evolution of the reacting plume and that this combined approach is needed for supplying the correct values in regional air quality models, which typically use grids of order of hundreds of meters, and hence the plume evolution is below this resolution.

References

1. Cao, L., Gao, M., Li, S., Yi, Z., Meng, X., 2019. Sensitivity analysis of the dependence of the Carbon Bond Mechanism IV (CBM-IV) on the initial air composition under an urban condition. Atmospheric Environment 215, 116860. https://doi.org/10.1016/j.atmosenv.2019.116860

2. Gkantonas, S., Giusti, A., Mastorakos, E., 2020. Incompletely Stirred Reactor Network Modeling of a Model Gas Turbine Combustor, in: AIAA Scitech 2020 Forum. Presented at the AIAA Scitech 2020 Forum, American Institute of Aeronautics and Astronautics, Orlando, FL. https://doi.org/10.2514/6.2020-2087

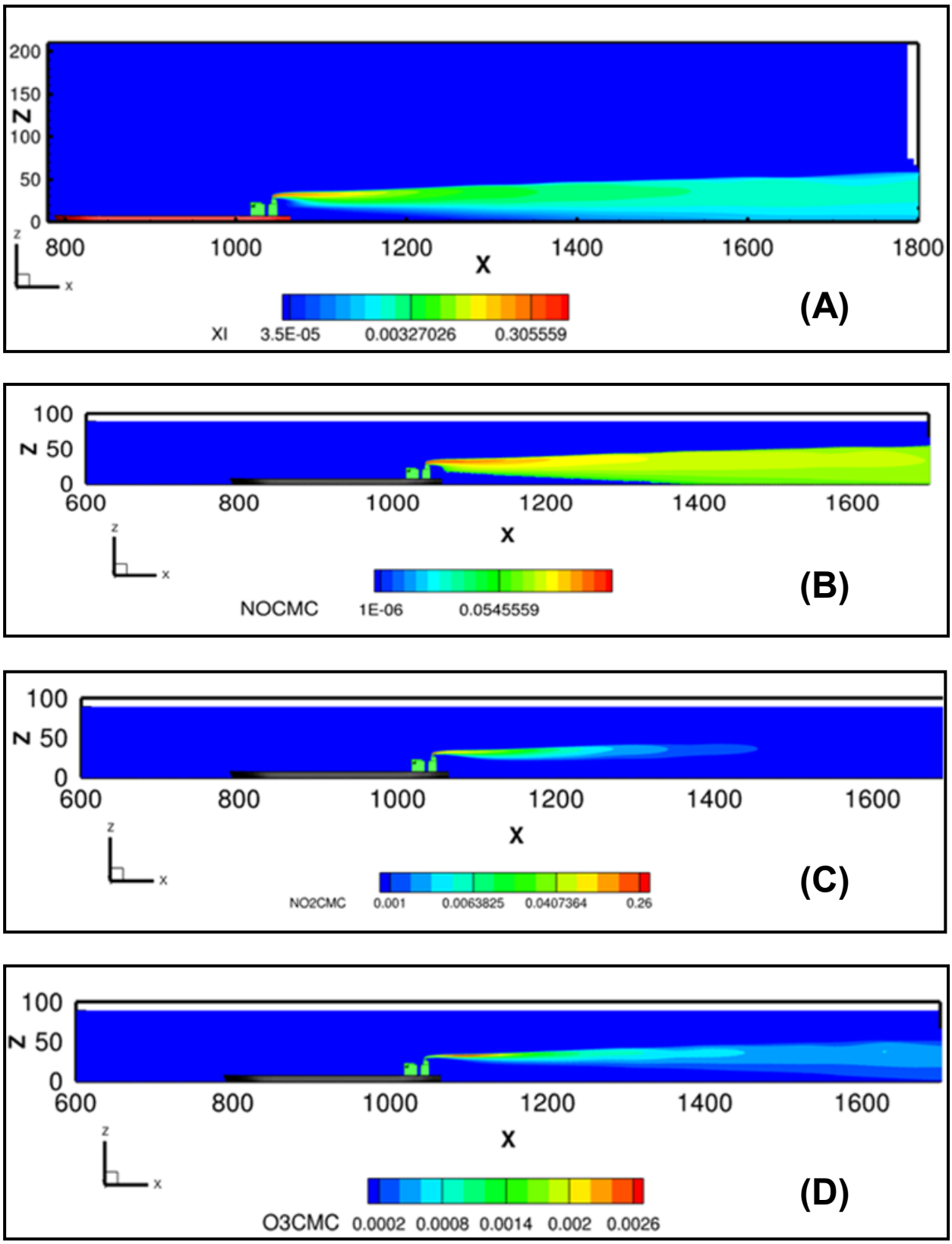


Figure 4.5: (a) Distribution of passive scalar Xi on the planes X and Z. The evolution of (b) NO; (c) NO_2; and (d) O_3 is shown after post-processing with ISRN. The spatial coordinates are in metres.

Dr Ramesh KOLLURU

Dr Molly HAUGEN (CARES Visiting Scientist, CAM) builds on her work of measuring particulate emissions with handheld devices and an aerial drone. Dr Haugen has been working on a variety of brake and tyre wear projects at the University of Cambridge. In particular, assessing the elemental composition of heavy and light-duty vehicle tyres, compared against a 25-elemental standard. This analysis contributes to building the largest database for unworn tyre composition. With the elemental analysis, correlations between elements have been used to give a fingerprint that can be used for source apportionment studies. By investigating the tyre composition in relative quantities, it can be used to determine if urban particles originated from tyre wear. The analysis included differentiating between side wall and tyre tread. The comparison noted that the components of the tread have 10 elements that are statistically different. The comparison between heavy goods and light-duty tyres revealed there were 6 elements that had statistically different concentrations between the two tyre types. These differences are directly related to the duty cycle requirements for each type of tyre.

The results of this work are useful for building the necessary knowledge base for the continuation of the particulate matter measurements in Singapore as they will allow greater differentiation between sources such as far-away forest fires, shipping, airplane or road transport.

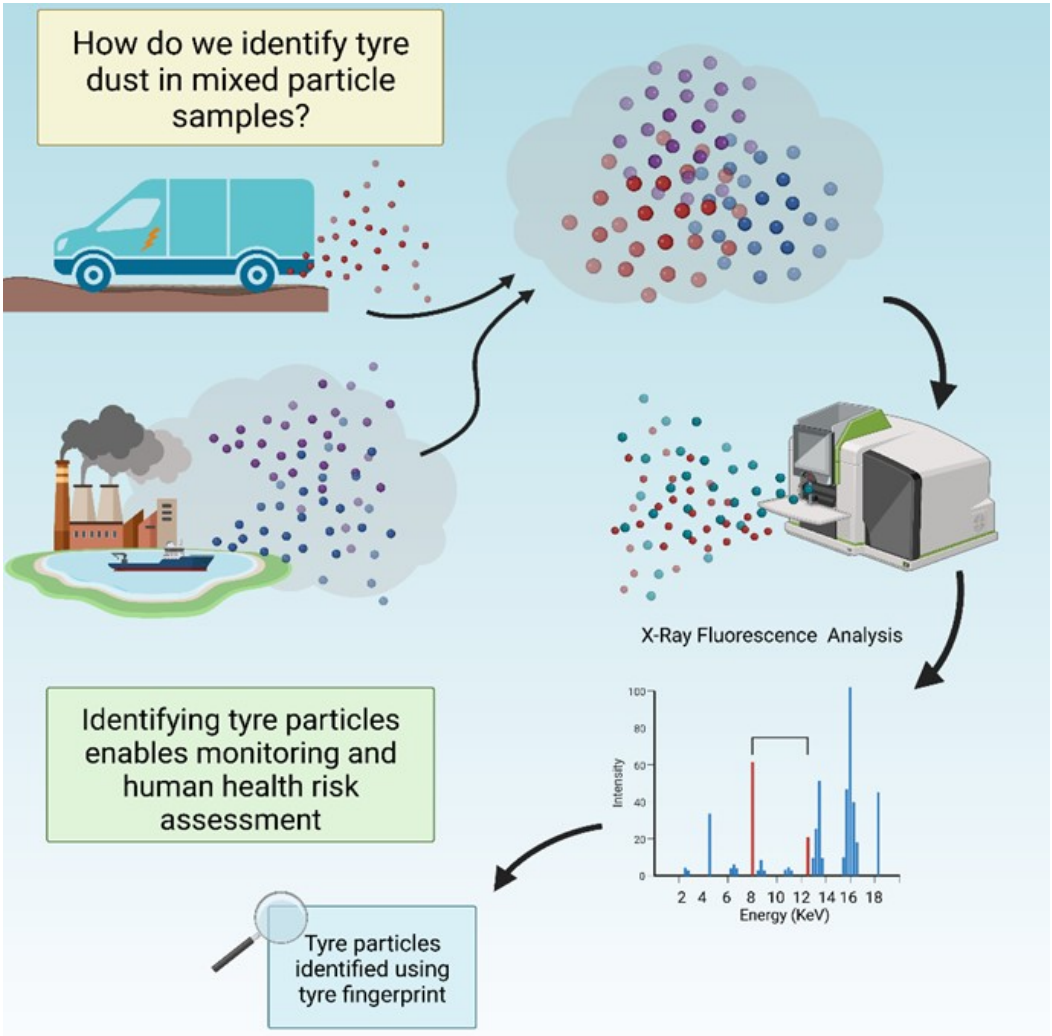


Figure 4.6: Flow chart for characterising non-exhaust emissions in the atmosphere based on laboratory speciation and analyses. Here, the framework is laid out for the current work, as well as future work needed for improving the quality of Singapore's air quality. Image created with BioRender.com

Dr Molly HAUGEN

Other activities and achievements

Dr Molly HAUGEN (CARES Visiting Scientist, CAM) presented her work on particulate dispersion in Port Rafina, Greece at three events:

- Two-part talk and drone demonstration on using drone technology for particulate monitoring at CREATE Tower and NUS campus on 20 April 2023 in Singapore.
- 33rd Coordinating Research Council Real World Emissions Workshop from 26 – 29 March 2023 in Long Beach, California. This was a platform presentation.
- Transport Research Arena 2022 Conference from 14-17 November in Lisbon. This was a rapid presentation.

Dr Haugen also won an Energy Interdisciplinary Research Centre Small Grant for composition studies on testing brake and tyre wear.

Prof Epaminondas MASTORAKOS (PI, CAM) presented "Systems analysis of low-carbon marine propulsion" at EU-Shipping-BCE 2022 from 19 – 21 September 2022 in Greece. Prof Mastorakos also participated in a panel discussion for the following talk.

Prof Mastorakos and **Dr Li Chin LAW (Research Engineer, CARES)** were panellists for the Solutions to Net Zero Seminar held by RINA Marine on 29 November 2022 in Singapore.

Prof Mastorakos has become a member of the Editorial Board of the Springer journal *Emission Control Science and Technology*, triggered partly by the recent work on emissions from shipping sources.

Dr Law reports that an NDA has been signed with RINA, a shipping classification agency, for discussions leading to future joint proposals and collaborations. A joint paper with a RINA engineer has also been submitted.

Discussions with CLEOS (a joint venture between Gaslog Ltd and Olympic Ship Management) on shipping decarbonisation have commenced, with CARES performing numerous presentations of the lifecycle assessment work to this industry.

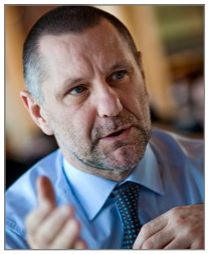
A website was also launched called https://lowcarbonship.com that utilises Dr Law's research measuring alternative fuels against shipping performance and design. The purpose is to engage stakeholders in the shipping industry to compare the design of future ships against current ships. Naval engineers from shipping companies have already provided valuable feedback and the website will continue to be refined.

IRP BB

BETTER BUSINESS: PATHWAYS TO INDUSTRIAL DECARBONISATION

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

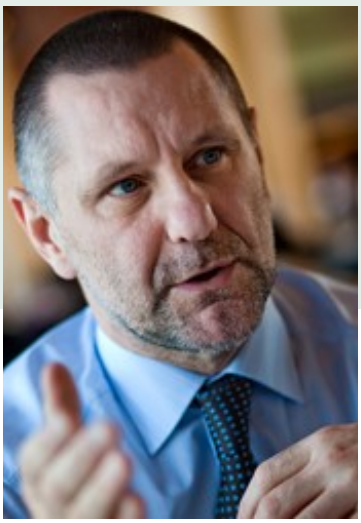
IRP BB Principal Investigators:



Professor Steve EVANS
University of Cambridge

Professor S. VISWANATHAN
Nanyang Technological University

Professor Kenneth HUANG Guang-Lih
National University of Singapore



OVERVIEW

Over the last few months, the group have continued to proceed with the existing projects and start new ones.

For the research on business model innovations related to solar energy adoption, WPBB.1 have revised the manuscript on the previous work. Meanwhile, they have also started a new research project discussing hybrid pricing mechanisms for solar third-party ownership models. The WPBB.3 project on how strengthening institutions for VC investment influences the pollution behaviour of firms in China's chemical and energy-intensive sectors has been invited to make a resubmission to one top journal, *Management Science,* and has also been accepted for international conferences. Based on the first study, we continue to conduct empirical analyses on the different roles of VC types (government VCs and private VCs) in influencing the green innovations of focal firms and their underlying mechanisms. For the related Emerging Opportunities Fund project, first-round results have been generated on the role of the Chief Sustainability Officer on a company's sustainability performance in terms of emissions and energy use. We are in the process of writing a manuscript titled "Decarbonization in the Oil and Gas Sector: Technologies and Strategies".

In addition, a new project on ecosystem-view transformation enabled and empowered by advanced digital technologies is in the process of finishing preliminary data collection from the industry and starting a new round of data collection with the refinement of design and strategy.

Professor Steve Evans, PI
University of Cambridge

Update on work package BB.1

Business model innovation potentials

Dr Lemy MARTIN (Research Fellow, NTU) and **Prof S. VISWANATHAN** (**PI, NTU**) have continued to work on the business model innovations related to solar energy adoption, the first manuscript has been finished for submission with additional sections on pricing algorithms for heterogeneous customers and buyback policies for selling solar energy back to the grid. They have also started the second manuscript discussing hybrid pricing mechanisms for solar third-party ownership models.

Update on work package BB.2

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

Dr Yan WANG (Research Fellow, NTU) and **Prof S. VISWANATHAN (PI, NTU**) collected ESG-related data (e.g., disclosure ESG, carbon per unit of production, scope 1, scope 2, scope 3, coal used, electricity used, etc.) and company key statistics (e.g., sales, profits, etc.) for 504 companies from 21 industries belonging to the S&P 500 from Bloomberg Terminal. Dr Wang has pre-processed the data and conducted the data analysis using mixed-effects regression models to evaluate the role of the chief sustainability officer (CSOs) on the company's sustainability performance in terms of emissions, energy use, etc. She obtained the first-round results which show that companies with CSOs overall outperformed companies without CSOs in terms of disclosure score. However, this positive effect on reducing carbon emissions is not evident except for certain industries, e.g., utilities. Based on the current results, she is in discussion to deepen their analysis to generate more insights. They expect to complete the first draft manuscript by October.

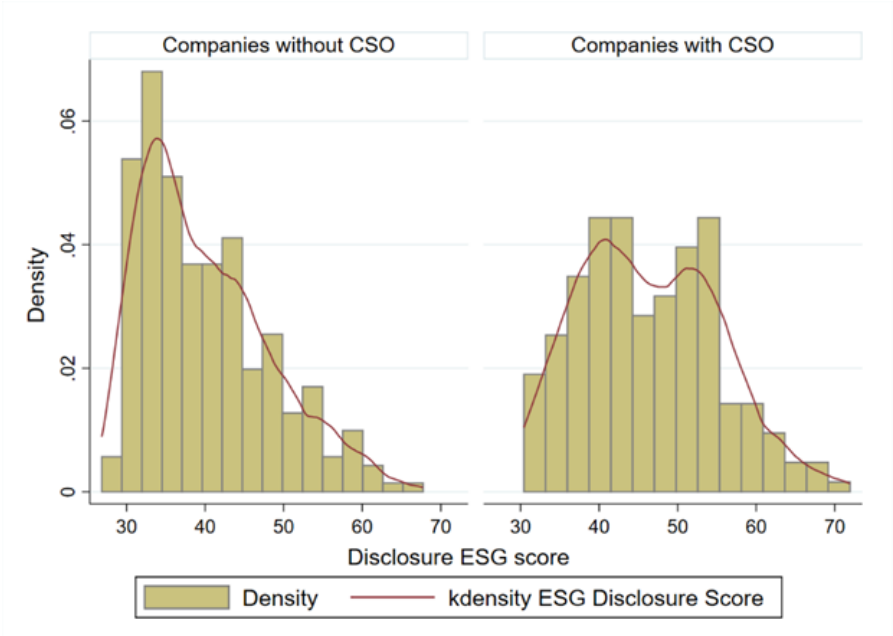


Figure 5.1: Illustration of the difference in disclosure ESG scores for companies with and without CSOs. The figure indicates that the distribution of ESG scores for companies without CSO is right-skewed, while it is relatively normal for companies with CSO.

Dr Yan WANG

Update on work package BB.3

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

Dr Michelle Xiaomin FAN (Research Fellow, NUS) continues to work with **Prof Kenneth G. HUANG (PI, NUS)** to analyse how strengthening institutions for VC investment influences the pollution behaviour of firms in China's chemical and energy-intensive sectors. After several rounds of revisions, this manuscript has been submitted to a top-tier journal, *Management Science*, and received an invitation for resubmission. The manuscript has been resubmitted after reframing and extensive revision based on the reviewers' comments. Meanwhile, this study has been accepted for presentation at several prominent international conferences, including the International Association for Chinese Management Research Conference from 14 – 18 June in Hong Kong, the INSEAD Doriot Entrepreneurship Conference from 15 – 16 June in Singapore, and the Academy of Management Annual Meeting from 4 – 8 August in Boston.

Building upon the first project, they continue to investigate the various roles of different VC firms in influencing the focal firm's green innovation in a new project. They are currently in the stage of conducting extensive empirical analyses. To do this, they have collected the data of all listed firms in the Chinese A-share market that have received VC funding from 1999 to 2019. Specifically, they identify and categorise the VC firms into government VC (GVC) and private VC (PVC) firms. By adopting an exogenous shock that has differential impacts on GVC (treatment group) and PVC firms (control group), they can ascertain the differences between the treatment group and control group after the policy shock regarding green innovations.

Update on work package BB.4

Industrial sustainability and ecosystem trends

Guided by **Prof Steve EVANS** (**PI, CAM**), **Ms Can CUI** (**PhD student, CARES**) has further analysed the challenging parts of constructing an ecosystem-view transformation. In addition, they have completed preliminary data collection from the industry and are now in the process of working on a new round of data collection by refining their design and strategy. They obtained initial findings on how to innovatively interact with novel partners beyond the traditional value chain to create sustainable value and how to help companies think outside their industry to formulate unconventional collaborations, etc. They conducted a comparison study by comparing SMEs and industrial group companies to analyse their different methods of unconventional collaborations and sustainability. Preliminary data reveals a difference between the two groups in terms of their attitudes and considerations, i.e., their understanding towards sustainability and collaboration, their partnership strategy with companies from different areas to drive sustainable value, and the challenges they face in forming collaborations.

Emerging Opportunities Fund

The team also worked closely with C4T Emerging Opportunities Fund 06 - Carbon reduction strategies of top chemical companies, see page 132 for further updates.

Other activities and achievements

Ms Can CUI (PhD student, CARES) and **Prof Steve EVANS (PI, CAM)** presented "Preliminary exploration of the role of stranger collaboration in delivering sustainability" at the 6th International Conference on Applied Research in Management, Business and Economics on 3 March 2023 in Switzerland

Prof S. VISWANATHAN (PI, NTU) participated as a panellist for "Sustainable Net-Zero Mechanisms for Tropical Cities" on 28 October 2022 at the Asian Clean Energy Summit for Singapore International Energy Week.

As PI through the Centre for Business Sustainability, NTU, Prof Viswanathan has been awarded a Research Consultancy Project by Land Transport Authority (LTA) for a study on transport decision-making.

Prof Viswanathan has also been awarded an NRF Intra-CREATE collaborative grant for "Singapore's Pathway to Carbon Neutrality: Analysis of New Technologies"

Prof Kenneth HUANG (PI, NUS) has been appointed the Dean's Chair (starting January 2023) at NUS in recognition of his outstanding and impactful scholarly accomplishments. He has also been appointed the Editorial Board member of a top-tier management journal, *Organization Science*

IRP JPS

THE J-PARK SIMULATOR

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

IRP JPS Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Raymond LAU Wai Man
Nanyang Technological University

Professor Iftekhar KARIMI
National University of Singapore

OVERVIEW

Over the past six months, we have significantly improved the architecture and underlying technologies of the J-Park Simulator (JPS) to increase its autonomy and connectivity to the physical world. We have augmented the existing Access Agent and time series classes and developed the Relational Database Access Agent to support the querying of relational databases. We have also developed a tool and an algorithm for dynamically generating user interfaces by querying the properties, subclasses, instances, values and units from ontologies uploaded to the knowledge graph. Furthermore, as part of an attempt to digitalise and automate the CARES Laboratory, we have developed an Android mobile application that allows users to view and control the real-time status of various laboratory equipment. We have also implemented a system to collect a wide range of environmental data and semantically mapped them to human activity for health-related the World Avatar (TWA) questions. We have worked on extending the 3D visualisation of the digital twin of the CARES laboratory to retrieve, consolidate, and visualise both static and real-time data associated with the laboratory building and its various equipment across multiple domains (chemistry, building management, and energy management).

We have worked on creating a digital twin for smart cities using knowledge graph technologies and evaluated the impact of potential flood scenarios in different domains to promote interoperability. Open-source data from various Application Programming Interfaces (APIs) and multiple data streams, such as geospatial city data, building metadata, environmental observation data, and transient information such as river water levels and flood warnings, were all instantiated into the knowledge graph.

We have also worked on an updated version of the Marie Knowledge Graph Question Answering (KGQA) system, which uses an Information-Retrieval method to answer questions by generating a set of candidate answers and ranking them. This update improves the system's robustness and response speed significantly.

Professor Markus Kraft, PI
University of Cambridge

Update on work package JPS.1

Big data — sensors and data modelling

Mr Simon RIHM (PhD Student, CAM), **Mr Wilson ANG (Software Developer, CARES)**, **Mr Shin Zert PHUA (Software Developer, CARES)** and **Ms Xinhong DENG (Software Developer, CARES)** have made progress on the automation of the CARES laboratory within the knowledge graph. This is part of an attempt to create a digital twin of the chemistry laboratory at CARES, encompassing all ongoing related efforts around chemistry, assets, and buildings as dedicated use cases. This digital twin integrates live data from various equipment with the Building Information Model (BIM) of the CARES laboratory, in order to create an interoperable system which allows monitoring of the energy consumption of the laboratory and its devices along with suggesting and implementing measures to reduce this usage.

Currently, Mr Rihm and Mr Ang are working on integrating live data (such as temperature and airflow) provided by the Building Management System (BMS) with the existing laboratory model in the knowledge graph to reduce its energy consumption and carbon footprint. For example, Mr Rihm and Mr Ang have analysed the data and detected anomalies in the operations of the walk-in fumehoods and the make-up air units in the laboratory. This issue was investigated together with the CREATE Building Management Office, and found that Mr Rihm and Mr Ang have correctly identified the faulty parts and non-optimal settings, which had not been detected by the standard sensor and notification system. The faulty parts are currently undergoing replacement. They also suggested changing the off-coil and supply temperatures of the make-up air units to optimise and reduce energy consumption, and are currently investigating the effects of the changes made.

Mr Ang also worked on a Radio-Frequency Identification (RFID) system that can track the in/out status of chemical containers for an explosive pre-

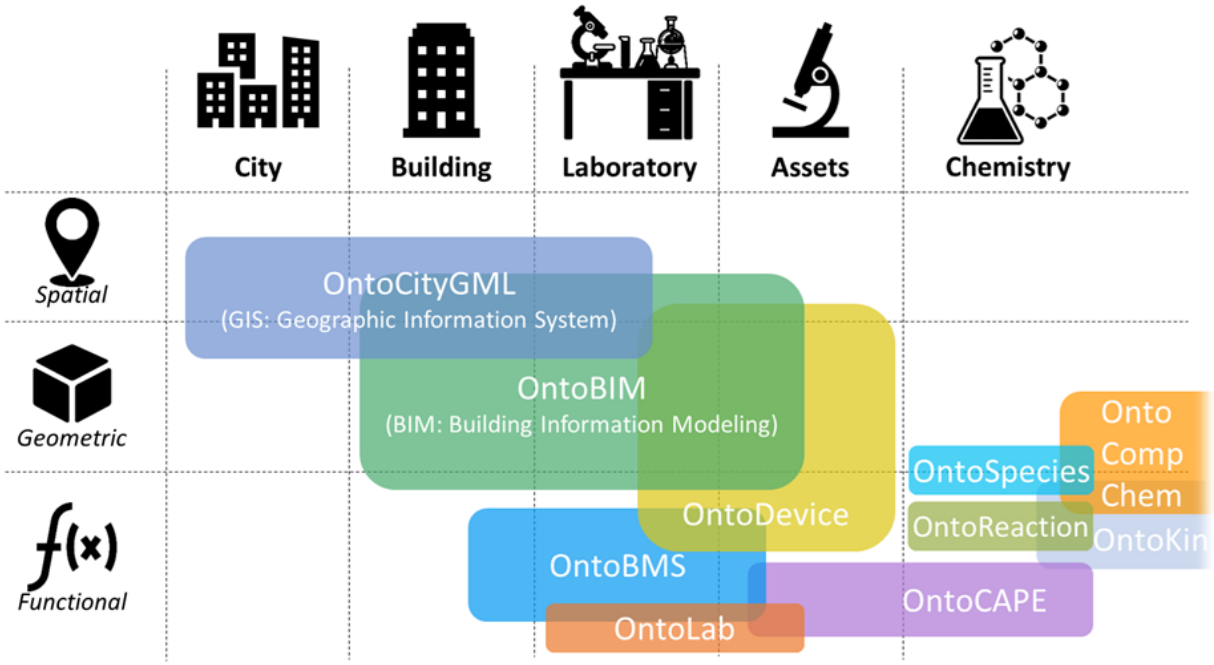


Figure 6.1: Representation of concepts across different scales to facilitate a digital twin of the chemistry laboratory. This entails the usage of existing ontologies such as OntoCityGML to describe building information or OntoCAPE to represent the chemistry domain. It also uses new ontologies such as OntoLab to represent experimental setups and OntoReaction to model the reactors and processes taking place in them. Combining these concepts will allow us to implement and connect existing use cases of 3D visualisation, data analysis of experimental setups, and chemical models based on first principles.

cursor cabinet using the RFID Query Agent, which works in tandem with several other agents such as the RFID Agent, RFID Update Agent, and Email Agent. The RFID Query Agent is designed to carry out a series of queries to the knowledge graph to retrieve information such as the RFID label tag's latest status, timestamp, tagged object label, chemical species label and chemical species Globally Harmonized System of Classification and Labelling of Chemicals (GHS) Hazard statements. With this information, the agent then determines whether the tagged item has been out of the cabinet for longer than allowed and, if so, triggers the Email Agent. The Email Agent is then responsible for crafting the alert email containing the information regarding the hazardous items and sending it to the designated personnel.

