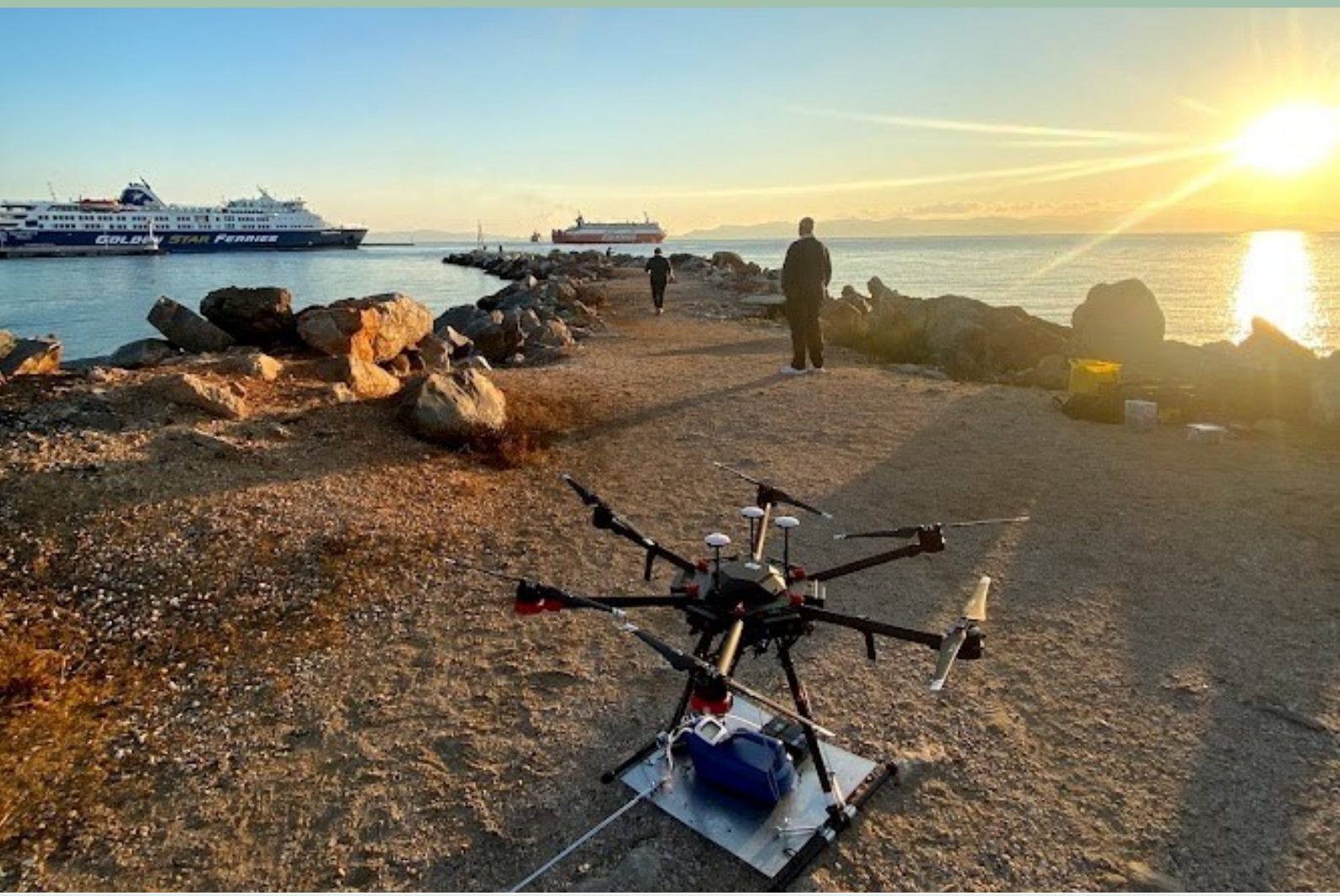
CAMBRIDGE **CARES**

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



Biannual Research Report

April - September 2021

CAMBRIDGE
CARES

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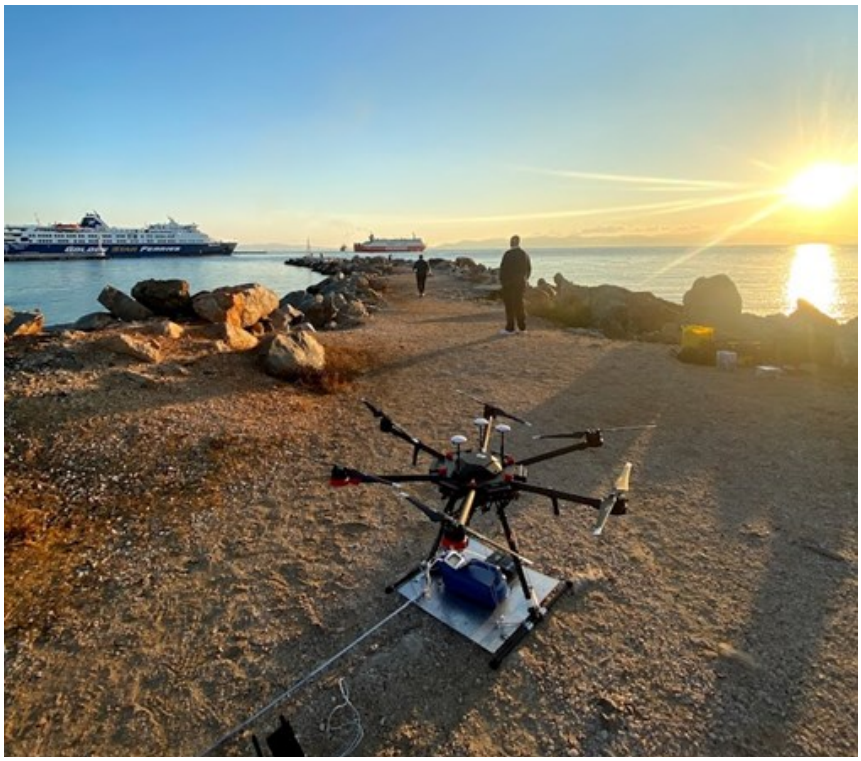

Drone with instrument platform for measuring shipping emissions ready for take-off at the port of Rafina, Greece.

Image by Dr Molly HAUGEN (Research Fellow, IRP 4). *See more on page 67.*

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

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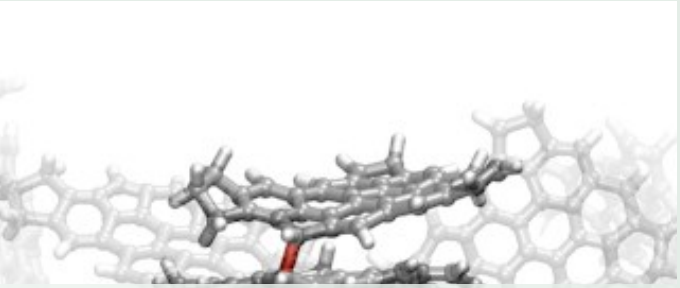

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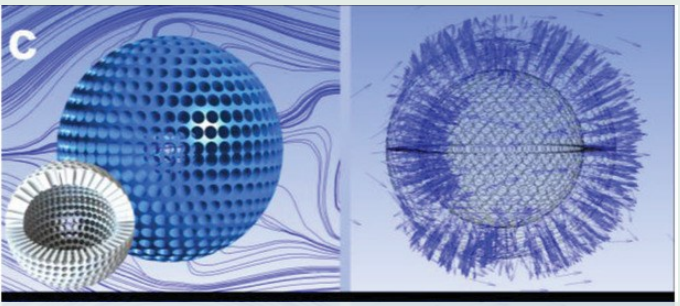

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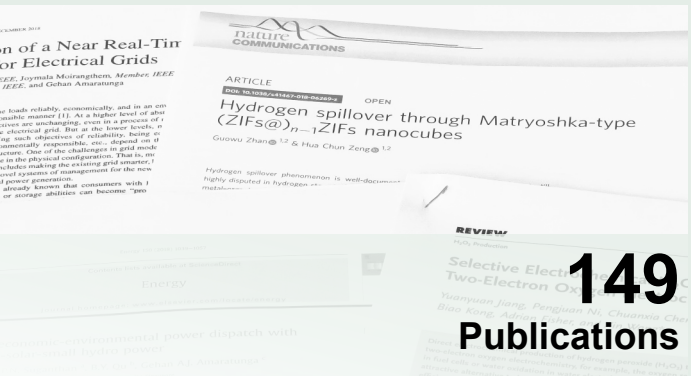

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FOREWORD

I am very pleased to present the 15th Biannual Research Report of the Cambridge Centre for Advanced Research and Education in Singapore (Cambridge CARES). The last few months have brought continued restrictions on work and travel but our researchers have carried on their excellent work and adapted well to virtual conferences and collaboration.