Figure 6.1 shows the representation of various concepts across different scales and domains that would be needed to facilitate a digital twin of the chemistry laboratory. To achieve true interoperability across these different scales and domains, Mr Ang has worked on extending an existing ontology called OntoDevice, in collaboration with **Mr Hou Yee QUEK (Research Associate, CARES)**, **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)** and **Dr Feroz FARAZI (Research Associate, CAM)**. The extension includes the addition of several concepts and properties to link Smart Applications REFerence Ontology (SAREF) to other existing ontologies such as Semantic Sensor Network (SSN), Ontology of Units of Measure (OM) and GeoSPARQL. These extensions can represent a device's capabilities, such as measurement range, accuracy and precision, the quantities and units associated with the measurements, and the device's location.

Mr Phua has been working on the semantic mapping of human activity for health-related questions. He has collected a wide range of data using the SensorLogger mobile application, including acceleration, magnetic flux density, gravity acceleration, location, speed, noise, ambient light intensity, and screen brightness. He has developed the Sensor Logger Mobile App agent which receives the data collected by the application and downsamples it based on the user-specified downsampling rate and type. The agent then instantiates this data into the knowledge graph to demonstrate a mapping between human activities and surrounding environmental data. Mr Phua also developed the Sensor Logger Mobile App Query agent which allows users to query for the instantiated data within a specific time frame

Figure 6.2: Trajectory of a human, augmented with weather data and simulated ship emissions dispersion data.

and location. This serves as a proof-of-concept of how environmental exposure, such as pollutant emissions, may affect human health, which is particularly important for workers in industrial plants, emphasizing the importance to take the necessary steps to decarbonise industries. By combining this data with data from virtual sensors that simulate the dispersion of pollutant emissions from ships, we can investigate the ships' activities on the health impact on humans (Figure 6.2). This is also explored in the EOF3 project "Impact of Singapore's Shipping Activities on Urban Air Quality" on page 127 where we study the dispersion of various pollutants from ships and other emitting sources, and the influence of a diverse range of factors on this dispersion model using the knowledge graph.

Ms Deng aims to create a lightweight and user-friendly mobile platform to link the real world to its digital twin in the knowledge graph, to significantly improve data accessibility. As part of this goal, she developed the BMS Query Agent to query data from the knowledge graph and an Android mobile application that allows users to view and control the real-time status of equipment in the CARES laboratory. The mobile application is integrated with the updated Digital Twin Visualisation Framework (Figure 6.3). Currently, she is developing a feature to allow users of a certain clearance level to have write access to the laboratory equipment via the knowledge graph.

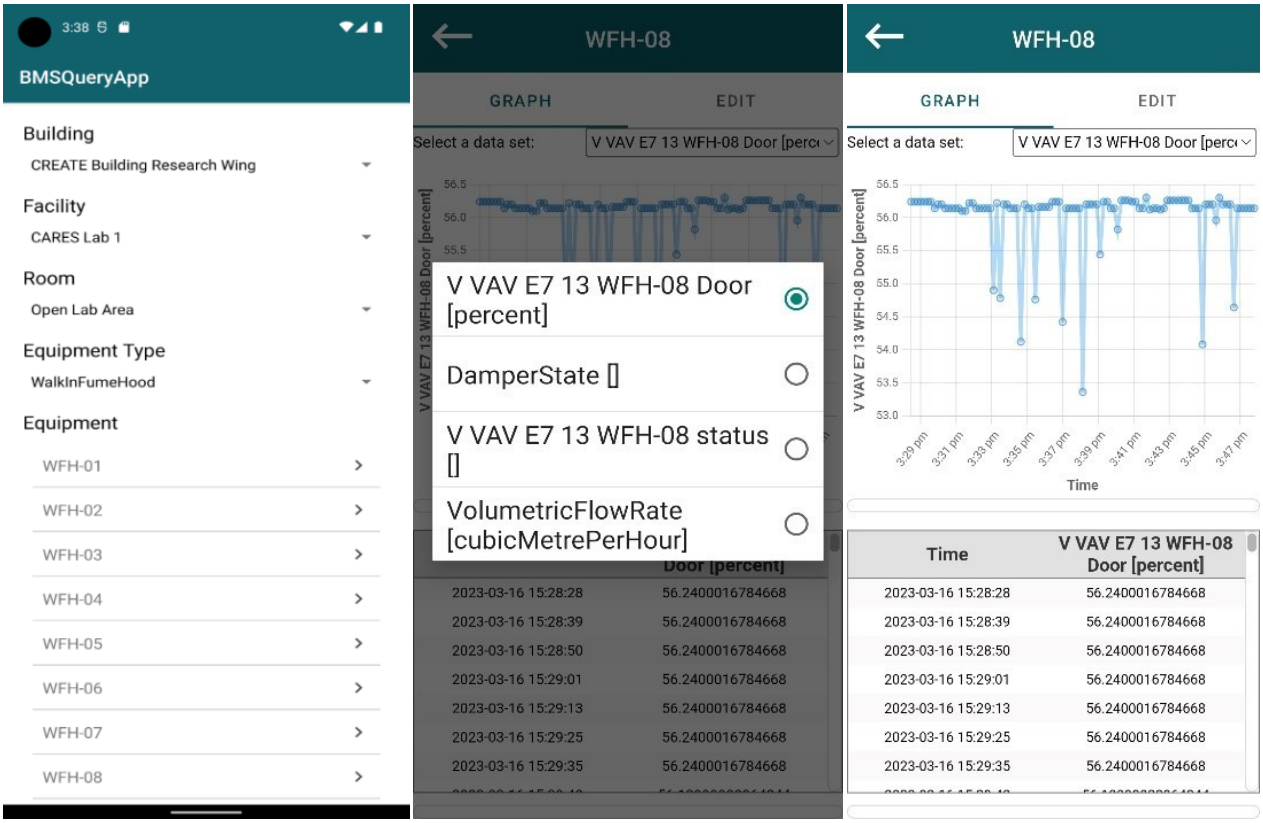


Figure 6.3: User interface of the Android mobile application which allows users to query for the status of different laboratory equipment and visualise the time series obtained.

Update on work package JPS.2

Surrogate models, superstructure and architecture development

Dr Sebastian MOSBACH (Senior Research Fellow, CARES), **Dr Casper LINDBERG (Research Fellow, CARES)**, **Dr Jethro AKROYD (Senior Research Fellow, CARES)**, **Dr Feroz FARAZI (Research Associate, CAM)**, **Ms Mehal AGARWAL (Software Developer, CARES)** and **Mr Shin Zert PHUA (Software Developer, CARES)** have been improving the World Avatar (TWA) infrastructure which includes augmenting the existing Access Agent and time series classes and developing the Relational Database Access Agent to query relational databases.

Ms Agarwal, in collaboration with Dr Lindberg, developed the Relational Database (RDB) Access Agent by extending the Store Client Interface and Access Agent framework to support the querying of relational databases. Relational databases are a widely used tool for large datasets; integrating the Access Agent to query such databases allows the use of existing, optimised solutions to tackle problems such as processing speed and storage, thereby helping in transitioning various real-world scenarios to use knowledge graphs.

She also developed the OntoRDBRouter ontology for representing RDB routing maps. She created a shared interface comprising general methods supporting both Triple Stores and RDBs and an interface with SPARQL-specific methods. She then developed the RDB Access Agent, which comprises the RDB Store Client, which can connect, query and update RDBs automatically, and the RDB Store Router, which maps user-specified RDB labels to the corresponding RDB Uniform Resource Locator (URL) used to establish a connection to the database. Ms Agarwal also developed the RDB Access Agent Caller, which is used to generate and send HTTP requests to the RDB Access Agent and integrated the RDB Access Agent into the Docker-compose stack for ease of deployment.

Dr Lindberg improved the Access Agent by adding a feature to remotely clear the StoreRouter cache and to allow an agent to use the Access Agent to retrieve the SPARQL query and update endpoints for a resource without performing a SPARQL operation.

Ms Agarwal also refactored the existing time series classes to update the process of instantiating time series based on the extended OntoTimeSeries ontology. The modified instantiation

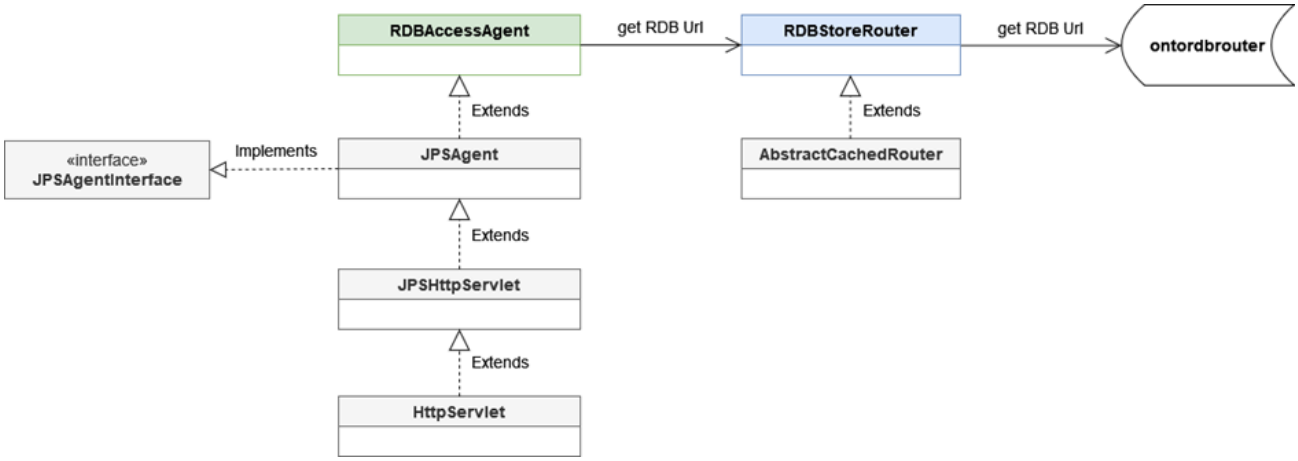


Figure 6.4: A diagram of the Relational Database Access Agent (RDBAccessAgent) implementation within the JPSAgent framework. The RDBAccessAgent receives an HTTP request for the URL of a target relational database resource. The RDBStoreRouter, which extends the AbstractCachedRouter class, either fetches the URL from the cache if it exists or queries the ontordbrouter triple store.

process accommodates the five types of time series, i.e., Instantaneous, Average, Stepwise Cumulative, Cumulative Total, and General time series. Mr Phua created a downsampling library that can downsample and aggregate time series using functions such as minimum, maximum, median, average count, sum, and instantaneous. This improves the efficiency of instantiating time series into the knowledge graph.

Dr Akroyd, Dr Mosbach and Dr Farazi developed a tool and an algorithm for dynamically generating user interfaces by querying the properties, subclasses, instances, values and units from ontologies uploaded to the knowledge graph. The tool has been tested by building the material passport user interface that will enable industrial users to provide data about recyclable composite material-made products and components of the automotive industry. The underlying algorithm takes a set of classes as the input and composes a query to retrieve all data associated with the input classes. The result is returned in a JavaScript Object Notation (JSON) object. The algorithm traverses through the object properties in the data by retrieving the classes defined in the range to identify their properties until the terminating condition is evaluated as true.

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES) is involved in training, supporting and providing guidance, especially to new team members, concerning documentation, questions on software design, agent development, and non-functional requirements such as performance and scalability. **Ms Srishti GANGULY (Project Engineer, CARES)** is involved in testing, deploying, and maintaining the various projects in TWA. Ms Ganguly has also migrated the projects in TWA from Java 8 to Java 11.

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)** created the material passport ontology to describe products, components and their constituent materials to enable the development and publishing of material passports. The ontology represents the component's identification properties such as name, brand/trade name, manufacturer details, the Global Trade Item Number (GTIN) or European Article Number (EAN), functionality and image. It also covers the component's physical (e.g., density, resistance, rigidity and weight), chemical, biological, temporal (e.g., expected lifetime and service life), and thermal properties. This ontology is used to develop a material circularity calculator and can simplify the automation of supply chain in industries, to promote circular economy and resilient logistics for achieving sustainable industry.

Furthermore, Dr Akroyd, Dr Mosbach and Dr Farazi modelled the domain knowledge of composite materials in an ontology called OntoCompMat, which reuses the Elementary Multiperspective Material Ontology (EMMO). The composite material was modelled with several subclasses based on matrix material, reinforce-

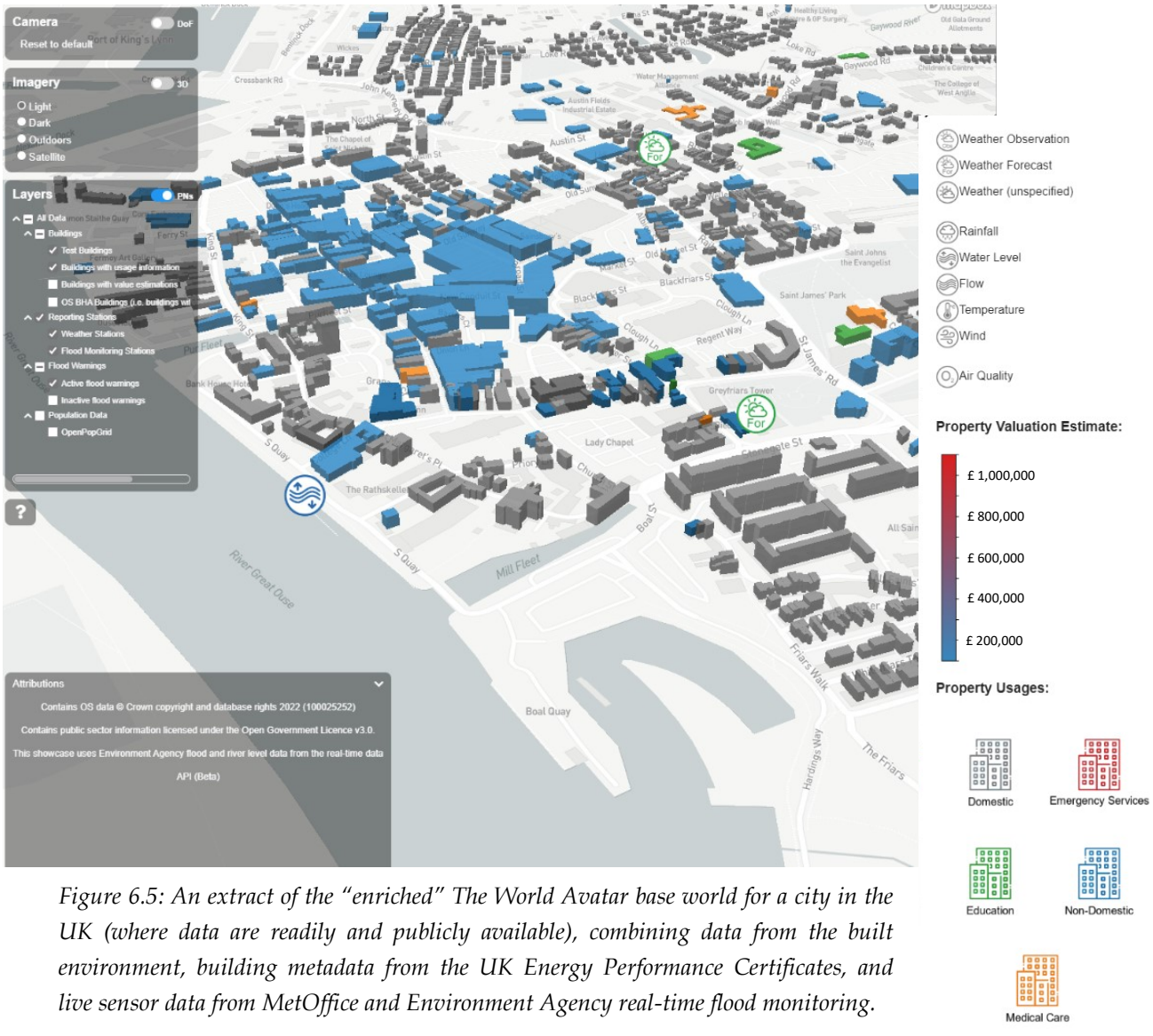


Figure 6.5: An extract of the "enriched" The World Avatar base world for a city in the UK (where data are readily and publicly available), combining data from the built environment, building metadata from the UK Energy Performance Certificates, and live sensor data from MetOffice and Environment Agency real-time flood monitoring.

ment type, manufacturing process, the orientation of reinforcement, functional requirement, resin type, fibre type and structure, with all these subclasses having further detailed classifications. OntoCompMat also included modelling manufacturing aspects, considering processes such as wet lay-up, resin transfer moulding, pultrusion, filament winding, compression moulding, injection moulding, vacuum infusion, and autoclave.

Dr Akroyd, Dr Mosbach and Dr Farazi also completed a background study to create an ontology for managing multi-hazard risks. This ontology will represent data about exposure and vulnerability, hazard, disaster damage, satellite and in-situ observation and climate projection.

Mr Markus HOFMEISTER (PhD Student, CAM) worked on creating a digital twin for smart cities using knowledge graph technologies. He evaluated the impact of potential flood scenarios in different domains to promote interoperability based on 'Findable, Accessible, Interoperable, and Reusable' (FAIR) data principles. This evaluation includes data from multiple data streams such as geospatial city data, information about buildings and their usages, near real-time environmental observation data, and transient information such as river water levels and flood warnings. This data was obtained from various open-source Application Programming Interfaces (APIs) and instantiated into the knowledge graph. Mr Hofmeister also developed computa-

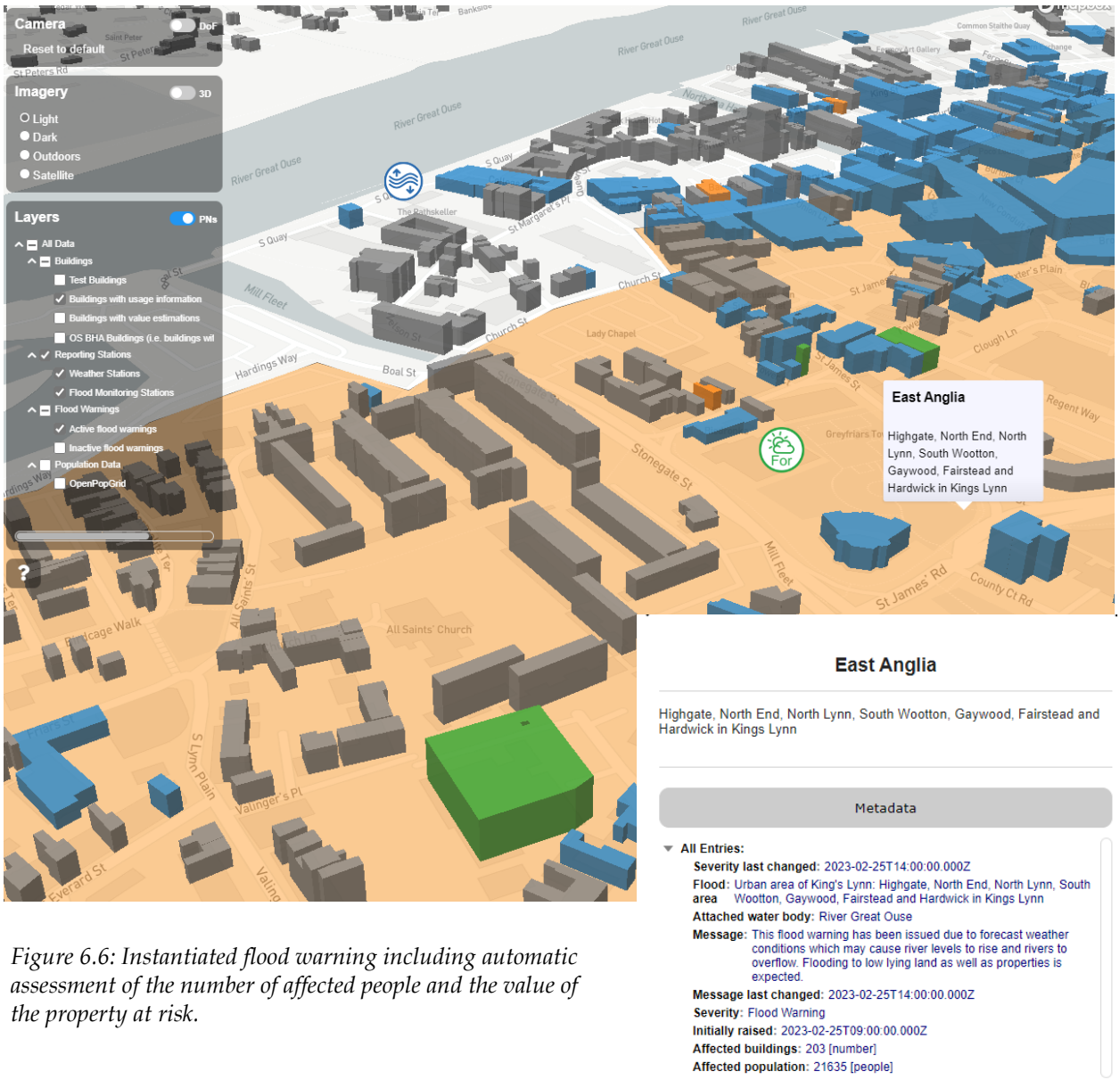


Figure 6.6: Instantiated flood warning including automatic assessment of the number of affected people and the value of the property at risk.

tional agents to estimate the effects of flooding events on the number of affected people and the value of the property at risk. The agents use the Derived Information Framework to assess the risk to people and property value during a flood warning and trigger automated cascades when data in the knowledge graph becomes outdated. **Ms Srishti GANGULY (Project Engineer, CARES)** supported Mr Hofmeister in improving some of these agents.

Mr John ATHERTON (PhD Student, CAM) extended the ontology that facilitates the storage of curtailment information to model wind farm energy curtailments in Britain. Along with market information, he also modelled co-located batteries with the goal of price arbitrage and curtailment reduction. He found a division between sites which directly reduced emissions by charging with otherwise curtailed energy and sites better able to arbitrage prices and achieve faster payback times.

Ms Wanni XIE (Non-C4T PhD Student, CAM) worked on a study that investigates how implementing a carbon tax can trigger the replacement of carbon-intensive power plants with Small Modular Nuclear Reactors (SMRs) to reduce carbon emissions. A knowledge graph consisting of a base world and a parallel world was developed. The latter depicted various scenarios with different numbers of replaced SMRs under four typical weather conditions. This allows a comprehensive understanding of the potential impacts of SMR replacement in each scenario.

Ms Xie used a high-resolution population data set from the UK (where data are readily and publicly available) to calculate the potential risks associated with reactor failure during the SMR site selection phase to ensure that SMRs are located in areas that pose the least risk to the population. The study shows that as the carbon tax approaches its saturated value, more SMRs are added. This is significantly influenced by wind and solar conditions. The study also indicates that the impact of the distribution effect (which implies placing SMRs in areas of high demand) becomes more significant in scenarios with insufficient solar or/and wind resources. Thus, in such scenarios, it may be necessary to carefully balance the distribution effectiveness factor with the risk factor of placing SMRs in populated areas when selecting the optimal location.

With colleagues from other CARES projects, the team have also improved the City Energy Analyst (CEA) Agent which can now query the knowledge graph to obtain more inputs such as surrounding building data and building usage; in terms of heating, ventilation, air-conditioning system settings, occupancy, and utility usage schedules. CEA can provide a more accurate and detailed analysis of energy use in buildings, thereby identifying opportunities to improve energy efficiency and reduce carbon emissions. The agent also has increased flexibility for optional parameters for endpoint specification. This has the potential to allow the user to customise the CEA agent to their specific needs, which can be important in developing effective decarbonisation strategies for different building types and locations.

Update on work package JPS.4

Model analysis and visualisation

Mr Hou Yee QUEK (Research Associate, CARES) worked on extending the visualisation of the digital twin of the CARES laboratory to retrieve, consolidate, and visualise both static and real-time data from different domains stored in the knowledge graph. Closely collaborating with **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, he designed the OntoBIM ontology to represent the Industry Foundation Classes (IFC) schema and link their assets to other ontologies from different domains such as OntoDevice (describes devices and their capabilities), OntoLab (represents experimental setups), and OntoBuiltEnv (represents information about properties). Mr Quek also developed several agents to instantiate IFC models using OntoBIM and to

Figure 6.7: Visualisation for the 3D Building Information Modeling (BIM) model of the CREATE Tower in a geospatial context via the Digital Twin Visualisation Framework.

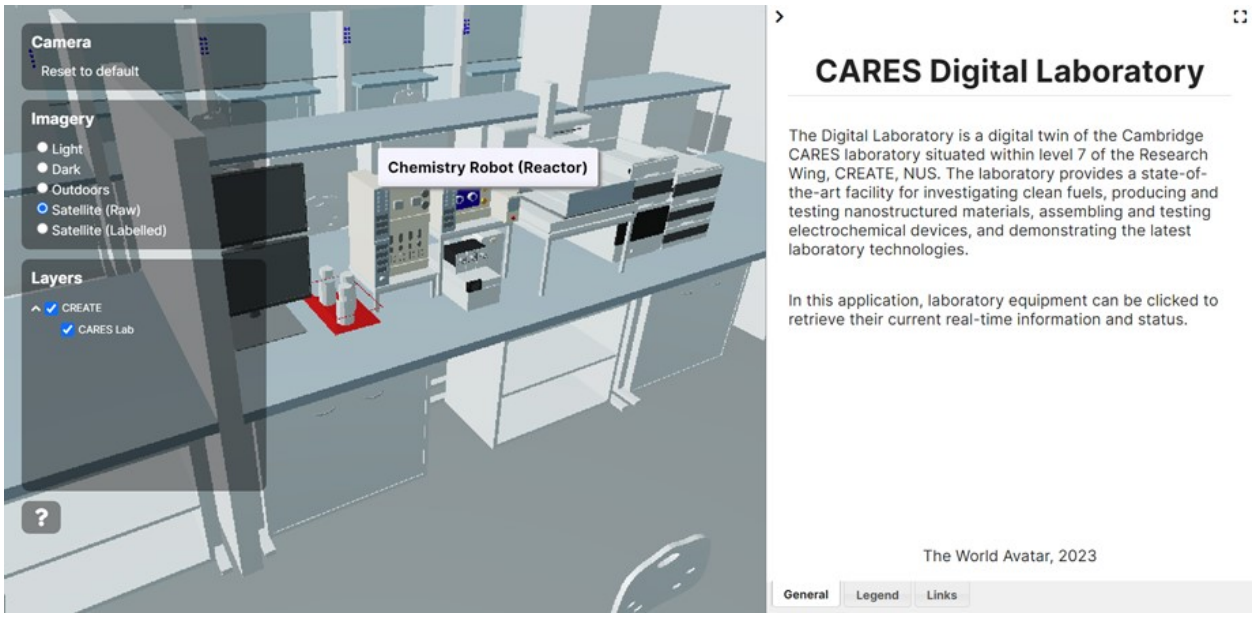


Figure 6.8: Visualisation of the CARES laboratory using its 3D BIM model.

visualise IFC models in a web-based platform. He is closely working with **Mr Dan TRAN (Software Developer, CARES)** to convert the IFC model into the '3D Tiles Next' format using the instantiated data in the knowledge graph. Using these agents and the updated Digital Twin Visualisation Framework, the IFC model of the CARES Laboratory and its assets are visualised, as shown in Figures 6.7 and 6.8. Furthermore, some of the instantiated sensor data and time series (described in work package JPS.1) have been consolidated and linked to the visualisation. This allows users on the web application to interact with different laboratory devices, such as the fridge and chemistry robots, to view their status, information, and time series via the knowledge graph, as seen in Figures 6.9. This allows users to monitor the status of various devices and make

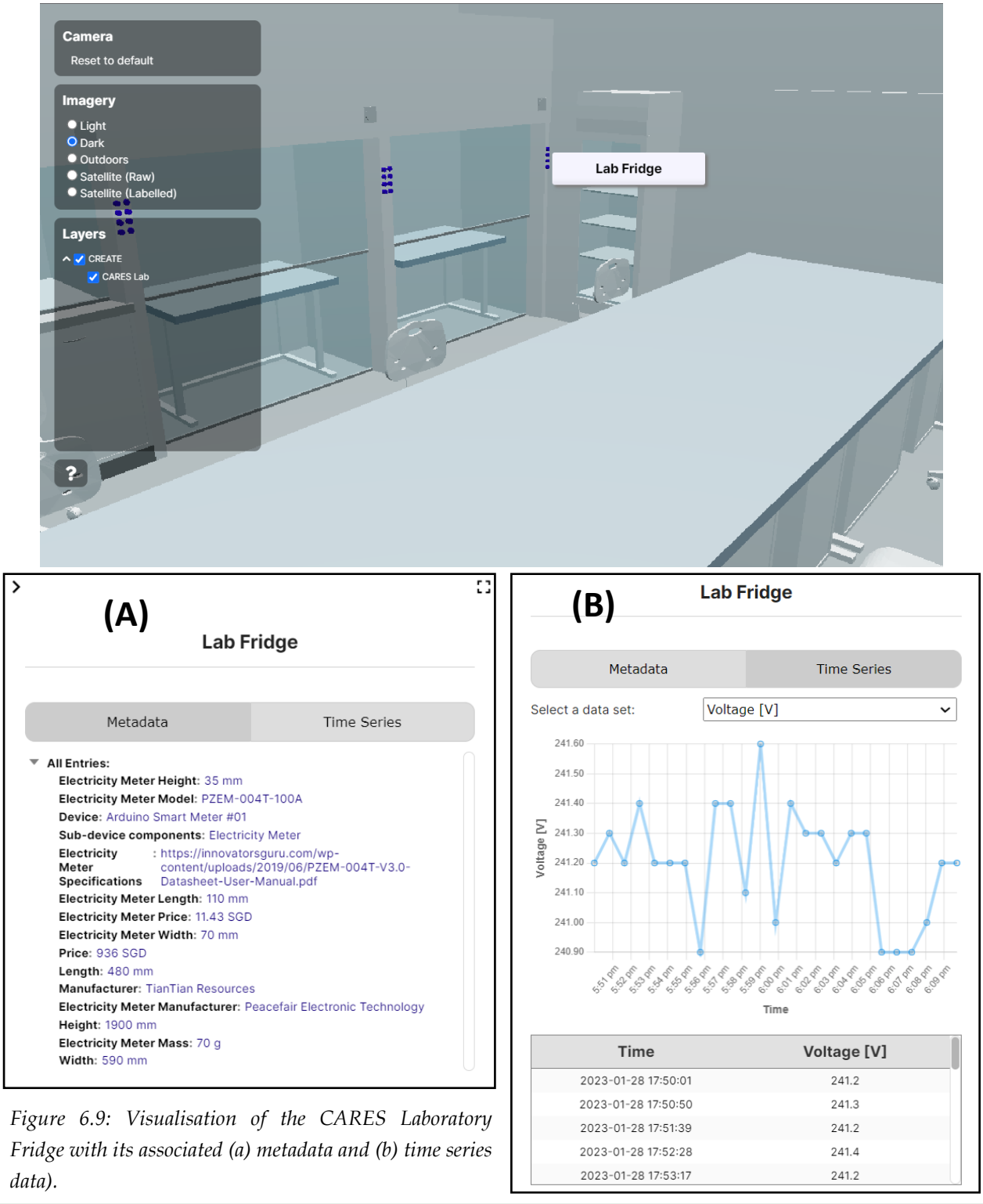


Figure 6.9: Visualisation of the CARES Laboratory Fridge with its associated (a) metadata and (b) time series data).

targeted decisions on the energy-saving potentials of those devices. For instance, the laboratory manager can monitor and adjust the energy usage of these devices for energy savings. Researchers can track their experiments historically, allowing them to fine-tune their experiments and reduce energy wastage. The CARES laboratory digital twin also serves as an example of a building with industry-grade equipment to simulate the optimised operation of an industrial plant.

Mr Wilson ANG (Software Developer, CARES) and Mr Rishabh Alexander JOHN (Non-C4T intern, NTU) have worked together to create the OntoCarPark ontology and an agent to instantiate Singapore's car park data in the knowledge graph based on this ontology. The data is retrieved from a publicly available Application Programming Interface (API). Figure 6.10 illustrates a visual representation of a car park and its available parking lots. This data can be used to monitor footfall and times of highest traffic for a given carpark, and also demonstrates how data from a publicly available government data source may be integrated into the knowledge graph and examine its effects on the real world. In this case, the car park data can be combined with routing algorithms to determine fuel/energy efficient ways of travel.

Mr Xiaochi ZHOU (PhD Student, CAM), Ms Shaocong ZHANG (Software Developer, CARES) and **Ms Mehal AGARWAL (Software Developer, CARES)** have been working on the updated version of the Marie Knowledge Graph Question Answering (KGQA) system, which aims to answer natural language questions, particularly in the chemistry domain. The Marie KGQA system can provide information on chemical reactions and properties relevant to energy storage and conversion technologies. This includes batteries, fuel cells, and catalysts for renewable energy systems. By providing insights into efficient and sustainable energy storage and

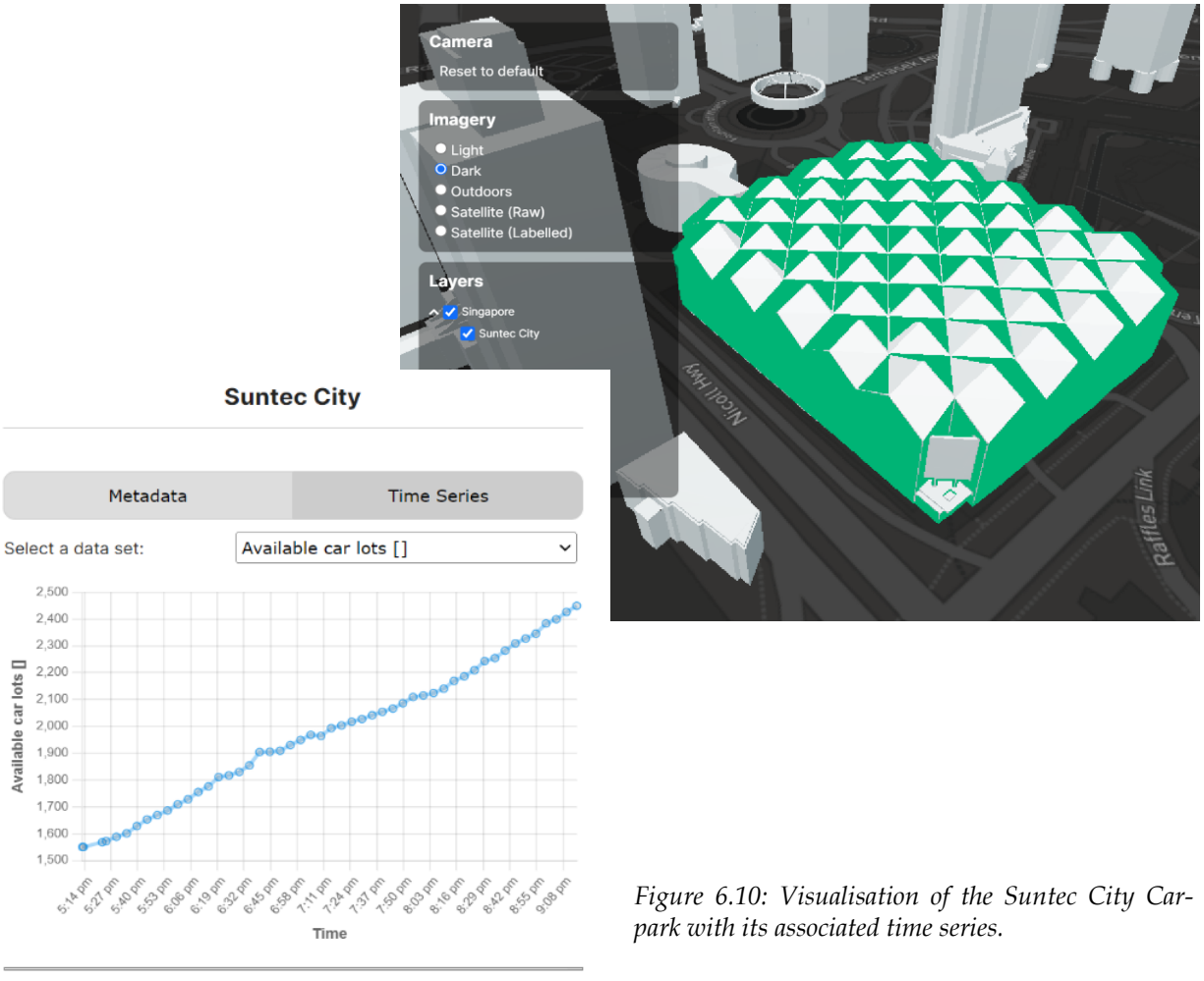


Figure 6.10: Visualisation of the Suntec City Carpark with its associated time series.

conversion, this system can support the development of cleaner energy systems and aid in the transition to low-carbon alternatives. The current version of the Marie KGQA system is based on Semantic-parsing techniques, which construct formal representations of the question to retrieve information from the knowledge graph. However, this method is not robust since formal representations are sensitive to semantic and schematic errors. The new design explores an Information -Retrieval method, which answers questions by generating a limited set of candidate answers and then ranking them.

The system first uses a joint entity recognition and entity linking system, which links natural language queries to knowledge graph entities. A Question-Answer (QA) model then produces a list of answer candidates and utilises a score function to measure the likelihood of the generated candidates' existence in the knowledge graph. Specifically, machine learning methods were used to learn the parameterised representation of entities and relations in the knowledge graph and subsequently measure the likelihood of a triple being the correct answer. This use of the new Information-Retrieval method not only improves the robustness of question answering by simplifying the semantic queries to tensor operations, but also improves the response speed significantly.

Ms Agarwal improved the system's robustness by implementing multi-threading which enabled the parallel processing of different QA Engines that operate on various chemistry ontologies namely, OntoSpecies (represents chemical species), OntoCompChem (represents computational chemistry calculations), OntoKin (represents chemical reaction mechanisms) and OntoMOPs (describes Metal-Organic Polyhedra formulations), and also chemistry databases, such as PubChem (describes chemical molecules). She also integrated several OntoAgent instances into the Marie KGQA system, allowing it to locate and invoke semantic agents to answer a range of questions posed by users dynamically.

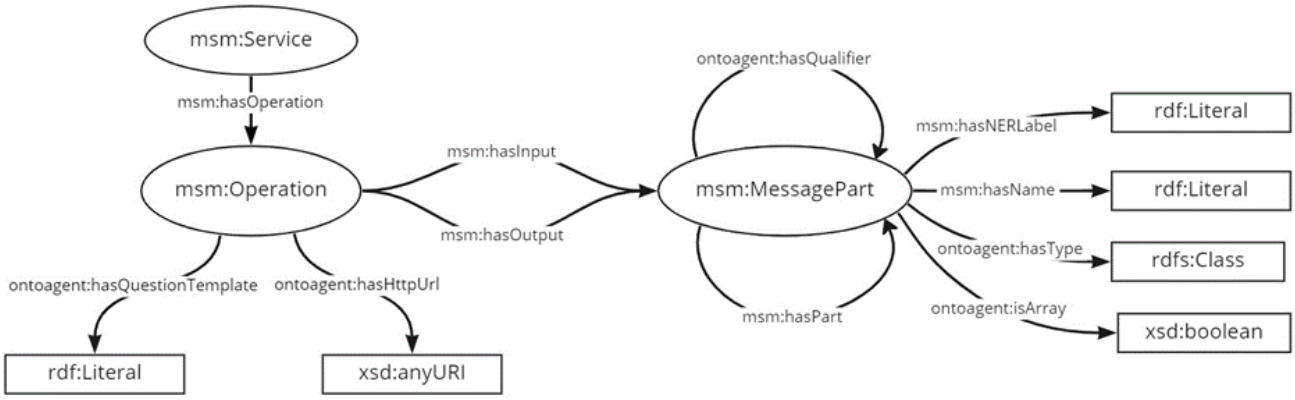


Figure 6.11: Schema of the OntoAgent ontology used to instantiate the agents and create their respective embeddings.

Scientific output

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

Cyber-Physical Systems in Decarbonisation
Oliver Inderwildi, Chuan Zhang, and Markus Kraft, *Lecture Notes in Energy*
DOI: 10.1007/978-3-030-86215-2_2

Abstract: Digital technologies such as advanced metering, big data, machine learning, and the Internet of Things are receiving significant attention as they provide the potential to facilitate the decarbonisation of industry while requiring limited investments. The orchestration of these novel technologies, so-called cyber-physical systems (CPS), provides additional synergetic effects that increase efficiency of energy provision and industrial production, thereby optimising economic feasibility and environmental impact.

Other activities and achievements

Dr Jethro AKROYD (Senior Research Fellow, CARES) presented a talk titled "Digital Twins and Semantic Technology" on 17 October 2022 at the UK Department for Business, Energy & Industrial Strategy. The talk gave an overview of the World Avatar (TWA) and CARES.

Prof Markus KRAFT (PI, CAM) presented TWA at a series of talks this reporting period:

- "Combustion/Soot Modelling and Digitalisation" was presented at Sandia National Laboratories, which is one of three research and development laboratories of the United States Department of Energy's National Nuclear Security Administration (NNSA) on 16 November 2022. The presentation highlighted how TWA can improve combustion and soot modelling.
- "Intelligent Decarbonisation – Can Artificial Intelligence and Cyber-Physical Systems Help Achieve Climate Mitigation Targets?" was presented at the University of Cambridge's "Accelerating the Energy Transition" event on 16 January 2023. The talk explored how Artificial Intelligence and cyber-physical systems can decarbonise energy supplies, urban systems, and industrial processes.
- Prof Kraft discussed how research around TWA aligns with the UN's Sustainable Development Goals to the United Nations (UN) Human Development Report Office on 17 January 2023
- "Digital Lab – The Next Generation" was presented by Prof Kraft and **Prof Alexei LAPKIN (PI, CAM)** at the Technology Networks Laboratory of the Future Symposium on 25 January 2023. The talk addressed important new laboratory automation developments, highlighting TWA's role in achieving lab interoperability and hardware independence.
- "The World Avatar Project – A Universal World Model" was presented at the Alan Turing Institute's Digital Twins Workshop on 2 February 2023. The lecture presented examples from TWA, including its aptitude in chemical knowledge creation, laboratory automation, building management, smart city operation, climate resilience and national energy scenarios.
- Prof Kraft presented TWA's abilities to the Institute for Economics and Peace on 24 February 2023 to discuss how it could align with their Positive Peace Index.
- Prof Kraft chaired a panel on "How can digital twins help save CO_2 in the manufacturing industry?" organised by Cambridge Zero on 23 March 2023.

CLIC

CENTRE FOR LIFELONG LEARNING AND INDIVIDUALISED COGNITION

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

Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

OVERVIEW

The team from the Centre for Lifelong Learning and Individualised Cognition (CLIC) have continued their focus towards meticulous data collection for the pilot study and in translating their initial findings. Researchers have also made significant headway in developing a day-to-day model of learning and cognitive flexibility, as well as understanding the relationship between social factors and structure learning.

The research team have had a particularly eventful past six months, with residency visits from Cambridge Principal Investigators as well as guests such as Professor Topun Austin and Professor Duncan Astle. Researchers from the workgroups have also presented their findings at international public events, workshops with the National Institute of Education (NIE), and have also been approached by the Singapore Examination & Assessment Board (SEAB) on a project to develop measures for inventive thinking. In particular, the Cognition Workgroup have also disseminated their findings to a diverse set of audience from webinars to symposiums. Most notable was a ground-breaking study which demonstrated that adult perceptual learning could occur through neuro-personalised entrainment stimuli which garnered interests from international media.

In October 2022, the workgroups worked closely with each other to present their developing findings from the adult and adolescent studies to the Scientific Advisory Committee (SAC). Using an inverse temperature parameter, the team underlined the relationship between structure learning and cognitive flexibility, including its relationship with outcomes such as creativity, language, and mathematics. Following the successful presentation to the SAC, the team is wrapping up Phase 1 of the project, with a majority of data collection completed, and are steadily working towards starting Phase 2 in the later half of the year.

Professor John Suckling (PI, WP0, CAM) visited Nanyang Technological University in March 2023, and offered guidance to the Neuroimaging team and helped finalise the main analysis approach of the project. This included the resting-state functional MRI analysis and the multi-parameter mapping analysis. Currently, the Neuroimaging Workgroup are hard at work with data collection and streamlining their data cleaning, organisation and storage. The team have far exceeded their target sample size in each intervention group and are still recruiting participants into the study.

The School Workgroup have conducted two more workshops and talks to stakeholders, namely from NIE, on the topic of what schools can and should do to ready Singapore's students for the future. This also includes an exciting collaboration with SEAB to develop and co-design an assessment tool on inventive thinking, which combines the efforts of both the School and Cognition Workgroup. The team are currently in discussions with SEAB to outline design principles and ideas to propose an appropriate measure.

The CLIC team are actively progressing with data collection and analysis, including the upcoming Writing Bootcamp in May 2023 with colleagues in Cambridge, where the researchers will get the opportunity to discuss, plan, and draft manuscripts for Phase 1 of the study. 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 contributed significantly toward the successful outcome secured at the Scientific Advisory Committee (SAC) review meeting in October 2022. Working in close collaboration with the other workgroups, **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM)**, **Prof Zoe KOURTZI (PI & Director, CAM), Prof Barbara SAHAKIAN (Senior Scientific Advisor, CAM), Prof Annabel CHEN (PI & Director, NTU)** and **Assoc Prof Victoria LEONG (PI & Deputy Director, NTU)** effectively presented the case for programme renewal based on promising emerging findings from the WP0.1 adult and adolescent studies. These highlighted the relationship between cognitive flexibility and structure learning (via an inverse temperature modelled parameter), as well as with other outcomes including creativity, language, and mathematics.

Between October 2022 and March 2023, the CLIC Cognition Workgroup continued diligent efforts on data collection for the WP0.1 adult characterisation study while developing a robust data analysis framework. As of March 2023, data has been successfully acquired from N=335 participants, which constitutes >95% of the total WP0.1 adult data collection target. The WP0.1 adult study protocol has also been submitted as a manuscript to the journal *PLOS ONE*, marking the first CLIC consortium-level publication involving all PIs and key research staff. **Dr Ke TONG (Research Fellow, NTU)** led the manuscript preparation with significant contributions from **Mr Kean Mun LEE (Research Assistant, NTU)** and **Ms Natalie HOO (Research Assistant, NTU)**.

The Cognition Workgroup welcomed two visiting professors from the University of Cambridge. Both events attracted CLIC staff and interested members of the public:

- World-renowned neonatologist **Prof Topun AUSTIN (Co-PI, CAM)** visited in November 2022. He delivered a talk, "Shining Light on the Newborn Brain," on his cutting-edge research on the application of functional near-infrared spectroscopy (fNIRS) with neonatal infants.
- Prof Duncan ASTLE (CAM) visited in March 2023. Prof Astle discussed preliminary findings with the CLIC Cognition Workgroup and provided valuable insights on data analysis and interpretation.

The Cognition Workgroup also actively disseminated research findings through various events, including webinars, presentations, and symposia during the reporting period. These outreach efforts engaged diverse audiences, further demonstrating the value and impact of the CLIC research programme. See "Other activities and achievements" in this chapter section for the full list.

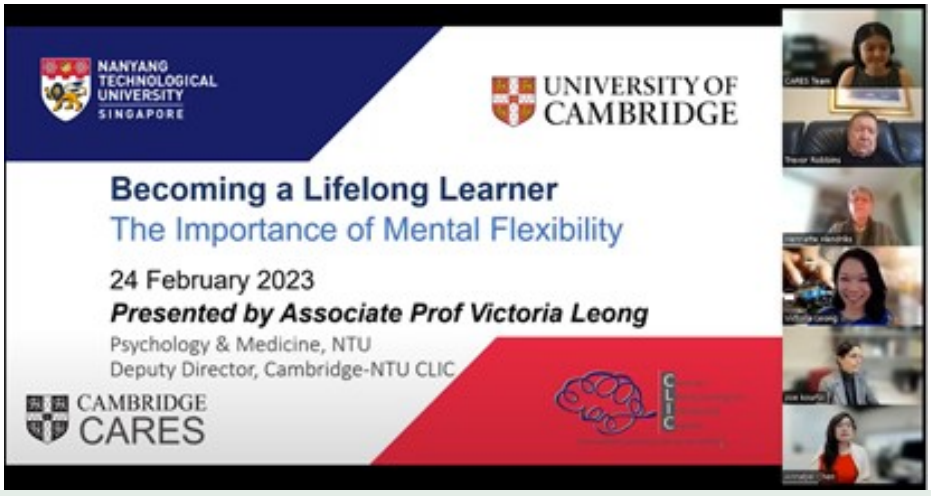


Figure 7.1: Assoc Prof Victoria Leong presented CLIC research to an international audience at the CREATE Webinar series on 24 February. A Q&A session was conducted with PIs from CLIC's Cognition, Neuroimaging, Social, and School workgroups.

The Cognition Workgroup also supported the collaboration between the CLIC School Workgroup and the Singapore Examinations and Assessment Board (SEAB) to develop inventive thinking assessments. Dr Tong, **Dr Xinchen FU (Research Fellow, NTU)**, and Mr Lee participated in the collaboration, bringing their expertise in cognitive research and data analysis to the partnership. This joint effort aims to create innovative and effective methods of assessing students' inventive thinking skills, ultimately helping to shape the future of education in Singapore.

Specific staff contributions

- Dr Tong contributes towards the development of the data processing and analysis framework for the WP0.1 adult characterisation study and other CLIC projects. He extracted critical constructs (such as cognitive flexibility, creativity, structure learning) and examined relationships among the constructs via modelling approaches. He is actively involved in the development, testing, and implementation of innovative tasks and analyses for the CLIC Phase 2 studies.
- Dr Fu has been involved in the analysis of infant explore-exploit behaviour within the context of a classic attention set-shifting task, specifically the object classification sequential touching paradigm. She is developing new computational metrics for quantifying explore-exploit behaviour (e.g., based on reaction time measures) in pediatric populations.
- Ms Hoo assumed the position of Coordinator for cognitive testing in January 2023, overseeing both in-person and RGT Hybrid testing procedures. She conducted RGT training sessions for newly appointed Student Assistants to ensure consistent data collection. She also prepares IRB amendments and documentation to comply with updated IRB guidelines.
- Mr Lee contributes significantly to the adult data collection, scoring (Torrance Test of Creative Thinking, Woodcock Johnson Test of Achievements), and data management efforts. He also assists in coordinating workgroup meetings and has been appointed the Cognition Workgroup Data Champion.
- **Mr Shamsul Azrin bin JAMALUDDIN (Research Associate, NTU)** joined the Cognition Workgroup in February 2023 and has commenced training in CLIC's cognitive task battery. He is involved in administering, scoring, and analysing data from creativity tasks such as the Torrance Test of Creative Thinking, Alternative Uses Task, and the Verbal Fluency Task. He is also representing the Cognition Workgroup in the CLIC Symposium organisation committee planned for 25 and 26 August 2023.