ECO_2EP

Our first large Intra-CREATE project, *eCO_2EP: A Chemical Energy Storage Technology* finished in June of this year. The project studied the viability of large-scale CO_2 reduction processes and explored a new energy-chemistry solution for a more sustainable future. The key achievements of the project can be found on pages 103-110.

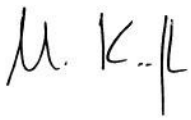
INTELLIGENT DECARBONISATION

Over the past few months, we have been gathering contributions from leaders in industry, government and academia that explore how we can best decarbonise our energy systems. These contributions, along with chapters written by CARES researchers, comprise the soon-to-be-released book *Intelligent Decarbonisation*. Written with Oliver Inderwildi and in collaboration with Springer, the book explains how digital technologies can be employed to reduce global greenhouse gases and meet the ambitious emissions reduction goals set out in the Paris Agreement 2015.

WORKING TOWARDS NET ZERO

At the time of writing, the 2021 United Nations Climate Change Conference (COP26) is fast approaching. CARES researchers have been closely involved with events in Singapore and Cambridge during the run-up to the event, including talks organised by the University of Cambridge's climate change initiative *Cambridge Zero*. The research being done in CARES, and indeed throughout CREATE, feels more urgent than ever and I am grateful for the opportunity that we have to contribute to scientific advances in this area.

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
September 2021

ABOUT US

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

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

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

The motivation for the C4T project is to integrate materials design and selection (i.e. for adsorbents and catalysts) with advances in process design to achieve improved selectivity and conversion. Such improvements will provide a reduced carbon footprint and energy demand for both established and new processes. Lowering the cost of CO_2 capture, and technologies and strategies for waste heat utilisation are also underlying drivers in the research. Our six collaborative Interdisciplinary Research Programmes (IRPs) combine state-of-the-art experimental analysis with advanced modelling research from Cambridge and Singapore. Whilst each IRP has clearly defined milestones and deliverables, denoted as work packages (WPs), there is significant interaction between the IRPs.

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

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

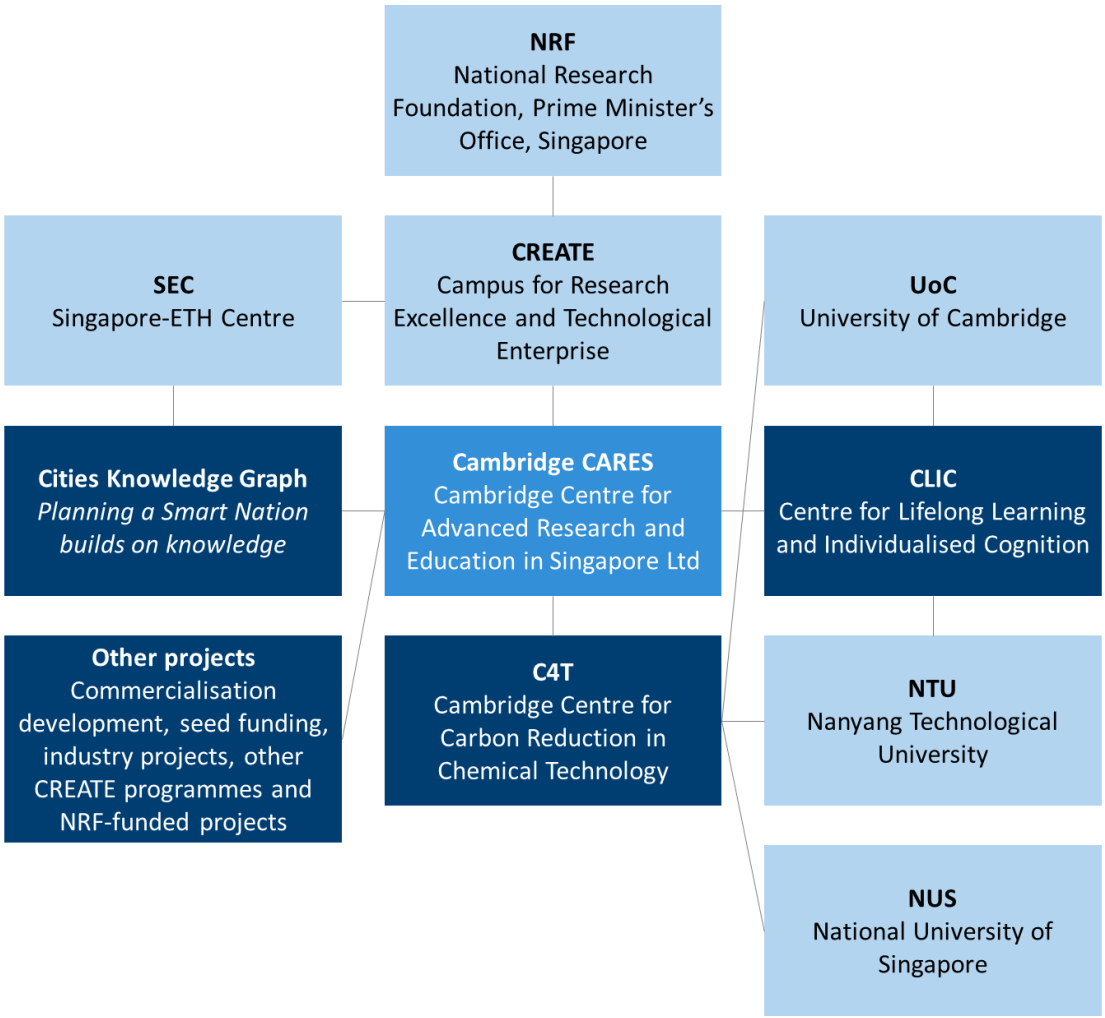
eCO_2EP, our first large Intra-CREATE grant, was a three-year programme that brought together researchers from the University of Cambridge,

the University of California, Berkeley, the National University of Singapore and Nanyang Technological University to develop ways of transforming carbon dioxide emitted as part of the industrial process into compounds that are useful in the chemical industry supply chain. eCO_2EP ended in June 2021.

In April 2020, CARES was awarded a further Intra-CREATE large grant for Cities Knowledge Graph, which brings together researchers from University of Cambridge and ETH Zürich to harness rapidly growing and diversifying data streams to improve the planning and design of cities. Cities Knowledge Graph will do this by developing an innovative digital platform designed to combine data and share knowledge about cities, and to inject new precision and responsiveness to static instruments of planning, such as the city master-plan.

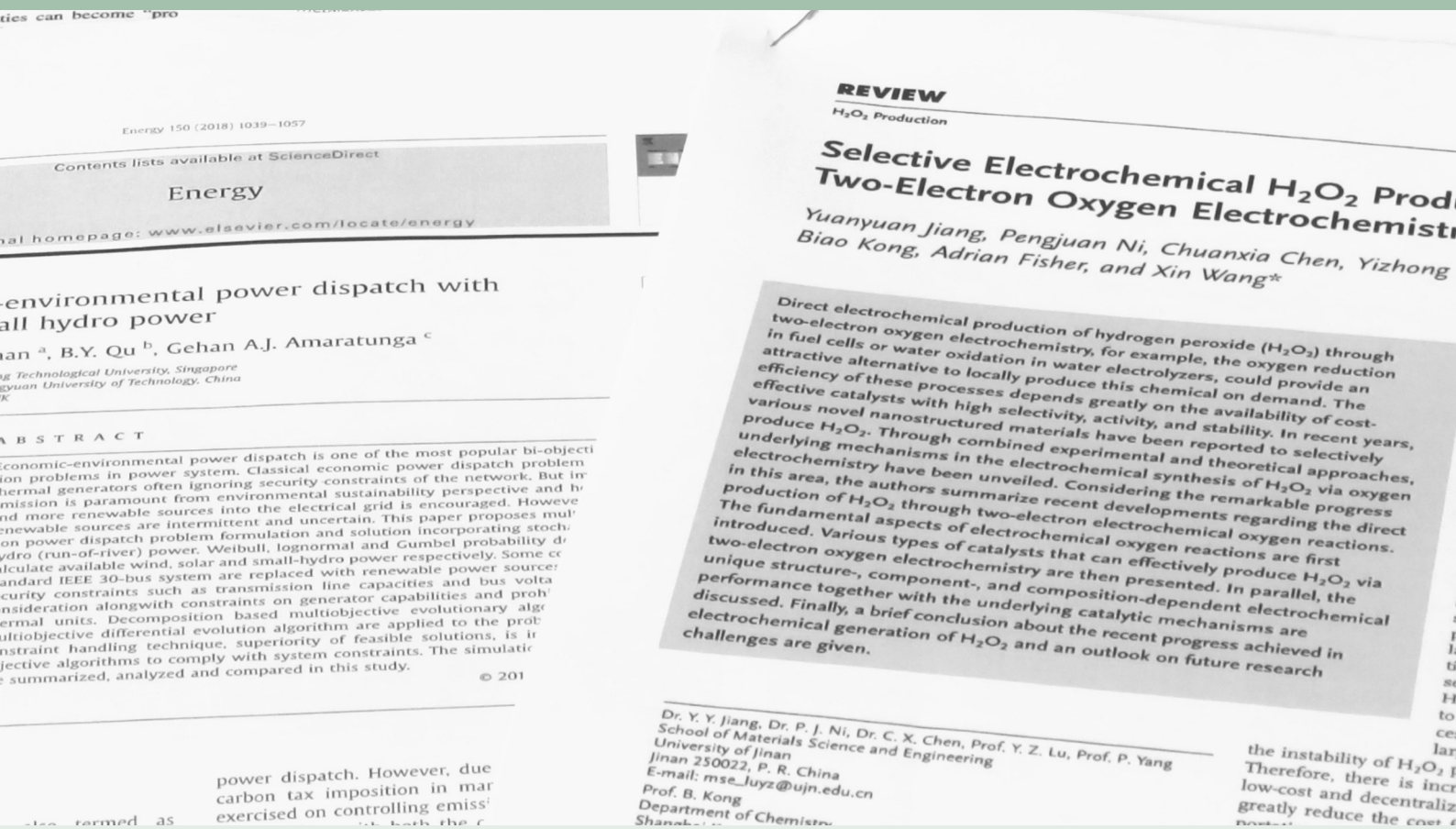
As well as these large Intra-CREATE grants, CARES has several smaller projects and spin-offs ongoing. There is one seed-funded, CARES-hosted Intra-CREATE project between University of Cambridge and the Singapore-ETH Centre (Consumer Energy Usage Data in Smart City Development), and three further projects under the Pharmaceutical Innovation Programme Singapore (PIPS) that involve industry funding. CARES also takes part in the Cooling Singapore 2.0 programme hosted by the Singapore-ETH Centre and is hosting the Asia-Pacific headquarters of the Cambridge Alternative Finance Collaboration Network. Details and updates for these smaller projects can be found from page 125.

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



HIGHLIGHTS

OUTSTANDING WORK FROM THE LAST SIX MONTHS OF CAMBRIDGE CARES RESEARCH



Discovery of circular production in big reaction networks

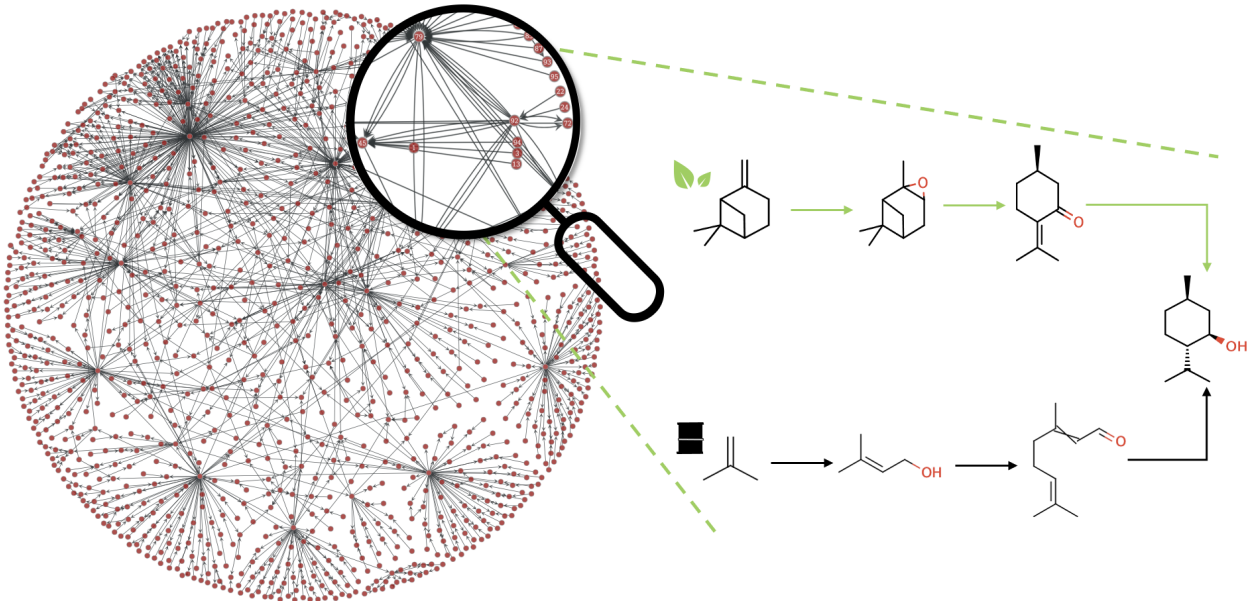
Dr Zhen GUO, Senior Research Fellow (IRP1) and Prof. Alexei LAPKIN, PI (IRP1)

From a sustainability point of view, the current mode of chemical production is far from optimised. For decades, chemical industry has been established on the basis of fossil resources, which leads to a linear production mode: *extract-make-use-dispose*. The consequences of this unsustainable mode are becoming increasingly pronounced. In contrast, circular economy, following a mode of *make-use-recycle*, has been proposed and is being adopted by many countries to achieve sustainability. One key element of circular economy is to exploit waste-streams as useful resources. However, successful utilisation of a waste-stream is determined by many factors, such as geographical distribution of wastes, complex compositions of wastes, existing infrastructure, available technologies, supply chain and market demand etc. To meet the challenge, a macro-system should be built on top of multiple sub-systems, while each sub-system is able to analyse the impact of one individual factor.

One indispensable sub-system is to discover circular production routes that are able to replace existing unsustainable routes. We find that analysis of big reaction networks is a straightforward and powerful strategy to answer the question. A reaction network is afforded by traversing molecules (as vertices) with reaction relationships (as edges), as shown in the figure below. The network can be featured by attaching various attributes to molecules and reactions, such as molecular information, reaction parameters, costs, origins, toxicities etc. However, to identify a promising route in a reaction network, one has to deal with three challenges. Firstly, raw reaction data should be gathered, cleaned and preprocessed before the construction of reaction networks, in order to improve the consistency, uniformity and reliability of the data. Generation of auxiliary and new data is required to mitigate the data scarcity issue. Secondly, efficient algorithms should be developed to represent and process molecules and reactions *in silico*. Molecular structures, in the form of small networks consisting of atoms and bonds, are highly diverse and complex. Chemical transformations and routes add additional layers of complexity to the problem. Thirdly, searching and analysing big reaction networks containing

Dr Zhen Guo obtained his Bachelor and Master degrees in chemistry at Wuhan University, China, and his PhD degree in chemical engineering at Nanyang Technological University, Singapore. Having worked in academia and industry for nine years, Dr Guo has experience in heterogeneous catalysis, organic synthesis, flow chemistry, design of experiments and machine learning. He focuses on development of in silico solutions for industrial challenges through chemoinformatics, data mining and machine learning. Dr Guo is a founding member of Chemical Data Intelligence, a Singapore-based spin-off company that builds on C4T research.

millions of molecules and reactions is also non-trivial. Idea algorithms should be scalable, fast and unbiased. Thanks to the evolution of new technologies in data-mining, machine learning, cheminformatics, graph theory and chemical engineering, an early version of automatic route searching system has been developed in our group, and more features are waiting to be implemented, aiming to achieve chemical data intelligence in this field.