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

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

Update on Schools Workgroup

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

Between October 2022 and March 2023, The School Workgroup completed the data collection of more than 350 secondary school students, including administering CLIC's task battery in Secondary Schools and in a laboratorial setting at NTU. The individual recruitment via Social Media was especially successful, with parents and students attending a short talk about NTU. The School Workgroup continued to conduct various modes of outreach activities to the larger community as part of the CLIC's science communication and engagement efforts and established a partnership with the School Examination and Assessment Branch (21CC group) in a research project on inventive and adaptive thinking.

Research Process: The School Workgroup continues to work with the Cognition and Social Workgroup to implement large-scale data collection in schools and ideal-condition study for the WP0.1 Adolescent Study. **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** has liaised closely with the Adults' Working Groups to ensure that data collection procedures, coding and analysis are properly aligned across all workgroups. Dr Lopes Fischer performed data cleaning and analysis of the adolescent data in collaboration with the Cognition and Social Workgroups. In October 2022, she also coordinated efforts to present key findings and the project's milestones for CLIC's Progress Report delivered to the Scientific Advisory Committee (SAC). Since October 2022, **Ms Phillis FU (Research Associate, NTU)** has been working on recruiting participants for the laboratory setting sub-set of the project. She manages CLIC's social media accounts and leverages this role to recruit participants via social media. The effort has shown to be fruitful, and she has completed recruitment of N=112 through this means. Ms Fu also ran the testing sessions diligently throughout this period, together with **Ms Yingqi CHUI (Research Assistant, NTU)**. Ms Fu and Ms Chui also worked on manually cleaning & coding complex creativity data (Alternate Uses Task & Verbal Fluency) and helped facilitate the professional development workshops with educators.

Neuroscience Research, Practice and Policy Nexus: **Dr Chew Lee TEO (Co-PI, NTU)** presented the CLIC research and Knowledge Building to the Director and Deputy Directors of Singapore Examination & Assessment Board (SEAB) in Dec 2021. This led to a series of meetings and discussion, including a 3-hour workshop explaining the battery of tasks and instruments in 2022. Finally, the CLIC School Workgroup and SEAB established a collaborative project on a development of measures for inventive-adaptive thinking.

The collaborative work involved co-design of new assessment items and implementing the items in school. This collaboration is significant in its contribution to understanding the nexus between neuroscience research, practice and policies. Both Ms Fu and Ms Chui supported the literature scan on this concept, outlined design principles and worked on ideas to design a measurement for inventive thinking. The School Team formed a sub-workgroup comprising representatives from the Cognition workgroup, **Dr Ke TONG (Research Fellow, NTU)** and **Dr Kean Mun LEE (Research Assistant, NTU)**; the Social Workgroup, **Dr Nadhilla Velda MELIA (Research Fellow, NTU)**; and Mr Timothy LEE (past-CLIC Research Associate). **Prof Michelle ELLEFSON (PI, CAM)** is co-leading this sub-workgroup with Dr Teo. The team has had two working sessions in February and March when Prof Ellefson was here on her residency (22nd March - 23rd April). Prof Ellefson joined the School Workgroup to meet a participating school's management team on 27th March where both teams explored several new opportunities.

Guided by **Assoc Prof Victoria LEONG (PI & 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 and social interactions.

Dr Ryutaro UCHIYAMA (Research Fellow, NTU) played an important role in performing the data analysis of the School Workgroup dataset for the CLIC's Progress Report which was delivered and presented to the SAC. Dr Uchiyama also collaborated with the Adult Working Group to implement the optimal foraging analysis and the semantic network analysis for the Verbal Fluency task performed by young adults while performing the CLIC's task battery.

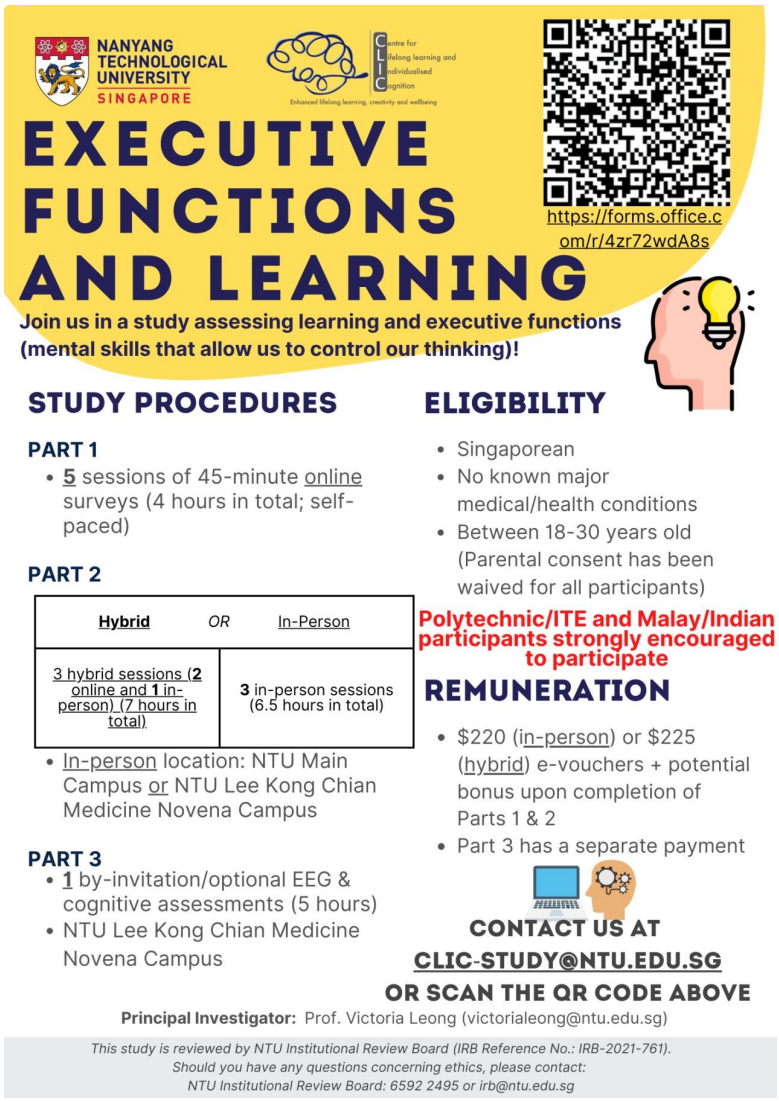


Figure 7.2: CLIC's participant recruitment poster

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

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

Update on Social Workgroup

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

The Social Workgroup focuses on the constructs pertaining to multilingualism, tolerance of uncertainty, perceived social support, social decision-making, and career development. Since April 2022, the Social Workgroup has been continuously collecting data from (online) questionnaires and (lab-based) cognition data for WP0.1. At the time of writing, N=340 adult participants have fully completed the WP0.1 study (both the online and face-to-face). Research Assistants from the Social Workgroup are also assisting the Neuroimaging Workgroup with data collection for WP0.2. The Social Workgroup Research Fellows and PhD student monitor the quality of incoming data by ensuring attentiveness while completing the online surveys or by tracking missing data. The team also monitor any issues with the online Qualtrics survey platform. The Social Workgroup has prepared and submitted pre-registrations for the hypotheses pertaining to the socio-cognitive variables in the adult study.

The team have been conducting data analyses of the social data. These preliminary findings were presented at the SAC meeting in October 2022, during which the team also presented four posters titled 'Social Decision-Making Tasks', 'Cooperativeness and Cognitive Flexibility', 'Multilingualism and Cognitive Flexibility', and 'Cognitive Flexibility and Lifelong Career Development'. Finally, the Research Fellows are also preparing for the Writing Bootcamp which will take place at the University of Cambridge in May 2023 where they will be preparing manuscripts for publication.

Assoc Prof Georgios CHRISTOPOULOS (PI, NTU) supervises **Dr Shengchuang FENG (Research Fellow, NTU)** and **Dr Nadhilla Velda MELIA (Research Fellow, NTU)** on their analysis of the relationship between social factors and variables of interest, including cognitive flexibility and structure learning. The group have provided measurements for social factors for WP0.2 and the adolescent data.

Prof Henriëtte HENDRIKS (PI & Deputy Director, CAM) has been closely involved in supervising Dr Melia's work on the preliminary analyses related to multilingualism and presented some of these and other preliminary findings regarding the social factors on behalf of the social group during the SAC meeting in October 2022. Currently, Prof Hendriks is helping to organise the Writing Bootcamp in May and is part of the committee in charge of organising the CLIC Symposium which will be held on 25 and 26 August 2023 in Singapore. Prof Hendriks will be visiting Singapore in May to facilitate further write-ups of work started at the bootcamp, planning the Symposium and Phase 2 of the project. In her role as deputy-director, Prof Hendriks is closely involved with the administration surrounding the signing of Phase 2 of the project. She also continues in her role of finance contact in Cambridge and attends the monthly CLIC Cambridge-Singapore meetings.

Dr Feng has contributed to the analysis of social decision-making variables and the testing of related hypotheses. Some preliminary results were included in the report and presentation to the SAC in October 2022. At the meeting, he presented two posters titled 'Cooperativeness and Cognitive Flexibility' and 'Social Decision-Making Tasks'. He also prepared and demonstrated two interactive social decision-making games to the committee members during the hands-on demo session. He has continued his work on the analysis of social decision-making questionnaires and tasks in the adult sample, including descriptive statistics, correlations, factor analysis, and regression analysis. He is currently preparing a manuscript describing the dataset from the social decision-making tasks. He is also collaborating with **Dr Chia-Lun LIU (Research Fellow, NTU)** from the Neuroimaging Workgroup to analyse the multi-parametric mapping data. His analysis focuses on the association between social decision-making variables and brain microstructure.

Dr Melia has been conducting data quality checks, pre-processing of the data, and data analysis from the socio-cognitive questionnaires. Specifically, she is responsible for analysing the social variables of tolerance of uncertainty, perceived social support, and multilingualism. She is conducting analyses such as descriptive statistics, reliabilities, correlations, exploratory and confirmatory factor analyses, and the moderating effects of these variables on the relationship between cognitive flexibility and structure learning. She included some of the preliminary results from these analyses in the report and presentation to the SAC in October 2022. At the SAC meeting, she also presented a poster titled 'Multilingualism and Cognitive Flexibility'. Currently, she is preparing literature reviews and data analyses for a paper to be written at the Writing Bootcamp. She is also collaborating with **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** from the School Workgroup to preprocess and analyse the multilingualism data. She is also working with the School Workgroup on the collaboration with the Singapore Examinations and Assessment Board (SEAB) on designing new assessment tools. Finally, Dr Melia is part of the organising committee for the CLIC Symposium.

Ms Emma Yoke Loo SAM (PhD student, NTU) has contributed to the general logistical and administrative planning for WP0.1 (e.g., preregistration and data analyses). She is also assisting with the participant recruitment for the WP0.1 study, such as determining the demographic characteristics of targeted populations. Ms Sam is also responsible for the cognitive flexibility and career transition/adaptation sub-study and prepared a pre-registration titled 'Cognitive and Social Aspects of Career Transition and Adaptation' under WP0.1. Specifically, for the report and presentation to the SAC, she examined how cognitive flexibility was associated with well-established career variables, i.e., career adaptability, career exploration, and perceived employability.

Mr Akshay ABRAHAM (Research Associate, NTU) has been engaged with CLIC since September 2022 by contributing to administrative duties within the study. His main responsibilities include participant screening, the running of experimental sessions for WP0.1, participant reimbursement, as well as data entry and backup. He is also engaged in the management of Student Assistants through the administration of training for data collection and the recommendation of claims.

Ms Hui Shan YAP (Research Assistant, NTU) contributed to the general logistical and administrative planning for WP0.1 and WP0.2 (e.g., setting up multiple survey forms for different studies, including designing ways to allow for questionnaires to be administered online, drafting and updating relevant SOPs, drafting IRB amendments and incident reports, etc.) used during the data collection process. She is also involved in the data collection for WP0.1 Adults and WP0.2 (social measures).

Ms Yuan Ni CHAN (Research Assistant, NTU) assisted in the general logistical and administrative planning for WP0.1 (e.g., setting up the online survey forms, designing the decision-making games, and updating the relevant SOP and manuals). She is involved in participant recruitment for the WP0.1 study (e.g., promoting study outreach through other schools and other methods) and in the data collection process for the WP0.1 Adults and WP0.2.

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

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

Update on Neuroimaging Workgroup

Neuroimaging: Structure Learning Training and Cognitive Flexibility

Since the last report, the Neuroimaging Workgroup continued data collection with the help of **Mr Wei Ler KOO (Research Assistant, NTU)** and **Ms Marisha Barth UBRANI (Research Assistant, NTU)**. Both researchers received relevant training on the CLIC study workflow with the support of the team. As of March 2023, the Neuroimaging Workgroup has collected data from 86 participants (training = 42, control = 44), beyond the estimated sample size of 70 in each intervention group.

Due to the intensive training intervention paradigm and cognitive testing required for WP0.2, the team maintains a group of well-trained student research assistants (RAs) to ensure sufficient manpower for data collection on a rolling basis. Two batches of student assistants were recruited to replenish this manpower pool (5 students at end of September and trained in October 2022, and 4 students hired and trained in February 2023). All student RAs underwent intensive training conducted by the Neuroimaging Workgroup that spanned a total of 12 hours across five days. The training covered theoretical explanations of the study, protocol administration and hands-on sessions to conduct cognitive tasks and preparing participants before MRI. In addition, they observed cognitive and MRI sessions conducted by more experienced student assistants. The Neuroimaging Workgroup's Research Associates and Research Assistants sat in during their first sessions and provided feedback. This comprehensive training gave the student assistants the opportunity to learn and practise before they were confident enough to conduct the sessions independently. As of 30th March 2023, there are 12 student assistants under the Neuroimaging Workgroup, 11 of whom are involved in data collection and another in charge of recruitment. More experienced student assistants took on double roles of data collection and operations, and participant compensation processes.

From October 2022 to March 2023, six more batches of participants (total = 60; training = 27, control = 24, withdrawn = 9) have been recruited. The recruitment process is overseen by **Ms Janet TAN (Research Assistant, NTU)** who ensures that the team meets its recruitment target while pacing the recruitment adequately to avoid overloading student assistants. Ms Tan also coordinates with Mr Koo to ensure that MRI slots are fully utilised and participants are scheduled for their sessions. Data analyses of baseline sessions and matching to assign participants into Training or Control groups are also handled by Ms Tan. At present, there are five participants undergoing various phases of the study, with 13 newly recruited participants in the latest batch.

Preliminary data-cleaning and analyses of behavioural and MRI data were conducted by **Dr Chia-Lun LIU (Research Fellow, NTU)** with assistance from **Ms Winlynn CHOO (Research Associate, NTU)**, **Ms Min HONG (Research Associate, NTU),** Mr Koo, Ms Ubrani, and Ms Tan. The team are currently focusing their efforts on data cleaning and analysis, and developing models for the cognitive flexibility tasks. This complements the structure learning (SL) intervention's results, including an examination into Diffusion Decision Model by **Dr Xiaoqin CHENG (Research Fellow, NTU)** and Ms Choo to decide its suitability for the analysis. Meanwhile, exploration into semantic network analyses for Verbal Fluency will be explored with the School Workgroup by Ms Choo and Mr Koo. Ms Ubrani has begun the data cleaning and preliminary analysis for nine cognitive-behavioural tasks from the Inquisit platform. The data cleaning process were kept consistent with that of WP0.1. These tasks include Colour Shape Task, Task Set Switch (Where), Task Set Switch (What), Trails Making A/B Task, Wisconsin Card Sorting Task, Stop Signal Time Task, Stroop, Raven's Progressive Matrices, and Reading Span task. 71 participants' data were used for this preliminary analysis to ensure consistency with the MRI data analysis. Measures of cognitive flexibility are being compared with WP0.2 (Cognition Workshop) for primary outcomes to

ensure consistency and replication. These behavioural results will be used for brain behavioural analysis for neuroimaging analysis.

The Neuroimaging Workgroup has also started to closely examine the training data of the SL task this March. To establish a link between the study's structure learning (SL) training intervention and cognitive flexibility, decision index (ICD) obtained from SL training were regressed on three modelling parameters of the Intra-extra dimensional (IED) task - a classic test of cognitive flexibility. Initial analyses of 24 training participants' data found a positive trend between decision index and inverse temperature extracted from IED task. This is expected as both maximising (quantified by ICD) and exploitation tendencies (measured by inverse temperature) share similar concepts. Moreover, the positive relation between decision index and learning rate from IED task suggests that participants who employ the maximising strategy in SL training have greater ability to obtain relevant information quickly. Likewise, the negative relation between decision index and dimension primacy indicates that maximisers are less likely to ignore new stimuli introduced at new stage of IED task. Considering the construct similarities in decision strategy derived from SL training and measures of IED task, this provides strong support for the SL training as an intervention to improve cognitive flexibility. Due to the heavy booking at the neuroimaging centre (CoNiC), the team works closely with staff at CoNiC to implement protocol to facilitate booking to maximise the available slots. This has greatly enabled the team to minimise cancellation fees. Similarly, behavioural and neuroimaging data organisation and storage pipeline has been streamlined and automated to ensure all the relevant data is placed in a best fit folder or file based on their nature. Ms Hong and Ms Tan are assisting with MRI data preprocessing and are supervised by Dr Liu. They

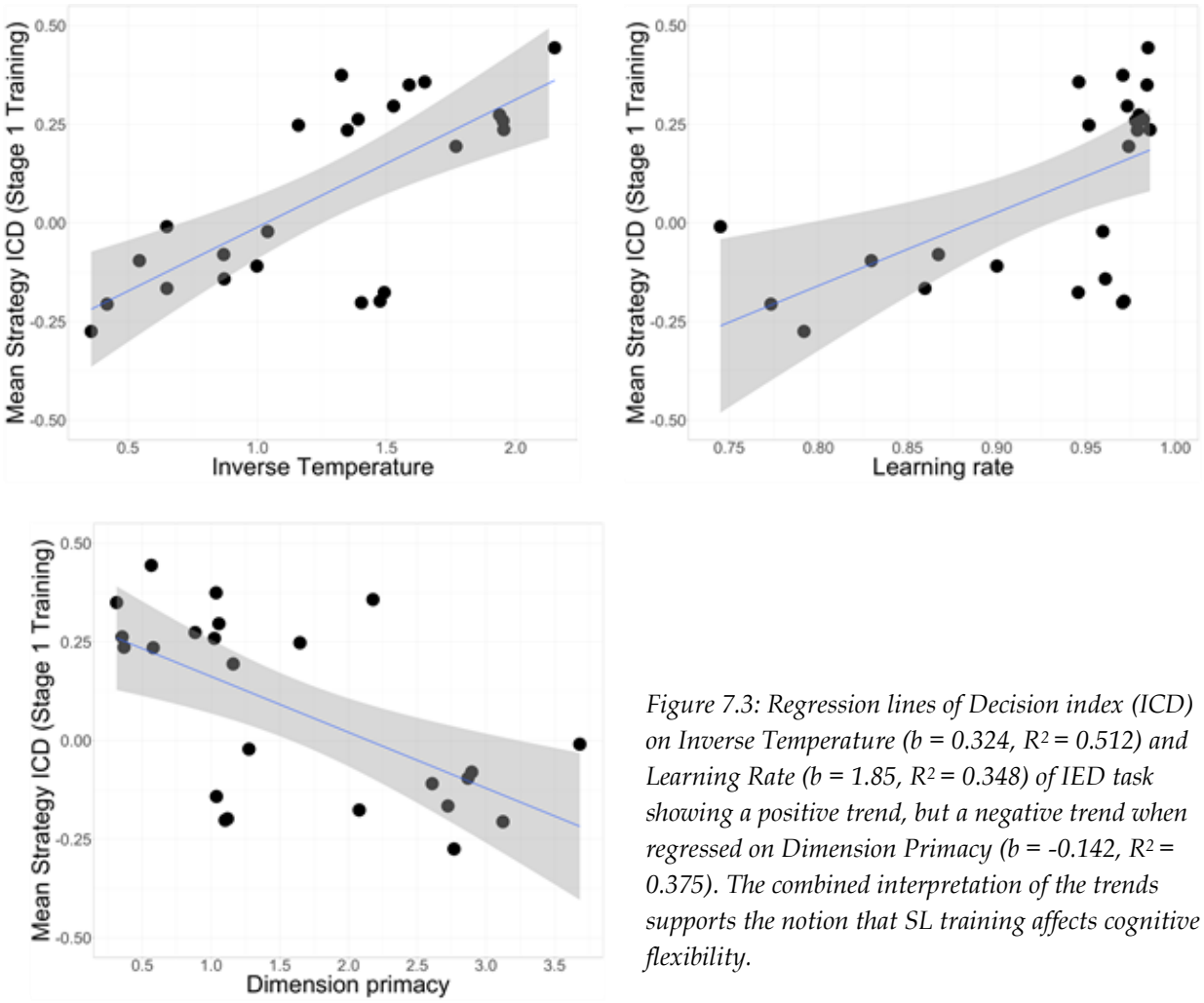


Figure 7.3: Regression lines of Decision index (ICD) on Inverse Temperature (b = 0.324, R^2 = 0.512) and Learning Rate (b = 1.85, R^2 = 0.348) of IED task showing a positive trend, but a negative trend when regressed on Dimension Primacy (b = -0.142, R^2 = 0.375). The combined interpretation of the trends supports the notion that SL training affects cognitive flexibility.

are also involved in image quality check of Multi-Parameter Mapping (MPM) images, i.e., rating all the participants' images on four MPM parameters (A, R_1, R_2* and MT_{sat}) according to a standardised guideline, followed by calculating the inter-rater reliability, and removing unusable images. Depending on the results from the inter-rater reliability analysis, the image quality check protocol will be adjusted until a good inter-rater reliability is obtained.

For the MRI data, the analysis steps employed the pipeline built last year. Dr Liu has updated the MRI results of MPM and resting-state fMRI based on 71 participants collected till March 2023. During **Prof John SUCKLING's (PI, CAM)** residency in Singapore, three data analysis meetings were held on 17th, 21st and 24th March with the team, including **Prof Annabel CHEN (PI & Director, NTU)**, **Prof Balazs GULYAS (PI, NTU),** and CoNiC. These meetings facilitated the finalisation of the main analysis approach. The two key points agreed upon from the meetings were to attempt replication of past findings and to provide new evidence of structure learning training from the brain network-level analysis from these replications. In short, resting-state fMRI analysis will focus on both functional connectivity within the cognitive flexibility network and functional connectivity between networks. For MPM analysis, the team will consider the decision strategy factor and age, in addition to the exploratory whole brain approach.

Dr Liu conducted analysis of MRI data for the WP0.2 Main Study with assistance from Ms Choo and other team members. Ms Choo ensures the smooth running of analyses pipelines on the Ubuntu server and two workstations. She supported the navigation and resolution of various network complexities, such as aiding with software installations and debugs, as well as machine maintenance (updates, billing, warranty, and services request) to minimise disruptions to the analysis. The team also plan to explore voxel-based morphometry if time permits.

In anticipation of heavy computational needs for WP0.2 Main Study, Ms Choo helps to maintain the 3 servers for CLIC and REDCap web server and ensures that any updates to the backend is successfully brought to production. She also provides support to clearing queries over Google Workspace and assists with the procurement of the new server for WP0.1 modelling analysis. She works together with Dr Liu and Ms Ubrani to ensure details of the Data Management Plan (DMP) provided are accurate.

Mr Koo has been assisting with both behavioural and neuroimaging data collection by coordinating the complex booking of linked MRI slots (for per-post scanning). He works closely with CoNiC's manager on billing and scan related issues and ensures smooth transfer of raw scan data to the database. In addition, Mr Koo has also been helping with data cleaning, data analyses of the behavioural data and developing R-scripts to automatise the process. Meanwhile, Ms Ubrani has been helping with data collection and provides oversight of the student research assistants to ensure participant payment and reimbursement procedures run smoothly. Ms Hong and Ms Ubrani manage the ethics documentation (NTU-IRB) for the workgroup by keeping amendments up-to-date and securing physical and digital documents. Ms Ubrani has been supporting the internal research audit processes with the Research Integrity and Ethics Officers to ensure proper documentation and record keeping. She also works with the broader CLIC team on ad-hoc projects and events as the workgroup's representative, such as the upcoming CLIC Symposium and Co-Principal Investigator visits.

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

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

Other activities and achievements

Cognition Workgroup

Prof Zoe KOURTZI (PI & Director, CAM) and **Assoc Prof Victoria LEONG** (**PI & Deputy Director, NTU)** published a groundbreaking study in *Cerebral Cortex* demonstrating that it was possible to achieve a 3-fold increase in adult perceptual learning through neuro-personalised entrainment stimuli tuned to individual brainwave frequency and phase. This story was picked up by the University of Cambridge in a press release "Tuning into brainwave rhythms speeds up learning in adults", and external outlets such as the Evening Standard and BBC World News.

Assoc Prof Leong was an invited speaker at two public events:

- "Becoming a Lifelong Learner - The Importance of Mental Flexibility" (virtual webinar) for the CREATE Webinar series on 24 February 2023.
- "Neural Sociometrics: Assessing parent-infant social dynamics in the context of developing cognition" (conference presentation) for the A*STAR Human Potential Programme Office (HPPO) "Early Life Scientific Symposium" on 2 March 2023.

Assoc Prof Leong was also the recipient of the Nanyang Research Award 2022 awarded by NTU which recognises individuals who have made outstanding contributions in extending the frontiers of knowledge.

The CLIC Cognition team is working with the Cambridge Adaptive Brain Group under Prof Kourtzi 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.

Social Workgroup

Ms Emma Yoke Loo SAM (PhD student, NTU) successfully received a grant titled "Ready For a Career Change? The Cognitive Science of Career Change and Transition" to examine the relationship between cognitive flexibility and career decision making under the supervision of both **Assoc Prof Georgios CHRISTOPOULOS (PI, NTU)** and **Prof Annabel CHEN (PI, NTU).**

School Workgroup

The School Workgroup have been in collaboration with the Ministry of Education's Singapore Examinations and Assessment Board (SEAB) since mid-January in the co-design of new assessment tools based on CLIC's research about cognitive flexibility. This work is part of CLIC's efforts in applying research findings to education.

The School Workgroup continue to develop and conduct Professional Development (PD) Workshops for external stakeholders (i.e., Singaporean Schools' Teachers) to: 1) familiarise them with the three core executive functions (i.e., working memory, inhibition and cognitive flexibility) concepts, its neurocognitive basis, development, relation to students' learning, and broad educational objectives; and 2) investigate how the teachers' executive function performance might interfere with the effectiveness of the PD workshop in promoting a positive change in the teachers' practices in classroom.

On 15 November 2022, **Dr Chew Lee TEO (Co-PI, NTU)**, **Dr Peter SEOW (Co-PI, NTU/NIE), Dr Nastassja LOPES FISCHER (Research Fellow, NTU), Ms Phillis FU (Research Associate, NTU),** and **Ms Yingqi CHUI (Research Assistant, NTU)** were invited by the Singapore-Hebrew University Alliance for Research and Enterprise (SHARE) to deliver a talk to a team of educators from a secondary school in Singapore's Ministry of Education as part of a 2-day Staff Learning Retreat to review and future plan school curriculum and facilitate dialogue on what schools can and should do to future-ready students for the challenges of tomorrow's world .

Dr Teo gave a lecture on Cognitive Flexibility and Knowledge Building during the Teachers' Award Ceremony in Oct 2022 at CLIC's partner school which was attended by the School Advisory Board and school leaders. The talk was well received and the school expressed interest to continue its partnership with CLIC.

Dr Teo, Dr Seow, and Dr Lopes Fischer conducted two Professional Development workshops on 27th January and 24th February at Kentridge Secondary School on Cognitive Flexibility and Innovative Pedagogy. The event was attended by close to 70 teachers.

Dr Katherine YUAN (Research Scientist, NIE/NTU), Dr Lopes Fischer, and Dr Teo conducted a talk titled, "Knowledge Building and Cognitive Flexibility" at the in-Learning Festival on 3rd March at the Google HQ in Singapore.

Dr Lopes Fischer was an invited peer-reviewer in two academic journals (*Educational Research Review* and *Quarterly Journal of Experimental Psychology*) and an invited lecturer for the National Institute of Education course titled "AGE06E Neuroscience, Computational Thinking and Artificial Intelligence in Learning" led by Dr Seow. Dr Lopes Fischer also conducted a talk at the National Institute of Education's Science of Learning (SoLEC) Brown Bag Seminar titled "Interactive minds: Collaborative learning and its neural processes" on 9 November 2022.

Dr Ryutaro UCHIYAMA (Research Fellow, NTU) gave a one-hour interview to the "The Dissenter" YouTube channel on cultural dynamics and our understanding of genetic effects, gene-environment interactions, and cognitive development. For more details, please refer to: https://youtu.be/j7HIP0AQwno

General

Research.com credited **Prof Trevor ROBBINS (Senior Scientific Advisor, CAM)** as the most highly cited researcher in both neuroscience and psychology in 2022.

Prof Robbins was also recognised as a Highly Cited Researcher by Clarivate in 2022 in the field of Neuroscience and Behaviour.

CKG

CITIES KNOWLEDGE GRAPH

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

CKG Principal Investigators:

Professor Markus KRAFT
University of Cambridge

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

Professor Martin RAUBAL
(July 2022 – present)
ETH Zürich

OVERVIEW

Cities Knowledge Graph (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 (FCLG) programme. The team is led by Principal Investigators from the University of Cambridge (Prof Dr Markus Kraft) and ETH Zürich (Prof Dr Martin Raubal). Dr Pieter Herthogs (Senior Researcher, SEC) is Co-Investigator and Project Leader. Dr Aurel von Richthofen (Team Leader Cities, ARUP Germany), Prof Dr Stephen Cairns (ETH) and Prof Dr Franziska Sielker (TU Vienna and CAM) are Co-Investigators of the project.

Over the past six months, we have made significant new additions to the knowledge graph architecture. We developed an Inference Agent to make intelligent choices and conclusions about tasks based on existing information in the knowledge graph. We developed a new ontology called OntoInfer, to represent the inference algorithms and tasks of cognitive agents. This new development allows agents to make more dynamic and context-specific choices based on existing data.

We extended various existing ontologies to include more concepts for measurable characteristics of buildable space on a plot, such as OntoZoning and OntoBuildableSpace. We extended the OntoUBEMMP ontology to include concepts for a more comprehensive representation of solar panels. We also developed a new ontology called OntoPlanningRegulations to semantically represent Singapore's planning regulations.

Furthermore, we improved some of the existing autonomous agents. For example, the City Information Agent can now transform multiple input parameters from the front-end application into complex queries for data retrieval and can filter the query results based on user input. The City Energy Analyst (CEA) Agent can now query the knowledge graph to obtain more inputs, such as building usage and surrounding building data, for CEA simulations.

The team further developed the Programmatic Plot Finder demonstrator to allow city planners to interact easily with the knowledge graph using a graphical user interface. We considerably improved the front-end application for this demonstrator, allowing users to easily navigate through regulatory information of various plots in Singapore. We are also designing the second demonstrator, the Suitable Site Selector, which will add evaluations and potential recommendations to the plots found using the first demonstrator. We have also been conducting several workshops with the Urban Redevelopment Authority (URA) in Singapore since December 2022 to showcase CKG research outcomes and obtain feedback on potential agency use cases. Lastly, we are starting up an international network for city knowledge graph developers, called the City Knowledge Graphs Network (CKGN); the first meeting took place in March 2023.

Professor Markus Kraft, PI
University of Cambridge

Professor Martin Raubal, PI
ETH Zürich

Update on work package 1

Developing master-planning ontologies

The team upgraded the OntoZoning ontology to improve its compatibility with the updated work on gross floor area calculations, inferencing, and urban energy modelling, for example, by introducing the concept of 'use quantum'. The *Journal of Urban Management* published the OntoZoning paper (with research led by **Ms Heidi SILVENNOINEN (Researcher, SEC)**) in a special issue on 'Digital technologies in urban planning and urban management'.

Ms Ayda GRIŠIŪTĖ (Researcher, SEC) developed the OntoBuildableSpace ontology, based on the existing OntoZoning ontology and the Units of Measure ontology (OM), to formalise measurable characteristics of buildable space on a plot. Concepts in this ontology were linked to Basic Formal Ontology (BFO) — a domain-agnostic upper-level ontology — to enable interoperability with other scientific research ontologies.

At the request of the Urban Redevelopment Authority (URA), the team organised an ontology validation workshop for CKG's OntoZoning, OntoPlanningRegulations, and OntoBuildableSpace ontologies of URA regulations. We created and shared with public officers of the planning authorities extensive documentation covering ontology modelling decisions and assumptions. URA is currently exploring the ontologies to provide feedback and potential implementation applications.

To automate allowable Gross Floor Area (GFA) calculations, Ms Grišiūtė and Ms Silvennoinen developed a semantic spatial policy model. They calculate allowable GFA by cross-referencing planning regulations for each plot from Singapore's Masterplan 2019 dataset and extracting the applicable number of storeys, setbacks, allowed site coverage and Gross Plot Ratio (GPR) values.

Figure 8.1: Explaining OntoZoning concepts and ontology competency questions to Singapore's planning authorities.

They also upgraded previously developed scripts for calculating allowed GFA for plots in the Singapore River Valley area to cover all plots across Singapore. Furthermore, Ms Grišiūtė merged and optimised individual scripts for residential and other types of plots, resulting in a more robust implementation.

The newly generated GFA estimates dataset for all plots in Singapore quantifies regulatory data and allowable built form at scale, which supports the integration of planning regulation into urban analytics. The dataset can be queried together with zoning data in the knowledge graph for more detailed programme-based plot-finding. Furthermore, semantically represented planning regulations and concepts can also be queried. This makes it feasible to perform systematic analyses on a subset of Singapore's planning policies or to check for any contradictions or discrepancies by leveraging semantic reasoning engines. The team also submitted a conference paper for the CAADFutures 2023 conference, led by Ms Grišiūtė, describing the proof-of-concept of this process.

Lastly, Ms Grišiūtė continued work on the OntoPlanningRegulations ontology to formalise Singapore's planning regulations. She examined and harmonised publicly available planning regulations by introducing consistent concept names, semantic structure and uniform data formats across regulations. Planning regulations generally fall into two distinctive classes: TypeRegulations and AreaRegulations. Area regulations are associated with a particular spatial boundary,

```
PREFIX opr: <http://www.theworldavatar.com/ontology/ontoplanningreg/OntoPlanningReg.owl#>
PREFIX om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>
PREFIX obs:<http://www.theworldavatar.com/ontology/ontobuildablespace/OntoBuildableSpace.owl#>
SELECT ?height_control_regulation ?absolute_height_value
WHERE { GRAPH <http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/planningregulations/>
      { ?height_control_regulation rdf:type opr:HeightControlPlan;
          opr:allowsAbsoluteHeight ?abs_height .
      ?abs_height om:hasValue/om:hasNumericValue ?absolute_height_value .
      FILTER(?absolute_height_value > 100 ) } }
```

Advanced features

Execute Clear

height_control_regulation	absolute_height_value
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_d1b3127d-0f9a-4533-8873-47d36096f6b7/>	104
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_eab67ad4-c7df-4ccd-aefa-e95dae8478e3/>	117
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_4bd7b4f2-0578-4cdf-b9d7-b1ecf6926744/>	117
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_3c5223d9-58a1-41b4-871b-330644240f59/>	250
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_2938925f-8d18-4fda-a55e-a2b9d851db9a/>	117
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_c9edf682-eed7-4aab-9544-9fc1141b5596/>	118
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_b688974b-067a-4f05-8c95-8302510dd9a4/>	104
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_921ea5cd-3177-4a15-bad0-f4403eeca81b/>	104
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_0f9ffa3c-c786-45e1-a49b-36ae1c86ecdb/>	153
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_e3f1cda8-8eff-4508-b90e-3ee97b34a7a1/>	250
<http://www.theworldavatar.com:83/citieskg/namespace/singaporeEPSG4326/sparql/cityobject/UUID_a7c67859-7040-4d31-b48d-69bb568753ee/>	153

Figure 8.2: An example query to search for URA regulation that allows absolute height of more than 100 metres. This illustrates additional query capabilities resulting from semantically representing a subset of Singapore's planning regulations necessary for allowed GFA calculation.

with Street Block Plans, Urban Design Guidelines, Height Control Plans, and Landed Housing Areas modelled as subclasses of this category. Type regulations are associated with particular land use types or other development properties, with Development Control Plans and Road Categories modelled as subclasses of this category.

Mr Yi-Kai TSAI (Software Developer, CARES) extended the OntoUBEMMP ontology to include concepts for a more comprehensive solar panel representation. More specifically, Mr Tsai improved the ontology to semantically represent the specific yield and the peak power generated by solar panels, the potential carbon dioxide savings that energy generators produce, and the solar radiation received by solar energy generators.

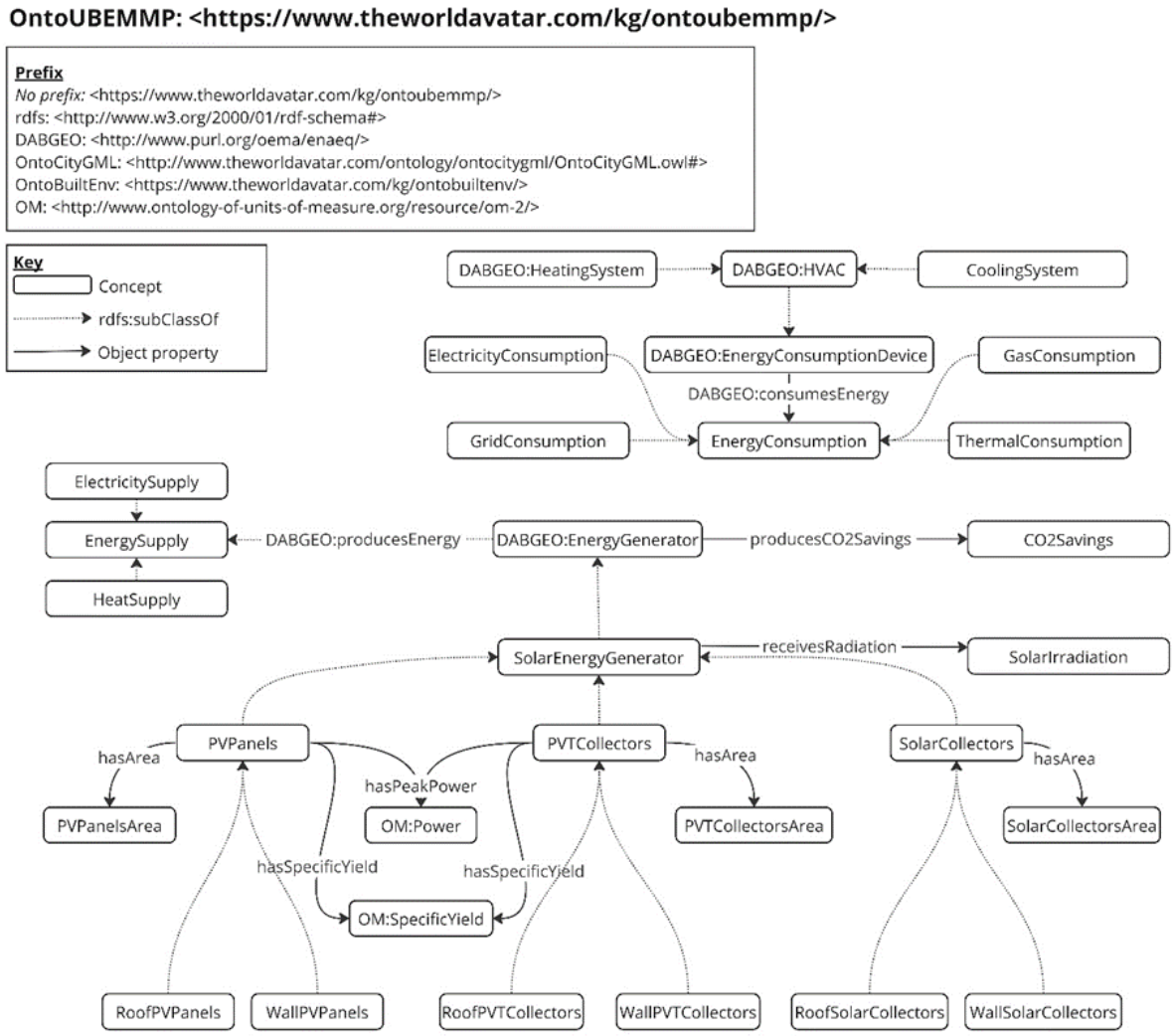


Figure 8.3: OntoUBEMMP ontology showing the types of energy consumption and energy generating devices that a building could install and the types of energy that these devices could consume or produce.

Update on work package 2

Developing the knowledge graph's architecture

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES) developed Inference Agents that were integrated into revised novel semantic web systems reference architecture for inferences. This also includes other components that can store and operate on knowledge graphs to infer new statements by an intelligent autonomous agent capable of making informed choices based on long-term memories about its tasks that implement inference algorithms. The research findings were described in a paper entitled 'Semantic 3D City Inferences - multi-domain reasoning on Dynamic Geospatial Knowledge Graphs' and submitted to the *Journal of Web Semantics*. Figure 8.4 shows the graphical abstract of the paper.

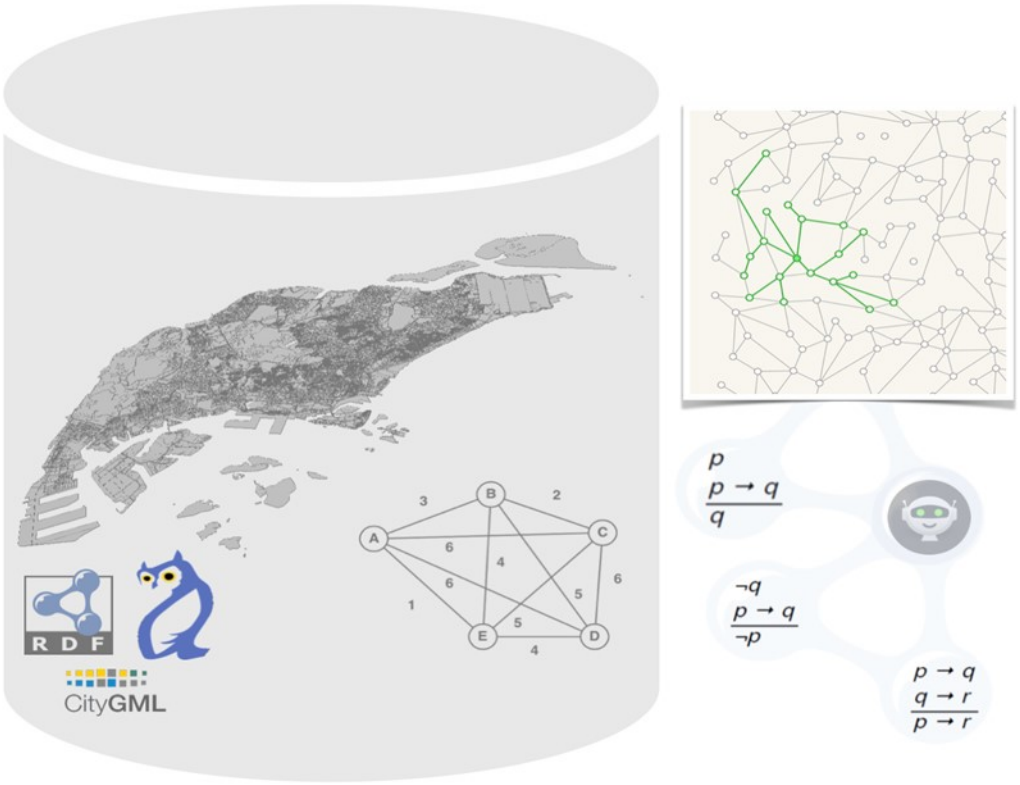


Figure 8.4: Graphical abstract of a paper describing extended novel system architecture for inferences on dynamic geospatial knowledge graphs.

Mr Chadzynski designed an Inference Agent to make informed choices based on long-term knowledge. The agent is supported by the newly developed OntoInfer ontology that encodes the taxonomy of inference algorithms linked to instances of the agent's tasks, thereby allowing the agent to make decisions based on the knowledge stored in the knowledge graph. This extended architecture can demonstrate the implementation of tasks designed to work as independently executed threads containing examples of known inference algorithms, using existing libraries and reasoning engines (Jena Jung and HermiT). Mr Chadzynski showcased the multi-domain reasoning capabilities on city object descriptions in terms of OntoCityGML, OntoZoning and OntoBuildableSpace on plot data converted into OWL 2 compliant knowledge base.

Mr Chadzynski also designed and developed the Owlconverter tool as a new architectural component which can produce fully dynamic knowledge graphs without the information loss

that usually occurs while attempting to store complex concept definitions in existing open-source dynamic triple stores.

Ms Shiying LI (Software Engineer, SEC) and Mr Chadzynski prepared the latest release for the Cities Knowledge Graph project. This included the Inference Agent described above and an updated version of City Information Agent, which allows transforming input parameters from the front-end application into more complex queries and filtering query results for the visualisation. The release also included the latest development of the front-end application (Programmatic Plot Finder demonstrator), such as different visualisation features for the query results and an information box. **Ms Srishti GANGULY (Project Engineer, CARES)** tested and deployed these new and improved agents as part of the release.

Update on work package 3

Developing agents to operate software and integrate data

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES) worked on the Inference Agent, built upon the JPS Agent Framework, which can answer with new insights to requests specifying objects described within the knowledge graph and types of desired reasoning methods. Within this architecture, a dynamic triple store provides a way to store long- and short-term memories about objects organised into larger structures described in the form of OWL 2 compliant Subject-Predicate-Object statements. The novel reference architecture places long-term knowledge corresponding to scientific theories (TBox) and knowledge about facts described in terms of those theories (ABox) in a dynamic store that allows for concurrent access and modifications to any functional processes by intelligent autonomous agents.

The Inference Agent uses the OntoInfer ontology described in Work Package 2 to make intelligent decisions based on the data in the knowledge graph about which task to operate to satisfy certain requests, as opposed to having this 'choice logic' implemented in the form of programming language code. This opens a possibility for agents to make more dynamic, context-based choices.

Because the two classes of inference algorithms used by the agent operate on different parts of the knowledge base, the agent is implemented as an abstract class in Java that groups the common functionality required to make all inferences. Instances of the concrete subclasses of the abstract class, namely Graph Inference Agent and Ontology Inference Agent, listen to and intercept requests pointing to either the whole graphs or into identifiers of classes and individuals within a graph, accordingly. Knowledge about different parts of the globe, geospatially described within separate and widely adopted Coordinate Reference Systems (CRS), is stored in separate namespaces within the knowledge graph. Every namespace is automatically assigned a unique

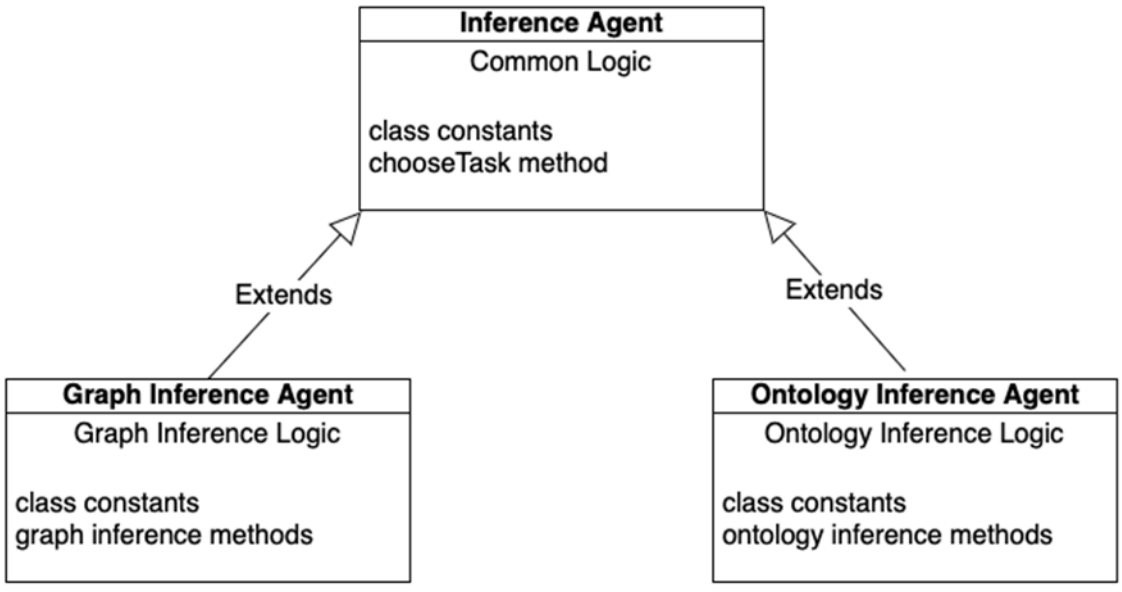


Figure 8.5: Class diagram of Inference Agent designed as an abstract class in Java that groups common inference agent logic and subclasses into Graph Inference Agent and Ontology Inference Agent that contain operations specific to two types of inference algorithms within Dynamic Geospatial Knowledge Graphs.

Internationalised Resource Identifier (IRI). Different parts of namespaces are separated into named graphs that describe distinct aspects of geospatial objects. Graph inference algorithms are provided with IRIs of named graphs containing knowledge in the form of TBox and ABox as inputs for analysis. Ontology inference algorithms operate on IRIs of classes, individuals or both to analyse their relationships within the knowledge base. The only exception is consistency checking, which (similar to the graph inference algorithms) requires whole graphs as an input. The relationship between Inference Agent and its two subclasses responsible for applying different classes of inference algorithms is depicted in Figure 8.5.

Mr Yi-Kai TSAI (Software Developer, CARES) updated the City Energy Analyst (CEA) agent to use more data retrieved from the knowledge graph as inputs for CEA simulations. The CEA agent now retrieves building usages and surrounding buildings' footprints from the knowledge graph to use as inputs for CEA. Mr Tsai also increased the flexibility of the agent by allowing optional parameters to specify the endpoints for the different queries for the CEA inputs mentioned above and to specify endpoints for the instantiation and querying of triples representing CEA results.

For building usage input, the agent first queries for the target building's usages and the respective usage shares, and the retrieved data is converted to the database file format CEA requires. The building usage input, as utilised in CEA, defines Heating, Ventilation and Air-Conditioning (HVAC) system settings, occupancy and utilities usage schedules, which could impact the consumption calculations done by CEA. For surrounding buildings' footprints, the agent retrieves this data from the knowledge graph and writes it into shapefiles for use by CEA as input. This allows CEA to use in addition to the default OpenStreetMap, additional data sources for surrounding buildings' footprints.