References:

- J. M. Weber, Z. Guo, C. Zhang, A. M. Schweidtmann and A. A. Lapkin, Chemical data intelligence for sustainable chemistry, Chem. Soc. Rev. (2021), DOI: 10.1039/D1CS00477H.
- P.-M. Jacob, P. Yamin, C. Perez-Storey, M. Hopgood, A. Lapkin, Towards automation of chemical process route selection based on data mining, Green Chem., 19 (2017) 140-152. DOI: 10.1039/C6GC02482C
- A. Lapkin, P.K. Heer, P.-M. Jacob, M. Hutchby, W. Cunningham, S.D. Bull, M.G. Davidson. Automation of route identification and optimisation based on datamining and chemical intuition, Faraday Discussions. 202 (2017) 483-496, DOI: 10.1039/C7FD00073A
- P.-M. Jacob, A. Lapkin, Statistics of the network of organic chemistry, React. Chem. Engng. 3 (2018) 102-118. DOI: 10.1039/c7re00129k
- J.M. Weber, P. Lio, A. Lapkin, Identification of strategic molecules for future circular supply chains using large reaction networks, React. Chem. Eng., 4 (2019) 1969-1981, DOI: 10.1039/c9re00213h
- Z. Guo, N. Yan, A. Lapkin, Towards circular economy: integration of bio-waste into chemical supply chain, Curr. Opinion Chem. Eng. 26 (2019) 148-156. DOI: 10.1016/j.coche.2019.09.010

For more information, visit www.cdi-sg.com.

FOCUS ON
FUNDAMENTAL SCIENCE

A molecular dance that could eliminate soot pollution

Dr Jacob MARTIN, former Research Fellow, C4T IRP3

A hidden molecular dance has been revealed that could hold the answer to the problem of soot pollution.

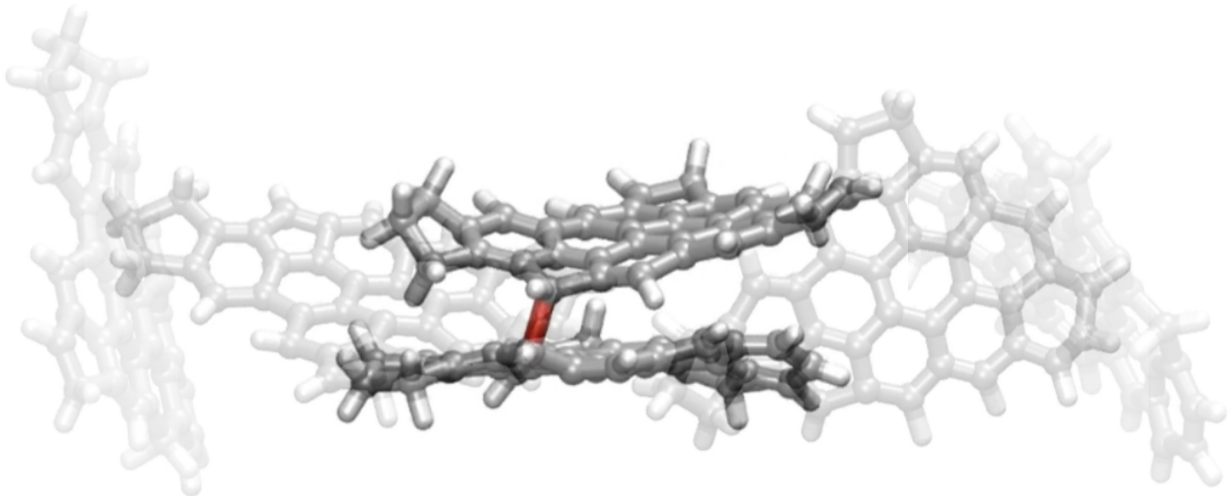
Soot pollution invades our bodies, causing cancer and blood clots as well as weakening us to respiratory viruses. Our atmosphere and glaciers are also blanketed by soot, leading to global heating and increased ice loss. Surprisingly, the way that soot particles form is still unknown but is of pressing concern to solve these global problems.

The reason for this long-running mystery is due to the extreme environment in which soot forms, the rapid speed of the reactions and the complex collection of molecules present in the flame. All of these obscure the pathway to soot formation.

Along with other researchers from the UK, Singapore, Switzerland and Italy, we have used two different microscopes to reveal the molecules and reactions taking place in a flame.

The first microscope operates by touch, feeling for the arrangement of atoms in the molecules of soot. These tactile maps provide the first picture of soot's molecular chicken wire shape. Quantum chemistry was then used to show that one of the molecules was a reactive diradical. A diradical is a type of molecule with two reactive sites, allowing it to undergo a succession of chain reactions.

The second microscope is entirely virtual and shows the reaction between the diradicals. Quantum mechanics guided a supercomputer to virtu-



Reaction dynamics between two aromatic diradical soot precursor molecules.

ally and realistically collide the molecules together and reveal the molecular dance in slow motion.

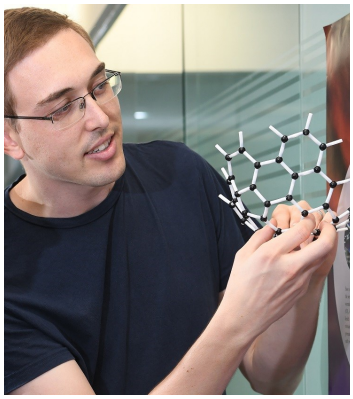
This simulation showed that the individual molecules are held together by intermolecular forces after they collide. This gives the reactive sites time to find each other and create a permanent chemical bond. Even after they have bonded they remain reactive, allowing more molecules to "stick" to what is now a rapidly growing soot particle.

This discovery could resolve the problems with previous attempts to explain soot formation via either a physical condensation or chemical reaction. In fact, both are required to adequately explain the rapid and high-temperature reactions.

If the concentration of these species is high enough in flames, this pathway could provide an explanation for the rapid formation of soot. This project brought together cutting-edge computational modelling and experiments to reveal a completely new reaction pathway which potentially explains how soot is formed.

Next, we hope to target these reactive sites to see whether the soot formation process can be halted in its tracks. One promising option is the injection of ozone into a flame, which has already been found to effectively eliminate soot in some preliminary results in other work.

For more information: The paper related to this research, "Diradical aromatic soot precursors in flames" (DOI: 10.1021/jacs.1c05030) is published in *Journal of the American Chemical Society* by researchers from Cambridge CARES, University of Cambridge, IBM Research Zurich, Consiglio Nazionale delle Ricerche and Università degli Studi di Napoli Federico II.



Dr Jacob W. Martin was a Research Fellow at CARES and completed his PhD in the University of Cambridge's Computational Modelling Group. Dr Martin has strong interests in renewable energy, pollution reduction and carbon nanomaterials. He uses physical models and simulations to describe the chemical world and is developing instruments to measure chemical properties. While at CARES, he studied the formation of soot in engines using molecular dynamics and quantum chemistry to look at gas-soot interactions and self-assembly processes within carbon materials. Dr Martin was the recipient of a 2021 Forrest Fellowship and is now working at the Department of Physics and Astronomy at Curtin University, Perth, Australia.

Highlighted research outputs from April - September 2021

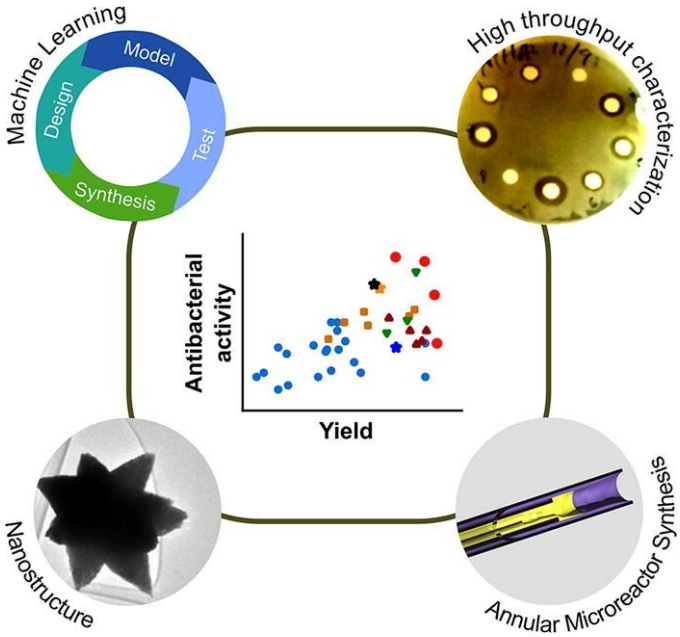
A selection of the top publications from across our programmes.

C4T IRP 1: Pushing nanomaterials up to the kilogram scale – An accelerated approach for synthesizing antimicrobial ZnO with high shear reactors, machine learning and high-throughput analysis

Nicholas Jose, Mikhail Kovalev, Eric Bradford, Artur M. Schweidtmann, Hua Chun Zeng and Alexei A. Lapkin, *Chemical Engineering Journal*

DOI: 10.1016/j.cej.2021.131345

Abstract: Novel materials are the backbone of major technological advances. However, the development and wide-scale introduction of new materials, such as nanomaterials, is limited by three main factors—the expense of experiments, inefficiency of synthesis methods and complexity of scale-up. Reaching the kilogram scale is a hurdle that takes years of effort for many nanomaterials. We introduce an improved methodology for materials development, combining state-of-the-art techniques—multi-objective machine learning optimization, high yield microreactors and high throughput analysis. We demonstrate this approach through the optimization of ZnO nanoparticle synthesis, simultaneously targeting high yield and high antibacterial activity. In fewer than 100 experiments, we developed a 1 kg day^{-1} continuous synthesis for ZnO (with a space-time-yield of 62.4 kg day^{-1} m^{-3}), having an antibacterial activity comparable to hydrothermally synthesized nano-ZnO and cetrimonium bromide. Following this, we provide insights into the mechanistic factors underlying the performance-yield tradeoffs of synthesis and highlight the need for benchmarking machine learning models with traditional chemical engineering methods. Methods for increasing model accuracy at steep pareto fronts, in this case at yields close to 1 kg per day, should also be improved. To project the next steps for process scale-up and the potential advantages of this methodology, we conduct a scalability analysis in comparison to conventional batch production methods, in which there is a significant reduction in degrees of freedom. The proposed method has the potential to significantly reduce experimental costs, increase process efficiency and enhance material performance, which culminate to form a new pathway for materials discovery.

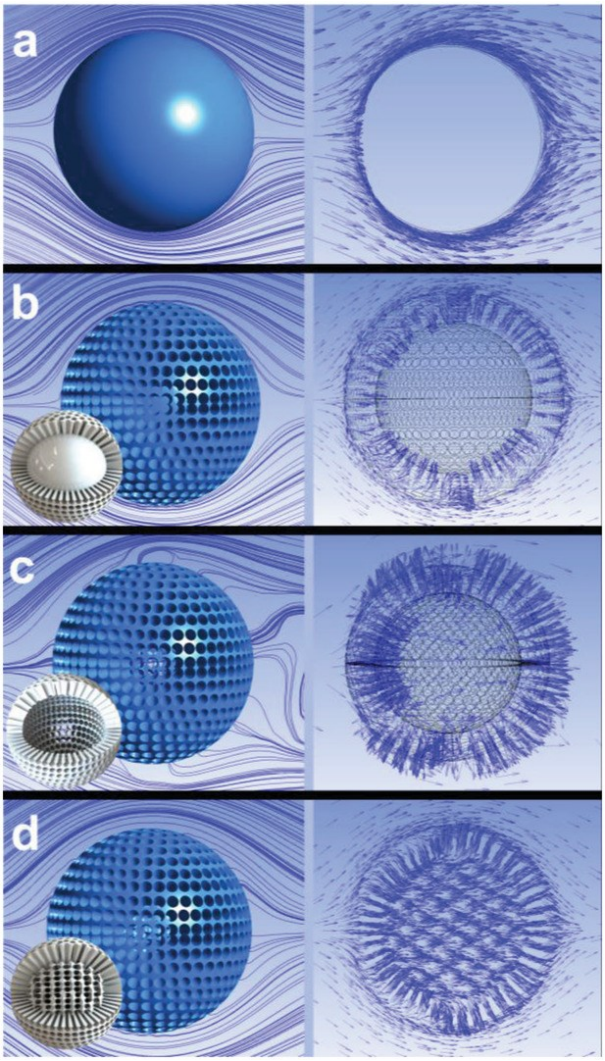


C4T IRP 1: Revamping SiO_2 spheres by core–shell porosity endowment to construct a mazelike nanoreactor for enhanced catalysis in CO_2 hydrogenation to methanol

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

DOI: 10.1002/adfm.202102896

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



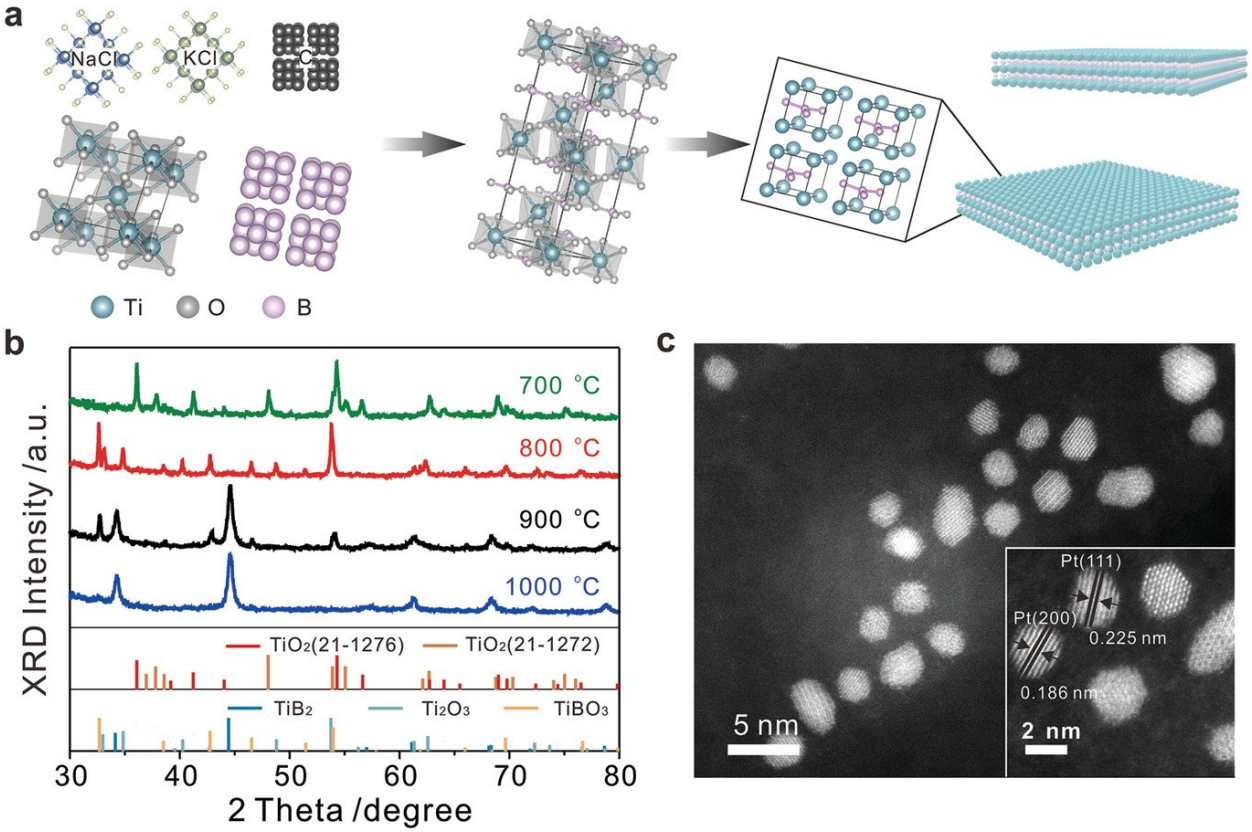
Simulations of four spherical materials including (a) rigid sphere, (b) mesoporous sphere with rigid core, (c) mesoporous hollow sphere, and (d) multi-voids mesoporous sphere, against a gas flow (i.e., air with flow rate at 0.01 m s^{-1}.