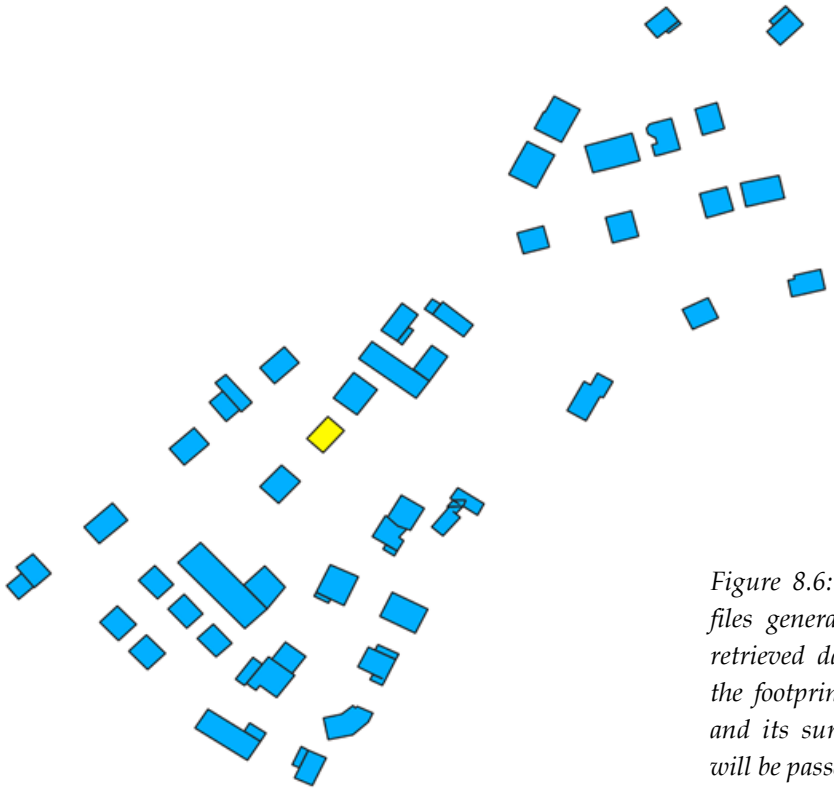


Figure 8.6: QGIS visualisation of the shapefiles generated by the CEA agent, with the retrieved data from the knowledge graph on the footprints of the target building (yellow) and its surrounding buildings (blue), which will be passed to CEA as inputs.

Update on work package 4

Developing interfaces and planning libraries for the CKG

The 3DCityDB-Web-Map-Client uses CesiumJS as its underlying technology and uses a dynamic loading technique to achieve seamless streaming of 3D objects for large city on the map. **Ms Shiying LI (Software Engineer, SEC)** implemented a feature into the 3DCityDB-Web-Map-Client which allows the querying of results over the whole of Singapore by creating an additional point data source for each query, so that points representing query results can be shown while the user waits for the 2D plot objects to load. Figure 8.7 illustrates the plot visualisation, point visualisation, and plot information. Ms Li also developed the interface element of the Programmatic Plot Finder demonstrator that summarises key information of the current and past queries and allows users to (de)select and delete query results and their visualisation.

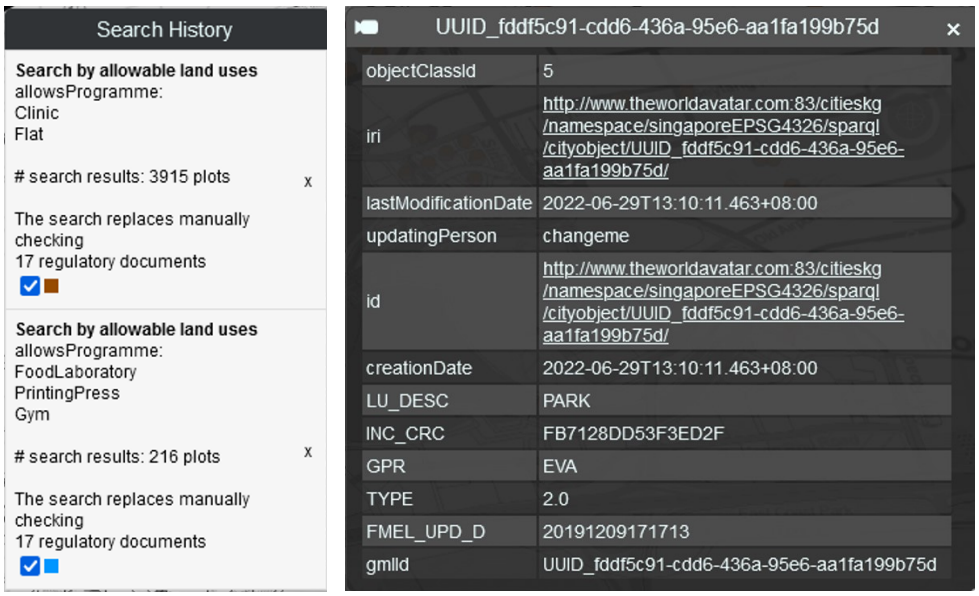


Figure 8.7: An instance of a point data source connected to the underlying plot and the relevant plot information (which can be retrieved by clicking on either the point or the plot). The white and grey command boxes are enlarged to the left.

Dr Jingya YAN (Research Fellow, CARES) worked on processing and visualising the Singapore CityGML Level of Detail 3 (LOD3) dataset. The data must be converted from triples to 3D Tiles to improve visualisation efficiency. To achieve this, Dr Yan developed a CityGML export function based on the 3D City Database Exporter tool. Figures 8.8 and 8.9 display the visualisation of LOD2 building models in Pirmasens, Germany and LOD3 building models in Singapore.

Figure 8.8: Visualisation of LOD2 building models in Pirmasens, Germany.

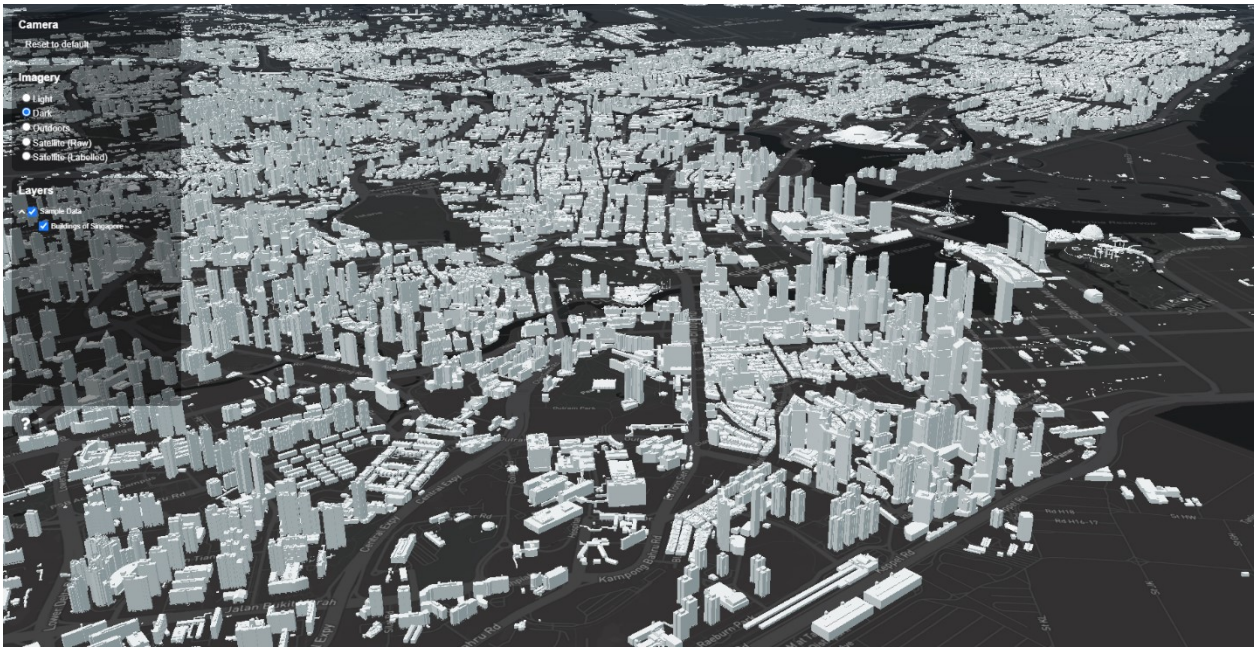


Figure 8.9: Visualisation of LOD3 building models in Singapore.

Update on work package 5

Developing Design Informatics Functions

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES), in collaboration with **Dr Pieter HERTHOGS (Senior Researcher, SEC)**, **Ms Shiying LI (Software Engineer, SEC)** and **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)**, started designing and developing a knowledge administration panel for the Cities Knowledge Graph (CKG). The application's aim is to open knowledge management to domain experts that are less proficient in lower-level programming languages, such as SPARQL, Java, and Python. It will provide intuitive user interfaces to manage ontologies and rules of inference within dynamic geospatial knowledge graphs. Following sustainable digitisation practices, existing open-source software will be adopted to achieve this goal. WebProtégé, a modernised version of the popular ontology editor, Protégé, will be augmented to work with ontologies stored in dynamic Resource Description Framework (RDF) stores. Existing Protégé plugins for the Semantic Web Rule Language will be adapted to work with web interfaces to allow for user-friendly management of knowledge inference rules by domain experts.

The team also scoped the underlying technologies and concepts of a second CKG demonstrator: the Suitable Site Selector, with multi-domain and multi-criteria evaluation of plots in Singapore. This demonstrator will extend the current Programmatic Plot Finder demonstrator, adding evaluations and recommendations to the sets of plots retrieved through programme-based search. The team is exploring a potential collaboration on this site evaluation demonstrator with Takenaka Asia Region (applied to Singapore).

Update on work package 6

Demonstrators: horizontal and vertical use cases

This work package aims to develop use cases that showcase horizontal (island-wide, strategic) and vertical (plot-based, built-form-related) planning synthesis support to demonstrate the potential applications and extensibility of the Cities Knowledge Graph (CKG) approach.

The development of the first demonstrator, the Programmatic Plot Finder (PPF) (demonstrating Representation and Search), led by **Dr Pieter HERTHOGS (Senior Researcher, SEC)** and developed by **Ms Shiying LI (Software Engineer, SEC)**, **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)**, **Ms Heidi SILVENNOINEN (Researcher, SEC)** and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, with inputs from the entire CKG team, was ready for hands-on user testing in October 2022. This was shared with the Urban Redevelopment Authority (URA) in Singapore for review.

The PPF demonstrator is a front-end application allowing planners to interact with the knowledge graph using a map-based Graphical User Interface (UI) to search for specific plots in Singapore, rather than having to query the knowledge graph directly using SPARQL query language. The 3DCityDB-Web-Map-Client serves as a base for the demonstrator. Based on a user's interaction with UI elements, the 3DCityDB-Web-Map-Client automatically generates a JSON object that is passed to the City Information Agent (CIA). The CIA uses it to construct relevant filtering SPARQL queries, and then sends these queries to the knowledge graph to retrieve information about plots. The results are processed using the CIA filtering functionality and the resulting plots visualised on the 3DCityDB-Web-Map-Client (Figure 8.10).

From the dropdown menus, users can select combinations of programmes or uses that should be allowed on a plot. Additionally, users can provide amounts for these programmes or uses. These inputs are also translated into a human-readable sentence, such as 'Where can I build a Clinic of 200 m² or more?', providing a tangible translation as feedback for the technical query process. After the CIA filters the query outcome, the resulting plots are highlighted in two levels of detail: using map pins when zoomed out and using coloured plot polygons when zoomed in.

Figure 8.10: CKG's Programmatic Plot Finder demonstrator.

The results of every query input are also summarised in an information box showing an overview of the initial input and the total amount of valid results. The UI is under active development, with the full feature list prioritised and road mapped and subject to change based on user feedback.

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. Further meetings took place with the Smart City Projects Office (Smart Nation and Digital Government Office (SNDGO)) in December 2022 and January 2023, and the Urban Redevelopment Authority (URA) Design & Planning Lab (DPL) and Strategic Planning in December 2022, January 2023 and March 2023.

During the December 2022 meeting, the team organised a hands-on demonstration and technical Q&A session with representatives from the Smart City Projects Office and URA. The team is developing a multi-agency workshop to showcase CKG research outcomes and obtain feedback on potential cross-agency use cases from different agency planners; SNDGO supports this initiative.

Dr Pieter HERTHOGS (Co-PI, SEC), **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)**, **Ms Shiying LI (Software Engineer, SEC)**, and **Ms Mei Qi LIM (Project Manager, CARES)** organised an ontology validation workshop for URA representatives in March 2023, in which they explained the modelling process of three URA regulation ontologies and received feedback. These ontologies and their potential applications within URA are currently being studied by the URA DPL. The team has been invited by the URA DPL to present at the Satellite of Excellence Smart Planning steering committee meeting in June 2023; this is a bi-annual forum co-chaired by the Housing & Development Board (HDB) and URA and attended by multi-agency counterparts involved in Research & Innovation efforts in the urban planning & design technologies, health & well-being and liveability domains.

By invitation of the Centre for Liveable Cities (CLC), Dr Herthogs attended a 5-day Complexity Science Studio Workshop at University College London in November 2022, where he presented CKG, as well as other projects. This workshop was organised by the CLC and the Centre for Advanced Spatial Analysis and attended by Singaporean public officers and university researchers.

Dr Herthogs also presented CKG in an invited lecture for a course of Prof Dirk HELBING (ETH Zürich) in October 2022. In this reporting period, the team has presented its research and demonstrator in meetings with ESRI, Aalto University, Takenaka R&D, NTU, University of Toronto, National University of Singapore Cities, and TU Braunschweig. A multi-project journal article, entitled 'The conundrum in smart city governance: Interoperability and compatibility in an ever-growing ecosystem of digital twins', with contributions by Dr Herthogs, **Prof Dr Franziska SIELKER (Co-PI, TU Vienna and CAM)**, **Dr Aurel VON RICHTHOFEN (Co-PI, Arup Germany)**, and **Prof Dr Markus KRAFT (PI, CARES)**, discussing the need for interoperability in digital twins and smart city governance was published in the journal *Data & Policy* in February 2023.

In October 2022, the team was approached by Prof Mark FOX (University of Toronto), a leading expert in city ontologies and standards, to explore collaborations. Together, we are starting up an international network for city knowledge graph developers, called the City Knowledge Graphs Network (CKGN); the first meeting took place in March 2023.

Dr Herthogs, Mr Genki UNNO (Visiting Scholar, Takenaka Corporation), Ms Li, and Ms Grišiūtė presented the Programmatic Plot Finder demonstrator to Mr Ryusuke KOJIO (General Manager Design and Global Solutions, Takenaka Corporation Asia Region). We will explore a potential collaboration on the Suitable Site Selector demonstrator, based on representative Takenaka client requests (applied to Singapore). Mr Unno, advised by Dr Herthogs, has developed a thematic evaluation framework for Smart Circular City projects and visions.

Scientific output

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

Defining archetypes of mixed-use developments using Google Maps API data
Zhongming Shi, Heidi Silvennoinen, Arkadiusz Chadzynski, Aurel von Richthofen, Markus Kraft, Stephen Cairns, and Pieter Herthogs, *Environment and Planning B: Urban Analytics and City Science*
DOI: 10.1177/2399808322114142

Abstract: Urban planning relies on the definition, modelling and evaluation of multidimensional phenomena for informed decision-making. Urban building energy modelling, for instance, usually requires knowledge about the energy use profile and surface area of each use that takes place within a building. We do not have a detailed understanding of such information for mixed-use developments, which are gaining prominence in urban planning. In this paper, we developed a methodology to quantitatively define the characteristics of mixed-use developments using archetypes of programme profiles (ratios of each programme type) of a city's mixed-use plots. We applied our methodology in Singapore, resulting in 163 mixed-use zoning archetypes using Singapore's master plan data and Google Maps API data. In a case study, we demonstrated how these archetypes can be used to provide more detailed data for urban building energy modelling, including energy demand forecasts and energy supply system design. To enable future automation of the workflow, the archetype definitions were represented and stored as a machine-readable ontology. This ontology can later be extended with for example, the mobility properties of archetypes; thus, enabling the archetypes' use in other urban planning applications beyond building energy modelling.

A semantic web approach to land use regulations in urban planning: The OntoZoning ontology of zones, land uses and programmes for Singapore
Heidi Silvennoinen, Arkadiusz Chadzynski, Feroz Farazi, Ayda Grišiūtė, Zhongming Shi, Aurel von Richthofen, Stephen Cairns, Markus Kraft, Martin Raubal, and Pieter Herthogs, *Journal of Urban Management*
DOI: 10.1016/j.jum.2023.02.002

Abstract: Semantic web technologies have the potential to significantly improve urban regulatory data access, integration and usability, with potentially large implications for planning practice. Ontologies are a cornerstone of the semantic web. In this paper, we describe OntoZoning, an ontology representing relationships between zoning types, land uses and programmes (more specific land uses) in Singapore. We link the ontology to geospatial data stored in a knowledge graph, which allows executing multi-domain queries on urban data. We demonstrate how such a semantic web based approach can improve access to and usability of land use regulation data, and in particular facilitate site selection and exploration. We also discuss the difficulty of defining some concepts in the land use regulation field, and how OntoZoning could be linked to a broader semantic-web based urban planning regulatory framework.

SMALL PROJECTS

OTHER CARES-FUNDED PROJECTS

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

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

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

An Accelerated Manufacturing Platform for Engineered Nanomaterials (AMPLE)

Central Gap Fund

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

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

Dr Nicholas JOSE (Project Lead, AMPLE) has developed a new UI for an automated, versatile flow synthesis system, which can be used for lab-scale low pressure materials and chemicals synthesis. He has also completed designs for a 100 kg/day "number-up" modular reactor which will be implemented, completed outdoor trials of anti-microbial coatings at Wolfson College in Cambridge, and led the team to completion of all required AMPLE Phase 1 deliverables to date.

Dr Jose's future goals are to integrate automated flow system with OPC Unified Architecture (OPC -UA) and knowledge-graph data-storage systems and oversee the commissioning of a 100 kg/day reactor.

Dr Mikhail KOVALEV's (Product Development Manager, AMPLE) has finalised the recipe formulation for three commercial additive products and developed their internal specifications. He has also purchased major characterisation equip-

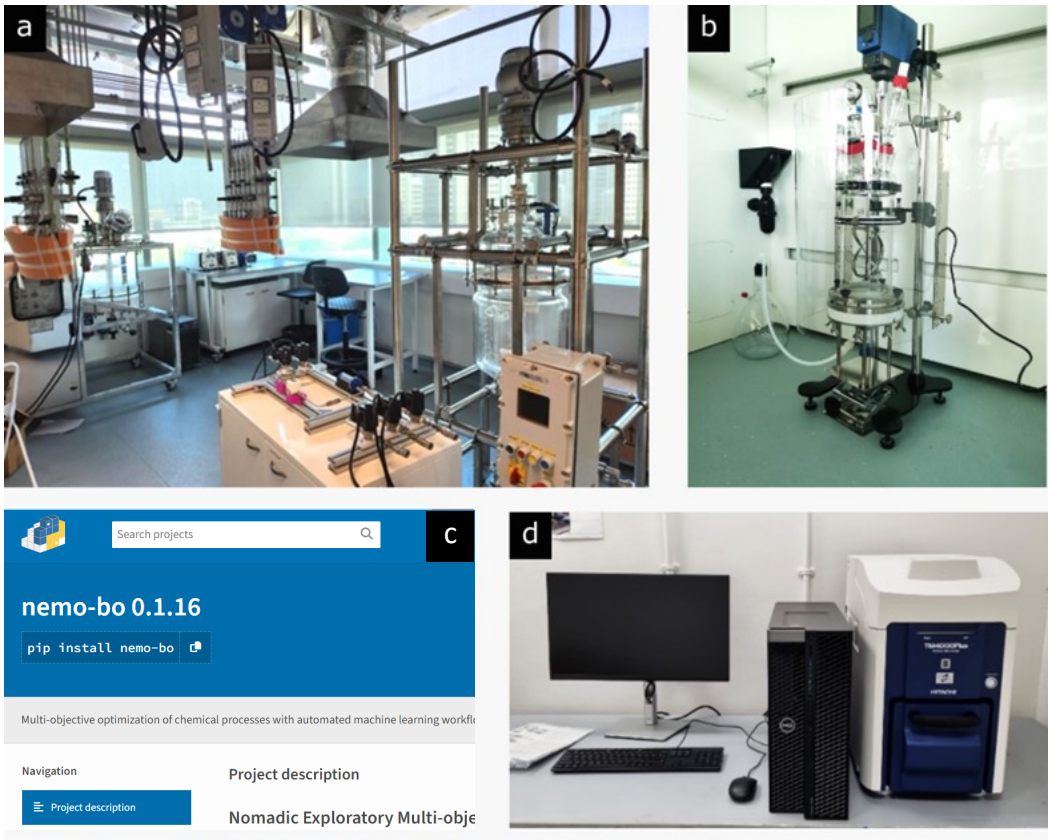


Figure 9.1: a) CARES Pilot Room being commissioned, (b) new pilot equipment being installed in the lab, (c) a screenshot of NEMO – a new machine learning method developed in the PIPS programme (following research update), being implemented in AMPLE, (d) a table top scanning electron microscope for product characterisation and quality control.

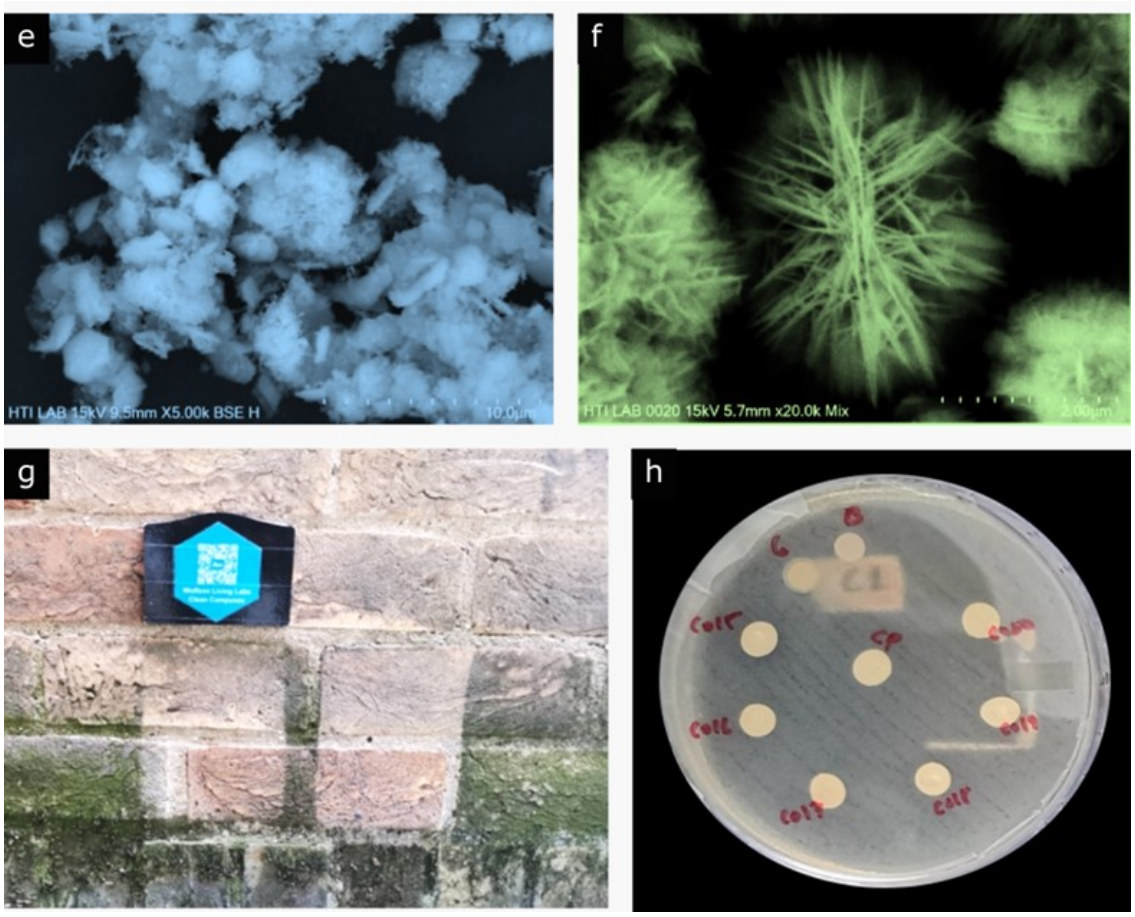


Figure 9.1 (cont): (e & f) SEM images of different ZnO morphologies synthesised, (g) the outdoor trial of ZnO coatings taking place at Wolfson College, and (h) antimicrobial assays of ZnO treated materials.

ment to support product development and quality control efforts. His future goals are to fine tune recipe formulation for the additive products, scale-up the products to multi-kilo scale, and complete characterisation of the product efficiencies.

Ms Satya KENCHA (Quality Control Scientist, AMPLE) obtained characterisation data for flow reactor synthesised ZnO nanoparticles using DLS, Raman, TGA, XRD and SEM to establish quality control protocols. She synthesised ZnO combined with paint samples and did Qualitative and Quantitative antibacterial testing on *E.coli*. These characterisation techniques were drafted into SOPs. Her future goals are to standardise all Quality Control protocols for characterisation of ZnO and coating formulations, and to standardise Quantitative and Qualitative assays for antimicrobial activity on both bacterial and fungal strains.

Dr Susithra LAKSHMANAN (Chemical Engineer, AMPLE) synthesised ZnO and performed its characterisation techniques. She also completed training for the operation of the g-scale annular micro reactor and built the reactor vessel which included vessel glass assembly and Purification module training. She also assisted in procuring fittings, dosing module assembly, Flow Meter calibrations and data analysis.

Dr Lakshmanan's future goals are to commission the semi-automatic kg–scale rig for demonstration; these include the Dosing, Reactor and Purification modules. She will also conduct experiments based on Design of Experiments and from these results and data analysis, conduct further experiments for high quality ZnO production.