C4T IRP 1: Strong metal–support interaction for 2D materials: application in noble metal/ TiB_2 heterointerfaces and their enhanced catalytic performance for formic acid dehydrogenation

Renhong Li, Zhiqi Liu, Quang Thang Trinh, Ziqiang Miao, Shuang Chen, Kaicheng Qian, Roong Jien Wong, Shibo Xi, Yong Yan, Armando Borgna, Shipan Liang, Tong Wei, Yihu Dai, Peng Wang, Yu Tang, Xiaoqing Yan, Tej S. Choksi and Wen Liu, *Advanced Materials*

DOI: 10.1002/adma.202101536

Abstract: Strong metal–support interaction (SMSI) is a phenomenon commonly observed on heterogeneous catalysts. Here, direct evidence of SMSI between noble metal and 2D TiB_2 supports is reported. The temperature-induced TiB_2 overlayers encapsulate the metal nanoparticles, resulting in core–shell nanostructures that are sintering-resistant with metal loadings as high as 12.0 wt%. The TiO_x-terminated TiB_2 surfaces are the active sites catalyzing the dehydrogenation of formic acid at room temperature. In contrast to the trade-off between stability and activity in conventional SMSI, TiB_2-based SMSI promotes catalytic activity and stability simultaneously. By optimizing the thickness and coverage of the overlayer, the Pt/TiB_2 catalyst displays an outstanding hydrogen productivity of 13.8 mmol g^{-1}_{cat} h^{-1} in 10.0 m aqueous solution without any additive or pH adjustment, with >99.9% selectivity toward CO_2 and H_2. Theoretical studies suggest that the TiB_2 overlayers are stabilized on different transition metals through an interplay between covalent and electrostatic interactions. Furthermore, the computationally determined trends in metal–TiB_2 interactions are fully consistent with the experimental observations regarding the extent of SMSI on different transition metals. The present research introduces a new means to create thermally stable and catalytically active metal/support interfaces for scalable chemical and energy applications.



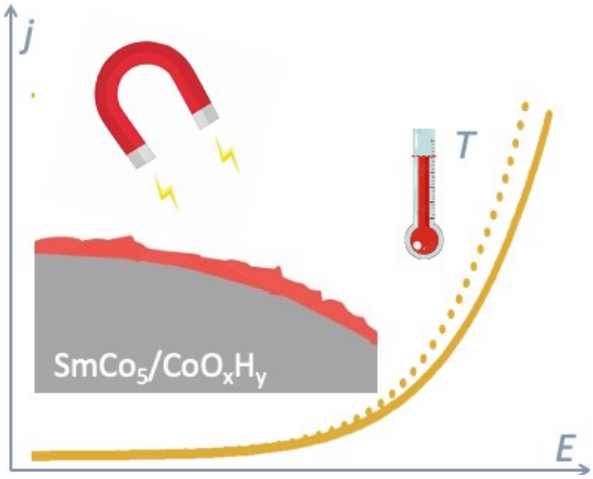
a) Schematic illustration of the molten salt-assisted borothermal reduction process to prepare TiB_2, (b) XRD patterns of the TiB_2 products prepared at different reduction temperatures, and (c) aberration-corrected HAADF-STEM image of Pt/TiB_2-600 (the inset shows the Pt(111) and Pt(200) crystal facets).

C4T IRP 2: $SmCo_5$ with a reconstructed oxyhydroxide surface for spin selective water oxidation under elevated temperature

Riccardo Ruixi Chen, Gao Chen, Xiao Ren, Jingjie Ge, Samuel Jun Hoong Ong, Shibo Xi, Xin Wang and Zhichuan Xu, *Angewandte Chemie International Edition*

DOI: 10.1002/anie.202109065

Abstract: The efficiency of electrolytic hydrogen production is limited by the slow reaction kinetics of oxygen evolution reaction (OER). Surface reconstructed ferromagnetic (FM) catalysts with spin pinning effect at the FM/oxyhydroxide interface could enhance the spin-dependent OER kinetics. However, in real-life applications electrolyzers are operated under elevated temperature, which may disrupt the spin orientations of FM catalysts and limit their performance. In this work, we prepared surface reconstructed $SmCo_5$/CoO_xH_y, which possesses polarized spins at the FM/oxyhydroxide interface that leads to excellent OER activity. These interfacial polarized spins could be further aligned through a magnetization process, which further enhanced the OER performance. Moreover, the operation temperature was elevated to mimic water electrolyzers' practical operation conditions. It is found that the OER activity enhancement of magnetized SmCo 5 /CoO x H y catalyst can be preserved up to 60 °C.



C4T IRP 2: Effects of Axial Functional Groups on Heterogeneous Molecular Catalysts for Electrocatalytic CO_2 Reduction

Libo Sun, Vikas Reddu, Tan Su, Xinqi Chen, Tian Wu, Wei Dai, Adrian C. Fisher and Xin Wang, *Small Structures*

DOI: 10.1002/sstr.202100093

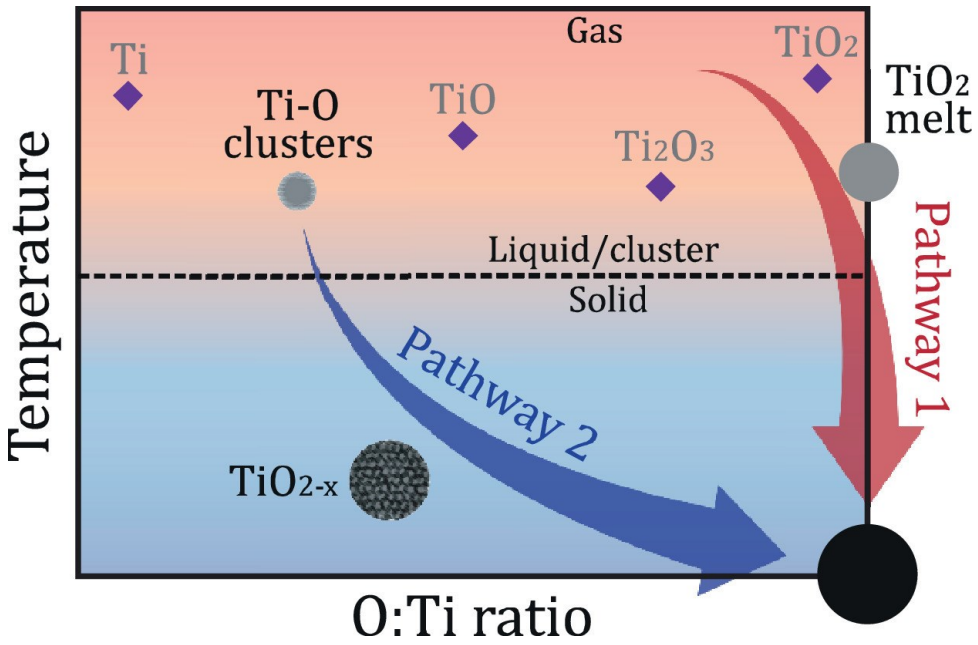
Abstract: Recent years have witnessed the development of heterogeneous molecular catalysts toward electrocatalytic CO_2 reduction. One effective strategy for such heterogenization is to decorate molecular catalysts directly through axial coordination to functionalized carbon substrates and it will be interesting to elucidate the influence of such functional groups on the activity. Herein, it is demonstrated that among several kinds of N-, O-, and S-derived functional groups-decorated carbon nanotubes, pyridine-based ones may play the role of a suitable linker and assist in achieving higher activity toward CO_2 reduction by a molecular catalyst. Density functional theory (DFT) calculation is also carried out to support the experimental results. This observation provides more insights into how a substrate can influence the intrinsic catalytic behavior of molecular catalysts via functional groups without venturing into the complexities involved with the synthesis of novel ligands.