Dr Mohammed JERAAL (Materials Engineer, AMPLE) designed and implemented an ML workflow that optimises the manufacture and performance of ZnO nanoparticles. Publicly available updates to the machine workflow have

resulted from this. Dr Jeraal has also specified and procured a large selection of fittings needed for the 100 kg/day scale dosing module, reactor module and filtration module. He has also developed and created SOPs for characterisation procedures needed to measure and improve quality of ZnO products.

Dr Jeraal's future goals are to further develop the aforementioned ML workflows and apply them in the development of specific customer products for specific performance characteristics. He will also focus on using the apparatus procured for the large rig to assist in the pilot scale reactor's construction, testing and operation. Lastly, he will address the gaps in the current product specification (crystallinity, dispersion stability) with the development and application of additional product characterisation techniques using equipment that will arrive in the next 6 months.

Ms Faye NG (Mechanical & Automation Engineer, AMPLE) assisted in specifying and procuring fittings and components for the Reactor module and Dosing module for both Automated and Backup Rigs. She also designed and fabricated custom jigs for both Dosing and Reactor modules to accommodate components and electronics. Lastly, she sourced and liaised with a system integration company for automation; established documentation, communication protocols, component preparation, and software architecture.

Ms Ng's future goals are to deploy and commission the fully automated Dosing and Reactor modules, ensuring readiness for manufacturing use. She will also integrate optimisation algorithms using FLAB with the team's Programmable Logic Controllers (PLCs) for closed-loop optimisation, and help to develop a more robust and transparent inventory tracking system to streamline operations.

Mr Kelvin YEO (Business Development Manager, AMPLE) completed his induction in scientific and engineering knowledge necessary for the role. This includes technical knowledge pertaining to scientific analysis (Raman, UV-vis, SEM, XRD, ICP, etc.) as well as reviewing existing preparations of AMPLE's going-to-market strategy. At the operational level, Mr Yeo provides support on events planning, budgeting, and corporate strategy with internal stakeholders. He has also initiated a call for the enhancement of the business development budget to support an initial events pipeline, marketing, and industry partner relationship acquisition.

Mr Yeo is currently taking the lead in planning and executing the AMPLE exhibition display in TechConnect World 2023 held in Washington DC. He is also working with six industrial partners on defining potential commercial use cases of ZnO in the fields of antimicrobial functions, cosmetics, and as an active preservative in the paints and coating industry.

Mr Yeo's future goals are to finalise collaboration agreements with at least three partners and develop a business plan and fundraising support for Accelerated Materials.

Other activities and achievements

Dr Nicholas JOSE (Project Lead, AMPLE) and **Mr Kelvin YEO (Business Development Manager, AMPLE)** attended the Nanotech Expo 2023 in Tokyo; Mr Yeo and **Dr Mikhail KOVALEV (Product Development Manager, AMPLE)** attended Korea Chem Expo 2023. The aim of these activities was to gather key insights on industry demands in APAC and connect AMPLE to important players.

AMPLE is actively working with industry partners to develop products and supply chains for nanomaterial production in Singapore. These partnerships are fuelling the Phase 2 (2023-2024) production trials.

NDA's have been signed with strategic industry partners including GlaxoSmithKline, Kowa Technologies and Corning. MOUs and RCAs for proof-of-concept and proof-of-value projects are in negotiation for the team's Phase 2 trials.

The team have also registered Accelerated Materials Pte Ltd in Singapore in March 2023, which will be the commercialisation engine for all technologies developed in AMPLE. Accelerated Materials began as an engineering services spin-off from IRP1 established by Dr Jose, Dr Kovalev, and **Prof Alexei LAPKIN (PI, CAM)**. Dr Jose aims to present work and fundraise for the seed-round of Accelerated Materials.

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

Intra-CREATE seed collaboration grant

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

In this reporting period, **Dr Casper LINDBERG (PI, CARES)** and **Ms Qi ZHOU (Project Officer Intern, NUS)** have focused on reviewing existing software and ontologies and determining the information needed to represent the NTU use-case. Existing ontologies are currently being extended to link the power network to their building load representations as well as the power consumption and solar generation time series data. Relevant power systems agents are also being updated to the latest agent framework, and new agents are being developed to instantiate data in the knowledge graph.

Ms Zhou instantiated a sample 15-bus power network with the OntoPowSys ontology. Optimal power flow (OPF) analysis was conducted on the sample network using the PyPower package contained within an existing agent, the ENAgent. The agent outputs were compared against sample data provided by NTU to evaluate the network instantiation and the functioning agent. Currently, Ms Zhou is working on a new containerised implementation of the ENAgent called the OPFAgent. This is an updated version of the ENAgent that uses the Access Agent framework to query the knowledge graph for details of the electrical network and then update the knowledge graph with the results of the OPF calculations. This transitions the agent from processing text and OWL files to interacting with triple stores within the JPSAgent framework.

Dr Lingberg and colleagues in other CARES projects (particularly **Mr Mingchuan TIAN, Cities**

Figure 9.2: Visualisation of the instantiated buildings on the NTU campus displaying historical power consumption data for the School of Physical and Mathematical Sciences (SPMS) building.

Software Developer) have developed an agent to retrieve historical NTU power consumption readings and instantiate them in the knowledge graph using the time series framework. The agent creates a relational database to store the data and links to time series instances within the knowledge graph. He also extended the existing ontologies to describe the NTU campus' power system. This will allow a large volume of historical and real-time data to be instantiated and interconnected with real-world entities, providing a solid foundation for future applications such as P2P energy markets and load flow optimisation to be deployed and tested within the knowledge graph.

Dr Hung NGUYEN (PI, NTU) and Dr Veerapandiyan VEERASAMY (Non-CARES Research Fellow, NTU) have been working on the NTU campus' 22kV distribution network. The microgrid setup in the Clean Energy Research Lab at NTU will be modelled and integrated into the NTU campus model within the knowledge graph. P2P energy trading will then be implemented within this microgrid setup to simulate the transactions.

Digital Workflow and Continuous Processing in Pharmaceuticals Manufacturing

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

Dr Dogancan KARAN (Research Fellow, CARES) is currently working on an industrially relevant multistep (2-step) process for synthesis of an active pharmaceutical ingredient. The project involves developing automated continuously flow reactors and gaining process understanding via machine learning. Earlier in the project, Dr Karan developed the continuously flow reactor for the first step of the project and performed fully automated machine learning optimisation. 75% yield with minimum process cost was identified. In this reporting period, he developed a new fully automated reactor platform for the second step of the process. The development involves analysis of the hydrodynamics and mixing characteristic via residence time distribution (RTD) studies, CFD simulations to understand the heat transport characteristics and deploying automation to control the whole workflow. The process was optimised for yield vs impurity as competing objectives by TSEMO algorithm. 94% yield and 4% impurity were identified as the optimum conditions in 39 experiments.

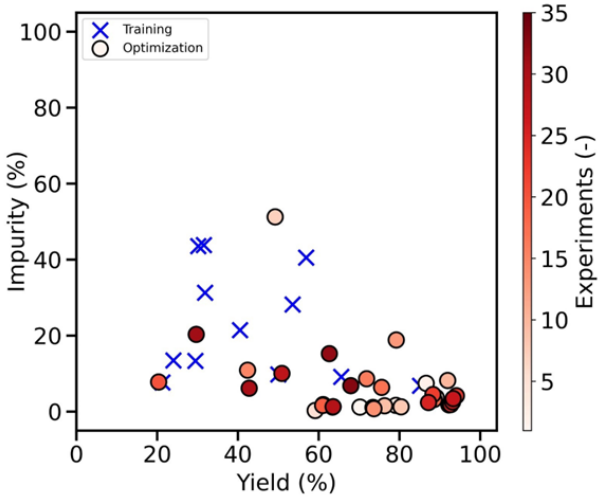


Figure 9.3: Plot of yield vs impurity for experiments related to optimisation of Step 2. The initial training set experiments and optimisation experiments combine to form a Pareto plot to highlight the trade-off between two objectives.

Cooling Singapore 2.0

In collaboration with the Singapore-ETH Centre

Cooling Singapore 2.0 aims to construct a Digital Urban Climate Twin (DUCT) for Singapore. This platform 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 their impact on urban heating.

CARES' contribution to Cooling Singapore 2.0 is to evaluate anthropogenic heat emissions from Industry in Jurong Island, Singapore, by developing computational energy models using the World Avatar (TWA) Knowledge Graph. Ultimately, these energy models will be fed into the Digital Urban Climate Twin. CARES will also develop scenarios to investigate the impact of the anthropogenic heat emissions from Industry in Jurong Island on Singapore.

Dr Karthik NAGARAJAN (Software Developer, CARES) and Ms Srishti GANGULY (Project Engineer, CARES) conducted an extensive literature search to gather data on the carbon emissions of chemical plants and logistics/storage companies on Jurong Island. The collected data was then instantiated into the knowledge graph, making it machine-readable. The data on carbon emissions was used to estimate the rate of heat emissions caused by industries on Jurong Island. TWA Knowledge Graph contains publicly available data on 119 companies, including their Singapore Standard Industrial Classification (SSIC) code, formation year, production technology, business activity, employee count, revenue, energy consumption, design capacity, and the amount of carbon dioxide they produce.

Dr Hansong XUE (Research Fellow, CARES) has further improved the Heat Emission agent to provide hourly profiles of heat emissions in GeoJSON required as inputs for the Weather Research & Forecasting (WRF) model in DUCT. At present, the hourly profile is assumed to be static due to the nature of the data available. In the knowledge graph, 568 anthropogenic heat emission points have been instantiated. Each point consists of the estimated heat emission rate and the centroidal coordinates of the heat emitting points.

Figure 9.5 shows the 3D visualisation of the various infrastructures on Jurong Island, along with their associated information, including their annual carbon emission and heat emission. Clicking on a structure displays the information box on the top right-hand corner, as shown in Figure 9.5. This information box is populated by querying all the data associated with a given structure from TWA knowledge graph.


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Figure 9.4: GeoJSON output of the Heat Emission agent for DUCT simulation. One anthropogenic heat emission point (centroidal coordinates highlighted in yellow) with assumed static hourly profile is illustrated here.

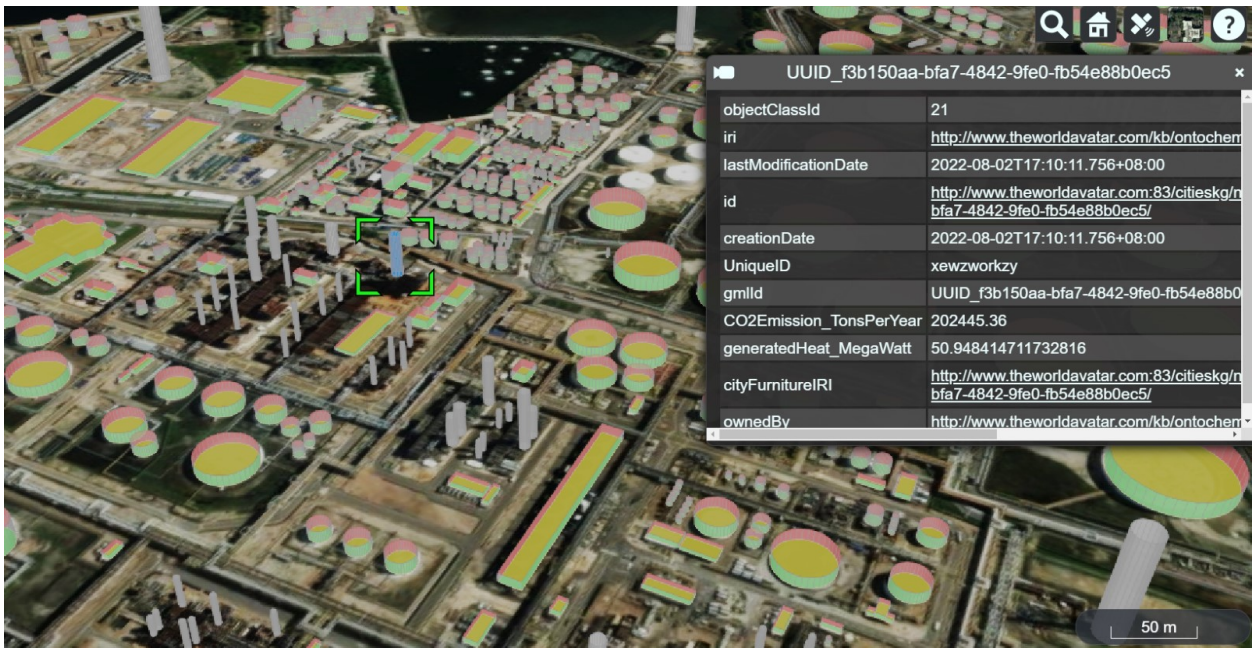

Figure 9.5: 3D visualisation of the various infrastructures on Jurong Island, along with their associated data queried from the knowledge graph.

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 source of air pollution in Southeast Asia and a factor of climate change. The project's experimental work has been finished in partnership with researchers from the Department of Environmental Engineering in NUS. The major result of the study is published in the journal *Atmospheric Environment*. The work provides insights into the potential impacts of blending fuels on the chemical and optical properties of BC and BrC emitted from engine combustion.

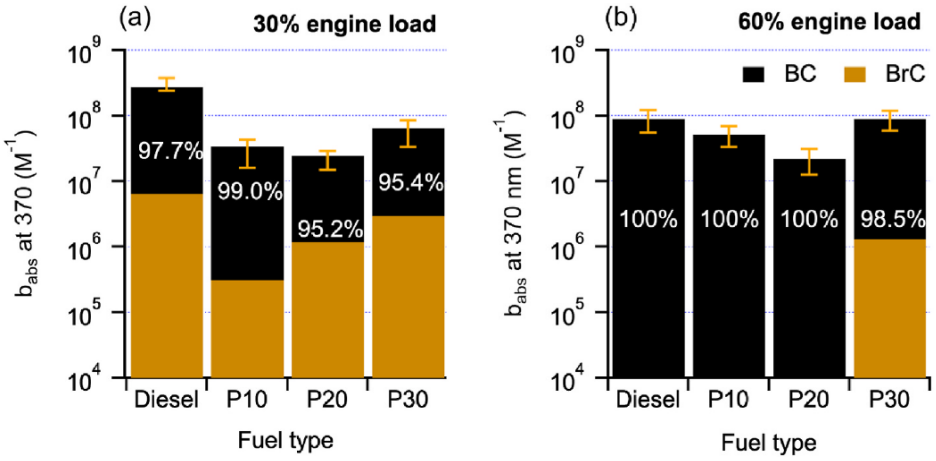

Figure 9.6: Brown carbon and black carbon emissions from blending fuel combustion

2) Chemical farming

Assoc Prof Ning YAN and Prof Alexei LAPKIN

Since the last report, the team led by **Assoc Prof Ning YAN (PI, NUS)** and **Prof Alexei LAPKIN (PI, CAM)** has studied the reaction mechanism of renewable organonitrogen compound formation. Based on the results, they hypothesised that the fed batch operation would further enhance product yield. Subsequently, they conducted a series of experiments under semi-batch, flow or co-fed mode, and obtained an optimised product yield higher than 50%, in contrast to their previous record (<40%). The new data has been added to the manuscript, and a revised version will be submitted to the journal *ChemSusChem*.

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

Prof Markus KRAFT and 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 generation and dispersion of the pollutants is influenced by an extremely diverse range of geospatial factors such that the data required to conduct a simulation of the dispersion of pollutants are highly heterogeneous, resulting in a demand for data interoperability. **Dr Karthik NAGARAJAN (Software Developer, CARES)** has been working on an agent that automates the AERMOD dispersion modelling system to run within the framework of the World Avatar. This agent retrieves the various inputs required for simulating the dispersion profile from the knowledge graph and then performs the required calculations.

The agent can query the knowledge graph for the location, height and diameter of pollutant sources, which gives users the flexibility to study the spatial distribution of pollutants arising from emissions. The agent can also detect buildings near each pollutant source and retrieve their geometrical properties to pass it to the AERMOD buildings pre-processor, BPIPPRM. It has been shown that the presence of buildings near pollutant sources may result in significantly higher pollutant concentrations at surrounding locations

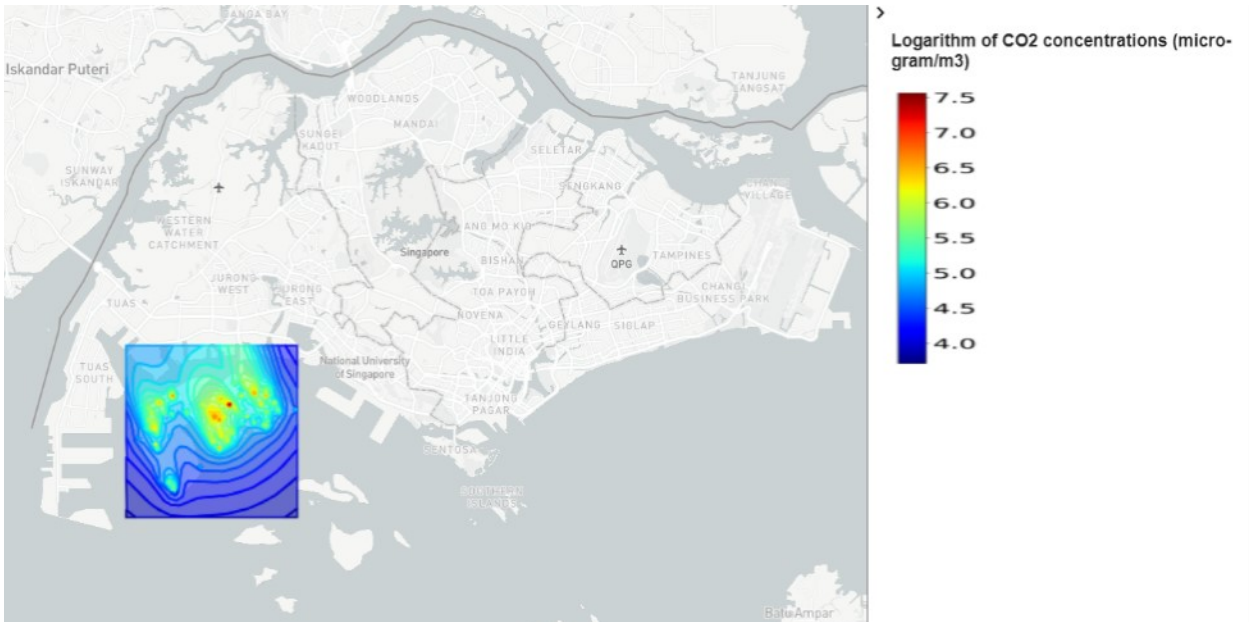

Figure 9.7. Spatial carbon dioxide distribution for Jurong Island.

due to downwash effects. This feature enables the user to investigate the increase in pollutant concentrations due to the presence of buildings. Finally, the agent runs the AERMOD terrain pre-processor, AERMAP, using terrain model raster data retrieved from the knowledge graph. The output from this pre-processor is subsequently used to run both BPIPPRM and AERMOD itself. This functionality enables the user to perform dispersion modelling for regions with geographic features such as hills and valleys, giving rise to significant variation in the surface elevation between different locations.

A sample visualisation obtained by running the AERMOD agent for estimating the dispersion profile for Jurong Island using publicly available data is shown in Figure 9.7.

4) Ignition systems for natural gas engines

Prof Epaminondas MASTORAKOS and Dr B HARIKRISHNAN

Dr B HARIKRISHNAN (Research Fellow, CARES) has been developing the solver dcmcConverge, which combines the CFD solver Converge with 3D doubly conditional moment closure (DCMC), which is an advanced turbulent combustion closure. As a next phase, Dr Harikrishnan will work on enabling the adaptive mesh refinement (AMR) capabilities on CFD and DCMC sides.

DCMC is the preferred solver for the complex turbulence-chemistry interaction problem. It includes the effects of advection, turbulent diffusion, dilatation, micro-mixing, and chemical source terms in the two-dimensional conversed scalar space (η and ζ are sample space variables for mixture fraction and reaction progress variable, respectively). As a result, the chemical source term can be first-order approximated.

The practical application is to study the turbulent jet ignition (TJI) process for different fuels/fuel blends with detailed chemistry. Lean-burn engines are getting significant attention due to their low emission and fuel consumption, enabled by the high compression ratio. However, this means they are harder to ignite using a typical spark ignition system, requiring TJI or dual-fuel injections of a more flammable fuel such as diesel. With its high predictive power and low computational cost, dcmcConverge can study complex ignition processes with any fuel, including new low/zero carbon fuels.

The current focus is to optimise the placement of the coarser DCMC cells to target more complex applications. In the future, various alternate fuels, such as ammonia, methanol, methane, etc., will be studied with the solver to understand their combustion and emission characteristics.

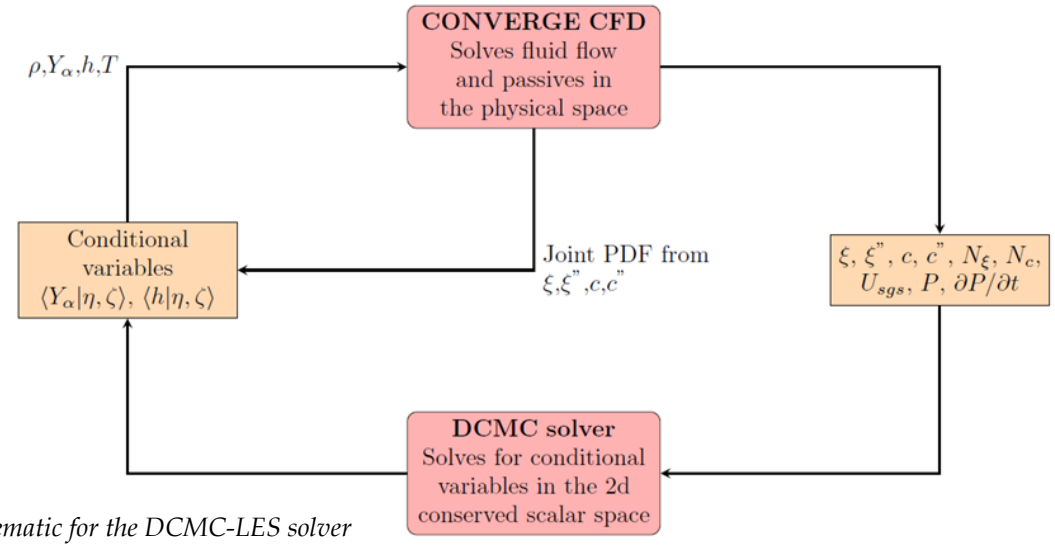

Figure 9.8: Schematic for the DCMC-LES solver

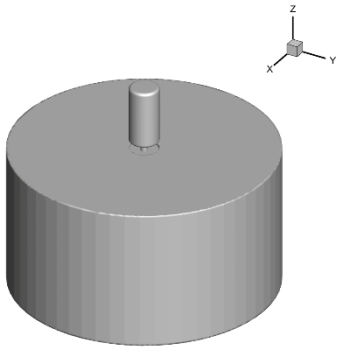

Figure 9.9: Geometry used for the numerical experiment

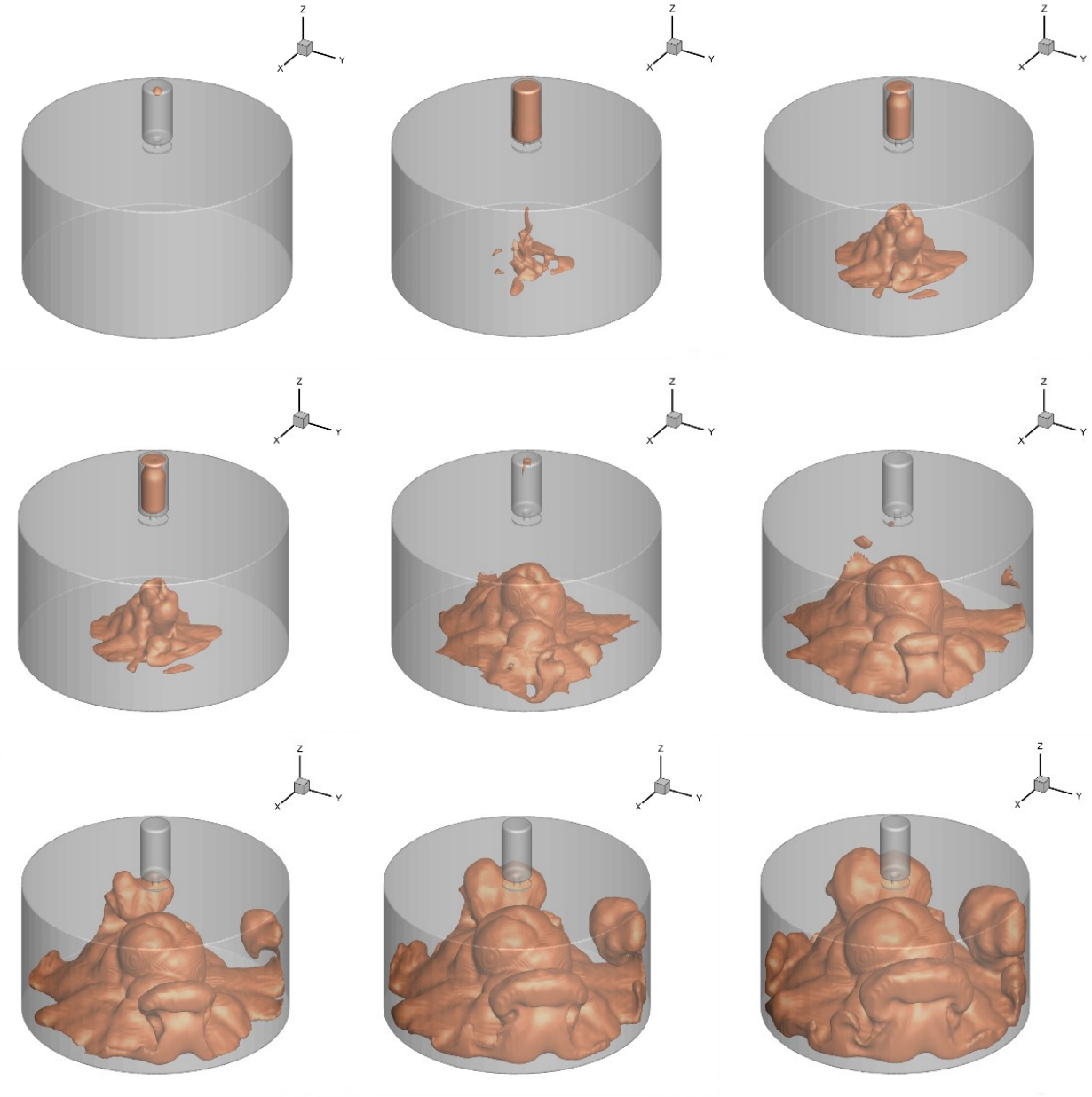

Figure 9.10: Turbulent jet ignition with $\phi_{PC} = 1.0$ *and* $\phi_{MC} = 0.5$

5) Future marine economy

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

Dr Li Chin LAW's (Research Engineer, CARES) launched https://lowcarbonship.com, a website for basic and advanced calculators for low carbon ship design. Based on the lifecycle assessment and fleet-level assessment work published in 2021 and 2022, an online interactive calculator was developed as a handy tool for the visualisation of ship performance when powered with low -carbon fuels. Here, the ship performance is defined and measured with four performance indexes: (i) cargo attainment rate, CAR (i.e., % of cargo that can be carried as compared to the reference ship powered by HFO); (ii) specific energy, ES (iii) specific cost, CS and (iv) carbon intensity indicators, CII. The calculator can benefit users who are interested in fuel transition for maritime decarbonisation. As part of the application, a numerical analysis was carried out for a specified low carbon containership with the aid of one of the calculators (Ship Performance Calculator). The result has been published in the recent paper – Numerical Analyses on Performance of Low Carbon Containership. In this paper, the performance of containership with onboard carbon cap-

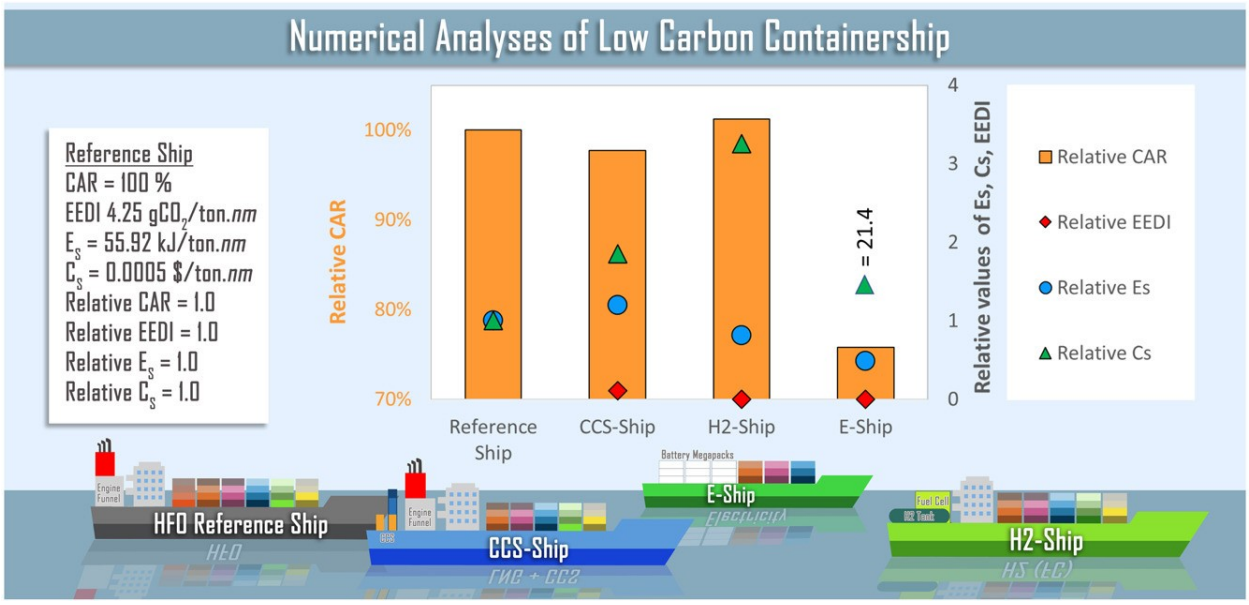

Figure 9.11: Graphical abstract of paper Numerical Analyses on Performance of Low Carbon Containership.

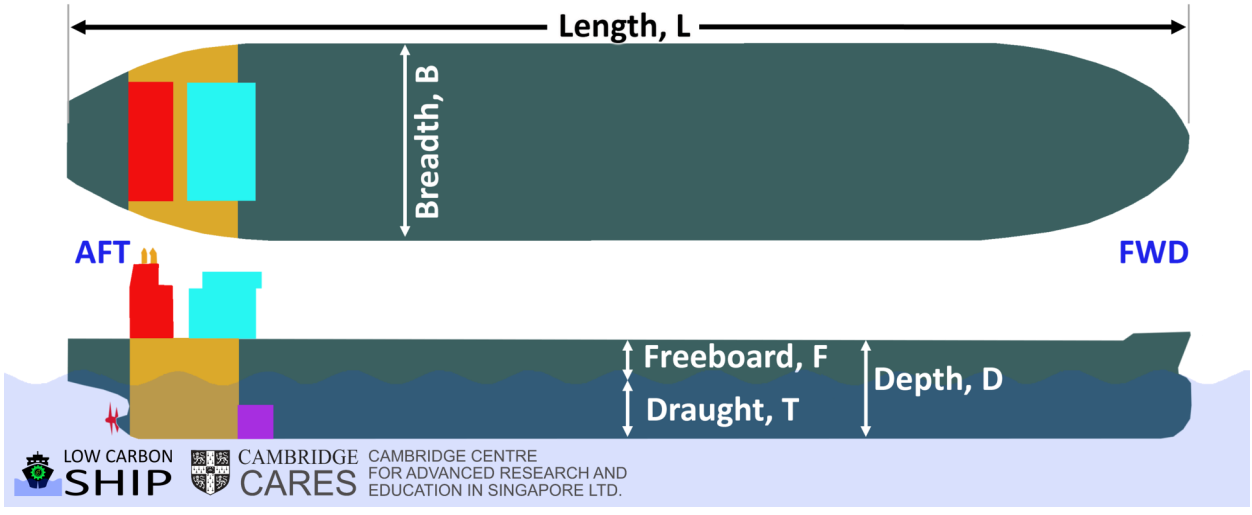

Figure 9.12: A screenshot of the Ship Sizing Calculator from the website.

ture (CCS-Ship) was compared with H_2-ship (hydrogen-fuelled ship), E-ship (electric-propelled ship) and conventional HFO-Ship. With the aid of the calculator, the implication of fuel transition for shipping was numerically analysed. In addition, a new approach to onboard carbon capture was researched. This interactive calculator aims to accelerate the efforts in maritime decarbonisation for the shipping industry.

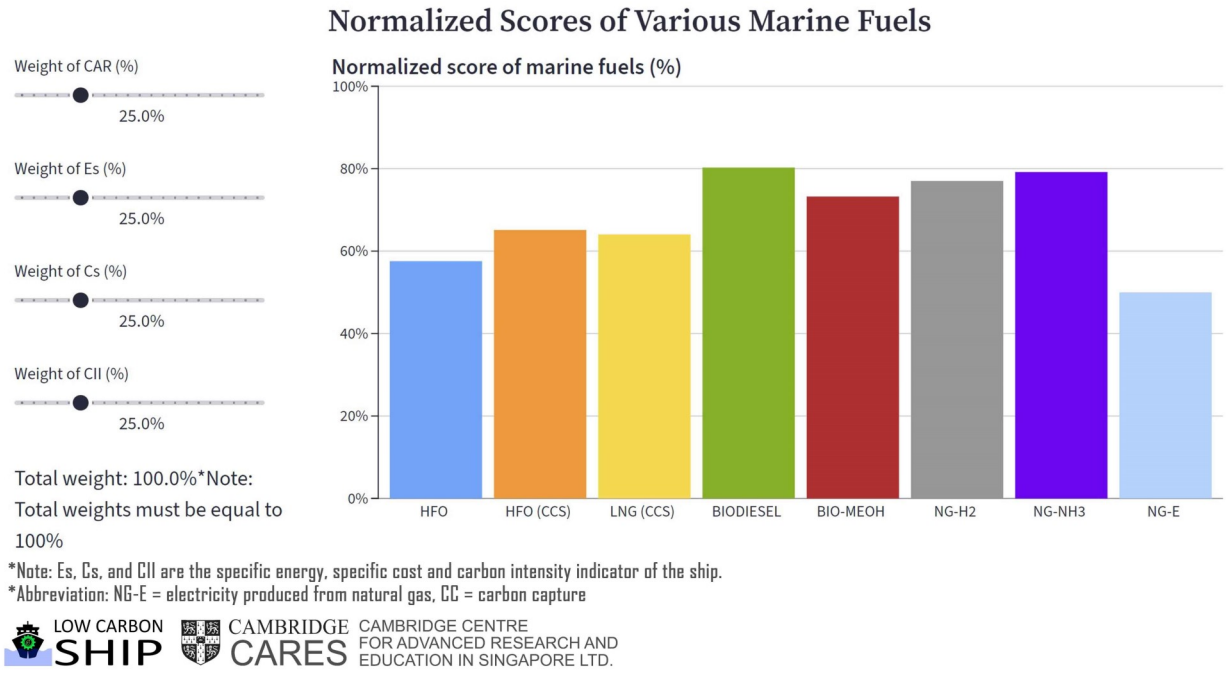

Figure 9.13: A screenshot of the Marine Fuel Comparison Calculator from the website.

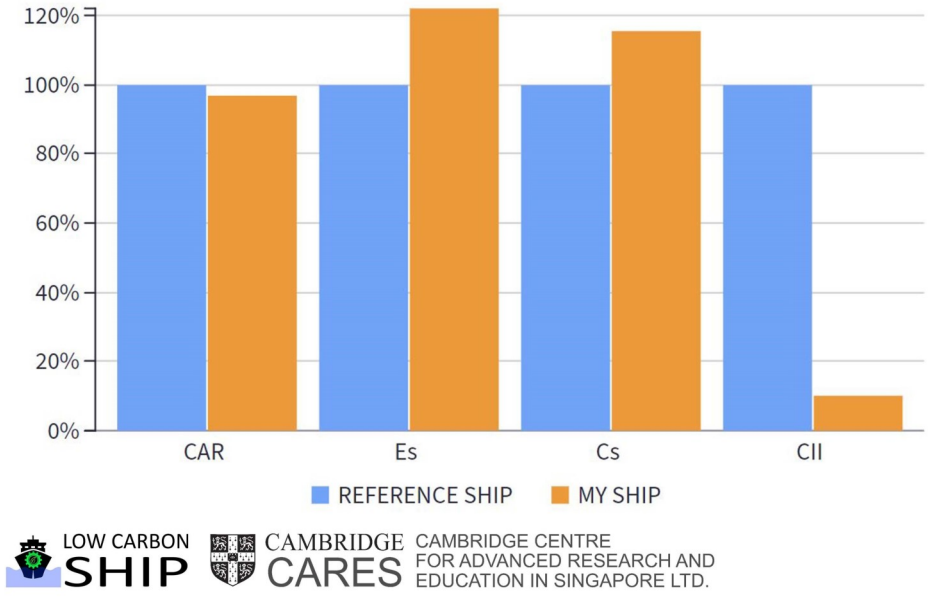

Figure 9.14: The comparative assessment between the HFO-fuelled ship (Reference) and user-defined alternative ship (My Ship) on the website

6) Carbon reduction strategies of top chemical companies

Prof S. VISWANATHAN, Dr Abhiruchi GADGIL, and Dr Yan WANG

Dr Abhiruchi GADGIL (Research Fellow, NTU) and **Prof S. VISWANATHAN (PI, NTU)** have analysed the Oil and Gas sector and are in the process of writing a manuscript titled "Decarbonization in the Oil and Gas sector: Technologies and Strategies". Some of the important insights from this study are as follows. The main decarbonisation strategies that Oil and Gas companies are pursuing (as articulated in their sustainability reports) are improving process efficiencies that reduce energy consumption; reducing fugitive methane emissions; investing and developing technologies for carbon capture, storage and utilisation (CCUS); and developing alternative pathways for fuel production (such as synthetic and sustainable fuels) and in production and processing of blue and green hydrogen. However, many of these technologies and projects are still at pilot scale and have not yet achieved scale economies or financial viability. Adoption and piloting of CCUS projects seems to be region agnostic and all the oil majors in this study are investing in the technology, irrespective of geography and regulations. On the other hand, the overall strategy of the oil and gas majors seems to be following the national decarbonisation policies based on the country where it is headquartered.

It was also found that though a majority of oil and gas companies have announced net-zero goals, the difference in the details of goal setting was significant. Amongst the firms studied, some firms have only announced a net-zero goal for 2050 without any details in the public domain on how they plan to achieve it, while others have published interim goals and detailed roadmaps to achieve net-zero by 2050. A subset of these firms has started their journey towards achieving these interim goals, by divesting from oil and gas, investing in renewable power sector and rebranding as energy companies.

A comparative study of the sustainability reports of the oil and gas companies has showed that the level of sustainability disclosure and the details provided in the sustainability reports depend directly on the level of environment and climate change related regulations in the region where the company is headquartered. It was also observed that the National Oil companies (NOC's) seem to have lesser details in the sustainability reporting compared to private firms.

In addition to the studies above, Dr Gadgil and **Dr Yan WANG (Research Fellow, NTU)** are carrying out a detailed review of the academic literature on decarbonisation technologies for the oil & gas industry. They aim to do a similar analysis for the Cement and Steel sector.

7) Decarbonisation of Singapore by 2050

Asst Prof Paul LIU, Prof Markus KRAFT and Dr Hui Ling TAN

Dr Hui Ling TAN's (Research Fellow, NTU) main research interest lies in the development of catalytic materials and technologies for renewable energy generation and CO_2 abatement. Recently, she has been focusing on developing roadmaps for different decarbonisation pathways for Singapore to decarbonise by 2050, as depicted in Figure 9.15. The technical potential of various decarbonisation techniques, such as energy efficiency improvement, electric vehicle adoption, industry electrification, solar power adoption, carbon capture and storage (CCS), and adoption of renewable energy sources, was studied. The roadmaps can be used as guidance to understand the impacts of the different decarbonisation techniques on Singapore's net carbon emissions by 2050 and to estimate the required implementation rates of the decarbonisation strategies to meet the decarbonisation goal in 2050. She has prepared a manuscript of the scenario analysis results for journal paper publication.

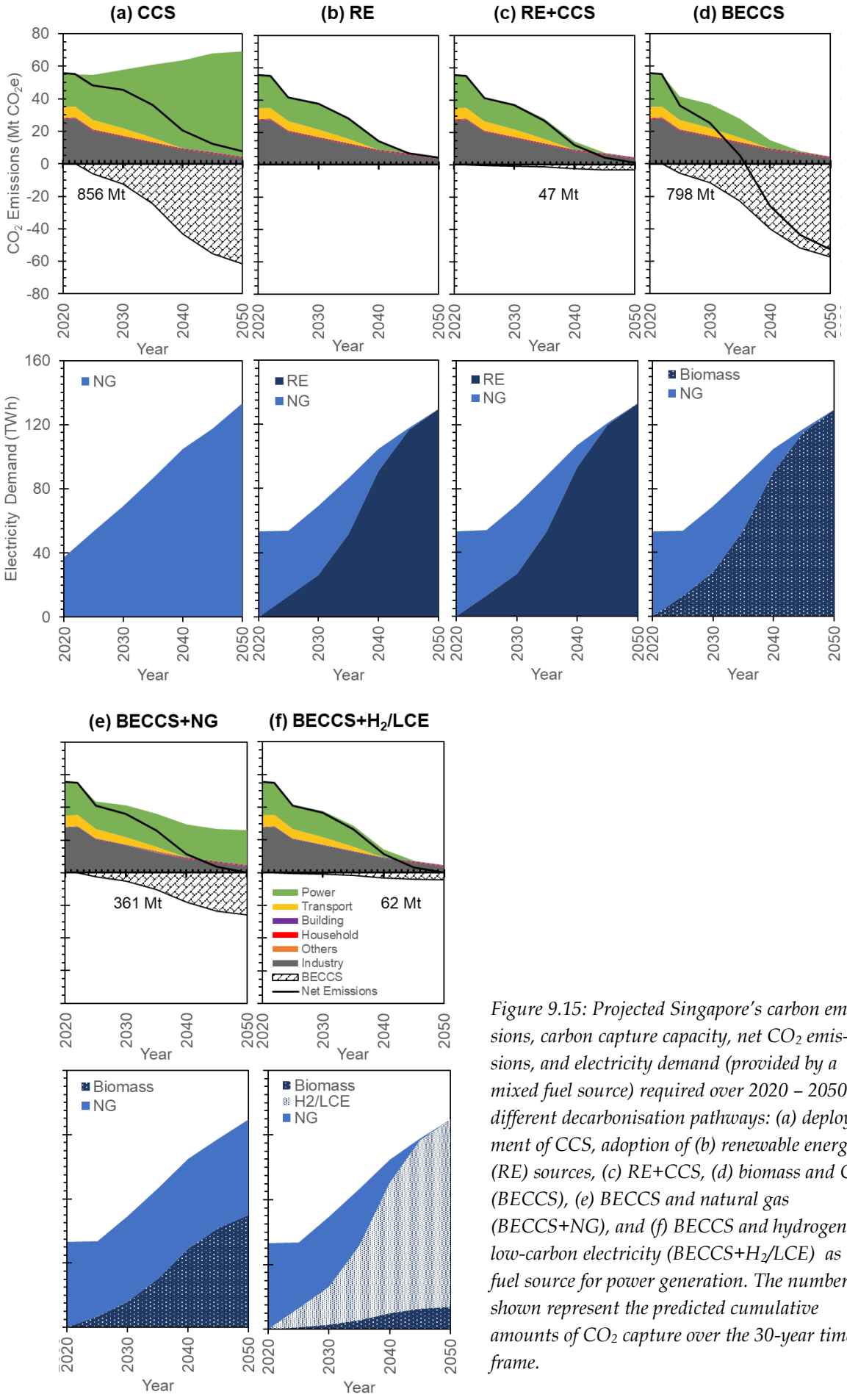

Figure 9.15: Projected Singapore's carbon emissions, carbon capture capacity, net CO_2 emissions, and electricity demand (provided by a mixed fuel source) required over 2020 – 2050 by different decarbonisation pathways: (a) deployment of CCS, adoption of (b) renewable energy (RE) sources, (c) RE+CCS, (d) biomass and CCS (BECCS), (e) BECCS and natural gas (BECCS+NG), and (f) BECCS and hydrogen or low-carbon electricity (BECCS+H_2/LCE) as the fuel source for power generation. The numbers shown represent the predicted cumulative amounts of CO_2 capture over the 30-year time frame.

8) Reaction Pathways of Formic Acid Conversion

Asst Prof Paul LIU and Dr Ari FISCHER

The previous Research Fellow for this project left CARES in January 2023. He will maintain an active research link with IRP1 to complete the write-up of his research findings.

Dr Ari FISCHER (Research Fellow, NTU) has joined recently to continue the work for this project.

9) Electrified Chemical Production

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

Dr Yubo CHEN (Research Fellow, NTU) work has been focused on increasing the number of available active Ir sites by preparing nano-sized Ir or IrO_2 with a high surface area. The most common method involves reducing Ir salts in a solvent. However, this method often requires multiple organic reagents, such as tetralin, dibenzyl ether, and oleylamine, which can be toxic and explosive. In addition, large-scale production of nanocatalysts using this strategy might be difficult due to the relatively low yield. Dr Chen developed a mesoporous IrO_xH_y catalyst with high activity and stability using the proposed cation leaching strategy. A K_4CdCl_6-structure-type Sr_4IrO_6 is designed as a precursor. Unlike rutile IrO_2 and Ir-based perovskites, in the unique crystal structure of Sr_4IrO_6, the Ir in such a composite oxide is fully coordinated (with six oxygen) and all IrO_6 octahedra are strictly isolated by Sr^{2+}. Therefore, the IrO_6 octahedron can be considered a "single molecular". The developed IrO_xH_y catalyst is obtained through the chemical leaching of Sr_4IrO_6, which induces aggregation of IrO_6 octahedra. To date, Dr Chen has not disclosed any techniques of using chemical leaching of Sr_4IrO_6 to prepare highly active and stable IrO_xH_y catalysts. This invention is the first application of using aggregation of IrO_6 octahedra to develop Ir-based catalysts for water oxidation.

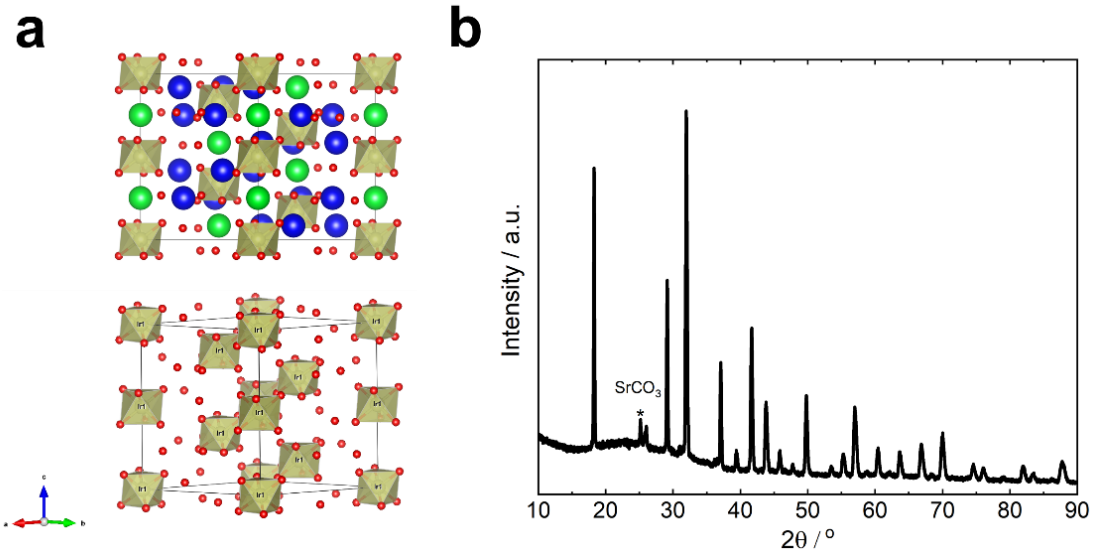

Figure 9.16: (a) The crystal structure and (b)XRD of Sr_4IrO_6

10) Electrolysis for renewable carbon utilisation

Prof Xin WANG Xin, Dr Xiaogang LI and Dr Hongwei ZHANG

Dr Hongwei ZHANG (Research Fellow, NTU) focused his research on the development of novel electrocatalysts in CO_2RR and ORR applications. He has published a review paper titled "Tailoring of Active Sites from Single to Dual Atom Sites for Highly Efficient Electrocatalysis" in *ACS Nano*.

Dr Xiaogang LI (Research Fellow, NTU) has been focusing on the design of electrocatalysts for H_2O_2 production. His work on isolated CoN_4 sites confined by metal-phthalocyanine (MPc) to modulate the OOH* adsorption towards high-efficiency H_2O_2 production has been published in *Advanced Materials*. Another manuscript based on sulfur-modified active sites which yield a selectivity of nearly 90% for H_2O_2 generation has been submitted to *Chem Catalysis* and is under revision now. Density functional theory calculations indicate that the incorporation of sulfur within Ni's coordination environment, together with oxidation of the active site motif, weakens the adsorption energy of OOH*.

Both researchers have left CARES.

PUBLICATIONS

ALL C4T PUBLICATIONS WITH CREATE ACKNOWLEDGEMENT

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

C4T joint IRP publications

IRP 1, IRP 2, IRP 3, and eCO$_2$EP

- **Ren, Hangjuan, Mikhail Kovalev, Zhaoyue Weng, Marsha Zakir Muhamad, Hongyang Ma, Yuan Sheng, Libo Sun, et al. 2022. 'Operando Proton-Transfer-Reaction Time-of-Flight Mass Spectrometry of Carbon Dioxide Reduction Electrocatalysis'. Nature Catalysis 5 (12): 1169–79. https://doi.org/10.1038/s41929-022-00891-3.**

IRP 1 and IRP 2

- **Li, Xiaogang, Shasha Tang, Shuo Dou, Hong Jin Fan, Tej S. Choksi, and Xin Wang. "Molecule Confined Isolated Metal Sites Enable the Electrocatalytic Synthesis of Hydrogen Peroxide."** *Advanced Materials* **34, no. 25 (2022): 2104891. https://doi.org/10.1002/adma.202104891.**

IRP 3 and IRP JPS

- **Kondinski, Aleksandar, Jiaru Bai, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2023. 'Knowledge Engineering in Chemistry: From Expert Systems to Agents of Creation'.** *Accounts of Chemical Research* **56 (2): 128–39. https://doi.org/10.1021/acs.accounts.2c00617.**

IRP 3, IRP JPS, and eCO$_2$EP

- **Rihm, Simon D., Mikhail K. Kovalev, Alexei A. Lapkin, Joel W. Ager, and Markus Kraft. "On the Role of C_4 and C_5 Products in Electrochemical CO_2 Reduction *via* Copper-Based Catalysts." *Energy & Environmental Science* 16, no. 4 (2023): 1697–1710. https://doi.org/10.1039/D2EE03752A.**

IRP 4 and IRP BB

- **Law, Li Chin, Epaminondas Mastorakos, and Stephen Evans. 2022. 'Estimates of the Decarbonization Potential of Alternative Fuels for Shipping as a Function of Vessel Type, Cargo, and Voyage'. *Energies* 15 (20): 7468. https://doi.org/10.3390/en15207468.**

C4T IRP 1: Sustainable reaction engineering

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