C4T IRP 3: Understanding the anatase-rutile stability in flame-made TiO_2

Manoel Y. Manuputty, Casper S. Lindberg, Jochen A.H. Dreyer, Jethro Akroyd, John Edwards and Markus Kraft, *Combustion and Flame*

DOI: 10.1016/j.combustflame.2020.12.017

Abstract: The relative stability of anatase and rutile in stagnation flame synthesis with stoichiometric mixtures is investigated experimentally. The measurements reveal a high sensitivity of anatase-rutile composition to the flame dilution. It is demonstrated that anatase formation is favoured in more dilute (colder) flames while rutile is favoured in less dilute (hotter) flames. A particle model with a detailed description of aggregate morphology and crystal phase composition is applied to investigate the anatase-rutile stability. A phase transformation model is implemented in which rutile is formed for particles larger than a "crossover" size while anatase is formed for those smaller. Two formation mechanisms/pathways are discussed and evaluated. In the first pathway, the nascent particles are assumed to be stoichiometric and the crossover size is determined solely by the surface free energy. This hypothesis captures the general trend in the measured anatase-rutile composition but fails to explain the sensitivity. In the second pathway, non-stoichiometric TiO_{2-x} oxide intermediates are assumed and the crossover size is hypothesised to be composition-dependent. This shows an excellent agreement with the experimental data. However, this hypothesis is found to be strongly influenced by assumptions about the initial particle growth stages. This study demonstrates the importance of a better description of the high-temperature chemistry and initial clustering mechanism in order to understand the crystal phase formation.

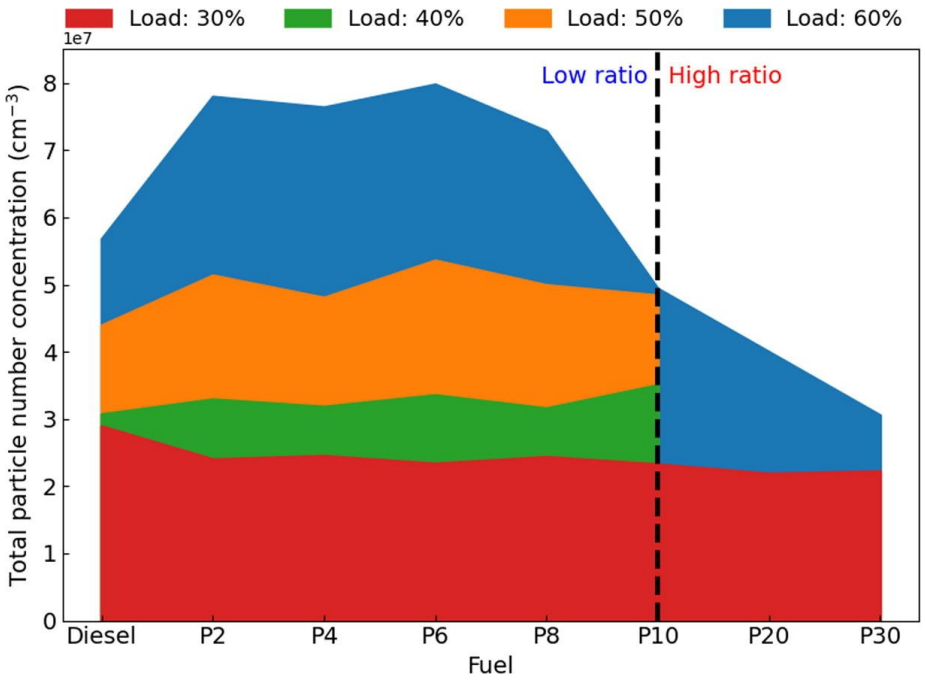


C4T IRP 3: Understanding the blending effect of polyoxymethylene dimethyl ethers as additive in a common-rail diesel engine

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

DOI: 10.1016/j.apenergy.2021.117380

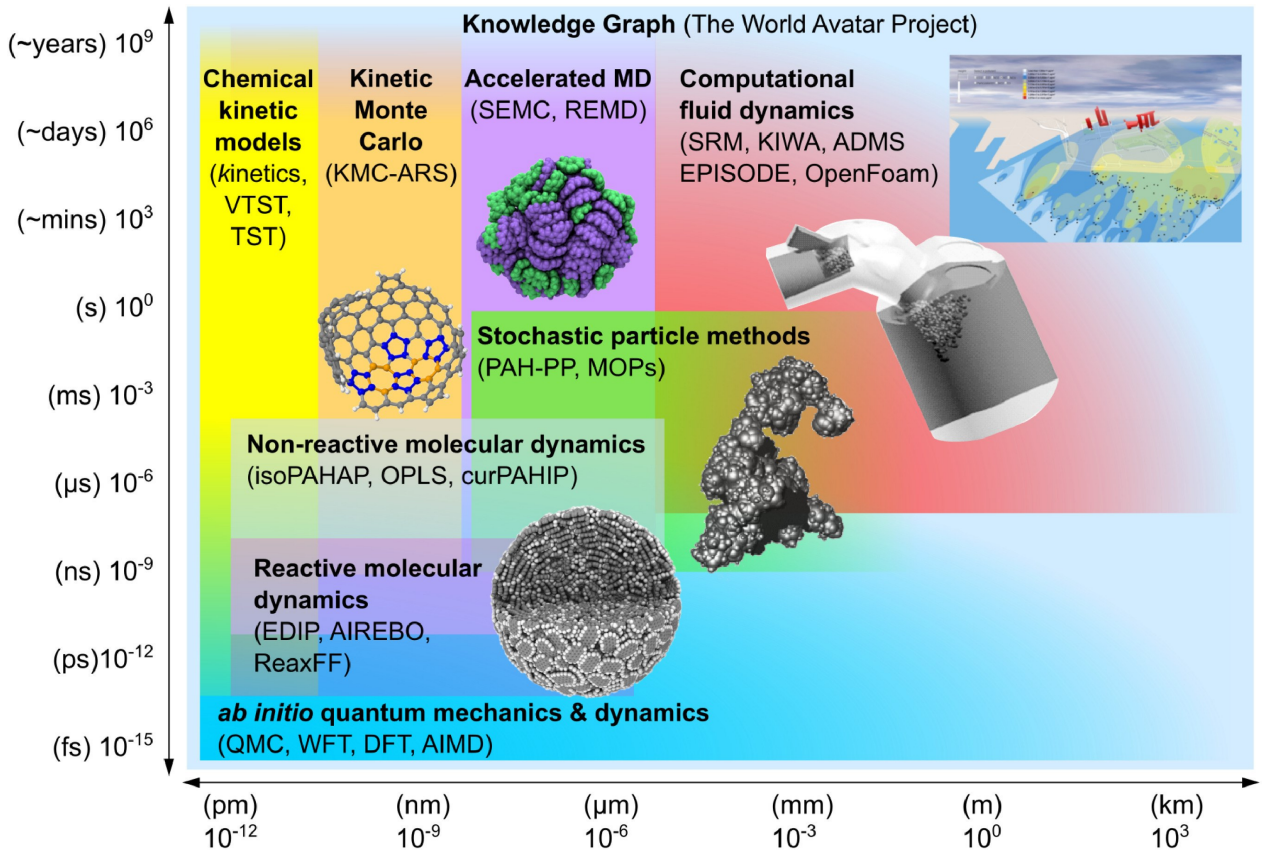
Abstract: Polyoxymethylene Dimethyl Ether (PODE) is known as a promising additive in the traditional diesel engine because it can reduce particulate matter emission in the exhaust gas. The reduction of the particulate matter emission when PODE is used as fuel additives is often attributed to the absence of C-C bond and the high oxygen content of the PODE molecular structure. In this paper, we have studied diesel-$PODE_3$ blends at both low blending ratio (<10%) and high blending ratio (10–30%). We have found that the high oxygen content effect of $PODE_3$ is only prominent in reducing the emission of particulate matter when there is a deficiency in the air supply of engine. Meanwhile, the effect of the absence of C-C bond has negligible impact on the emission of particulate matter. Moreover, an increase in the emission of the particulate matter was observed for the fuel blends containing low blending ratio of $PODE_3$. This is attributed to the decrease in the mean chamber temperature for the $PODE_3$-diesel blends as the lower heating value of $PODE_3$ is much lower than diesel. Despite this, high blending ratio of $PODE_3$ in diesel was found to still capable to decrease the emission of particulate matter. A summary chart has been proposed in this study to enable the prediction of the particle reduction ability of $PODE_3$ additive under different blending ratios and engine loads. In addition, the combustion characteristics and gas emissions (HC and NO_x) are also discussed in this paper.



C4T IRP 3: Soot inception: Carbonaceous nanoparticle formation in flames

Jacob W. Martin, Maurin Salamanca and Markus Kraft, *Progress in Energy and Combustion Science*
DOI: 10.1016/j.pecs.2021.100956

Abstract: The route by which gas-phase molecules in hydrocarbon flames form condensed-phase carbonaceous nanoparticles (incipient soot) is reviewed. These products of incomplete combustion are introduced as particulates and materials revealing both their useful applications and unwanted impacts as pollutants. Significant advances in experimental techniques in the last decade have allowed the gas phase precursors and the transformation from molecules to nanoparticles to be directly observed. These measurements combined with computational techniques allow for various mechanisms known to date to be compared and explored. Questions remain surrounding the various mechanisms that lead to nanoparticle formation. Mechanisms combining physical and chemical routes, so-called physically stabilised soot inception, are highlighted as a possible "middle way".



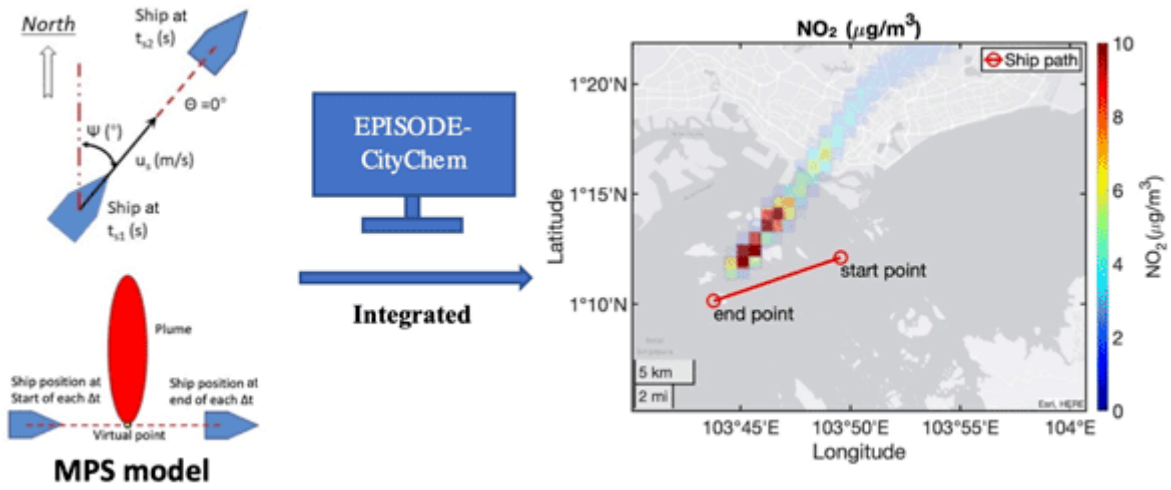
Linking spatial and temporal scales for modelling nanoparticle formation and pollution dispersion.

C4T IRPs 4 and JPS: Development of a moving point source model for shipping emission dispersion modeling in EPISODE–CityChem v1.3

Kang Pan, Mei Qi Lim, Markus Kraft and Epaminondas Mastorakos, *Geoscientific Model Development*

DOI: 10.5194/gmd-14-4509-2021

Abstract: This paper demonstrates the development of a moving point source (MPS) model for simulating the atmospheric dispersion of pollutants emitted from ships under movement. The new model is integrated into the chemistry transport model EPISODE–CityChem v1.3. In the new model, ship parameters, especially speed and direction, are included to simulate the instantaneous ship positions and then the emission dispersion at different simulation time. The model was first applied to shipping emission dispersion modeling under simplified conditions, and the instantaneous and hourly averaged emission concentrations predicted by the MPS model and the commonly used line source (LS) and fixed point source (FPS) models were compared. The instantaneous calculations were quite different due to the different ways to treat the moving emission sources by different models. However, for the hourly averaged concentrations, the differences became smaller, especially for a large number of ships. The new model was applied to a real configuration from the seas around Singapore that included hundreds of ships, and their dispersion was simulated over a period of a few hours. The simulated results were compared to measured values at different locations, and it was found that reasonable emission concentrations were predicted by the moving point source model.

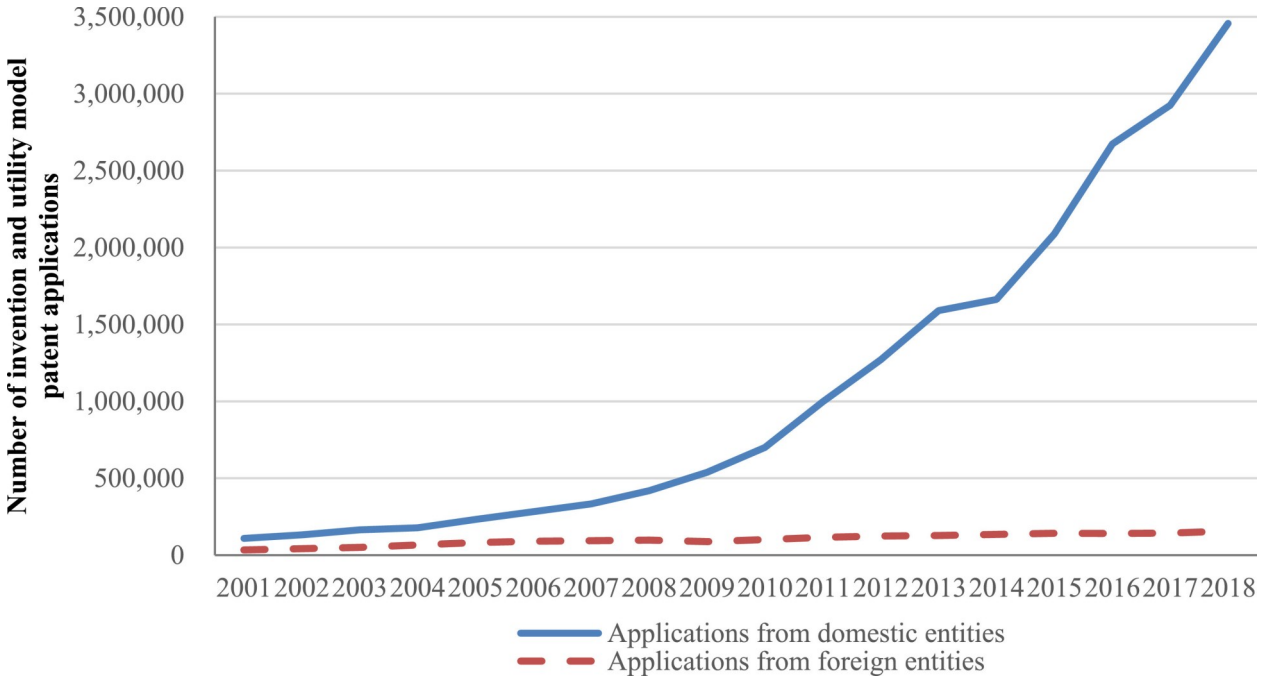


C4T IRP BB: Assessing the value of China's patented inventions

Kenneth Guang-Lih Huang, Can Huang, Huijun Shen and Hao Mao, *Technological Forecasting and Social Change*

DOI: 10.1016/j.techfore.2021.120868

Abstract: This study provides one of the first systematic and direct assessments of the value of China's inventions and examines the strategic factors influencing their value, using patents granted to firms by the China National Intellectual Property Administration (CNIPA). To do this, we first review the theoretical background of these factors and the inventor survey approach to estimating patent value. We then conduct the analysis using the large-scale, comprehensive annual Inventors Survey database (ISDB) collected by CNIPA, which consists of 12,869 firms linked to 30,693 patents granted between 2010 and 2012. We find that the median and average revenues from firms' implementation of their patents are RMB 0.75 million and 8.04 million respectively. Furthermore, we find that patents involving higher R&D investments, invention patents, patents essential to standards and belonging to patent pools command a higher value. State-owned enterprises (SOEs) produce lower value patented inventions relative to domestic private firms and foreign firms. Larger firms and those with intellectual property departments and aggressive in patent litigation have higher value inventions. Our findings yield important theoretical, methodological and policy implications.



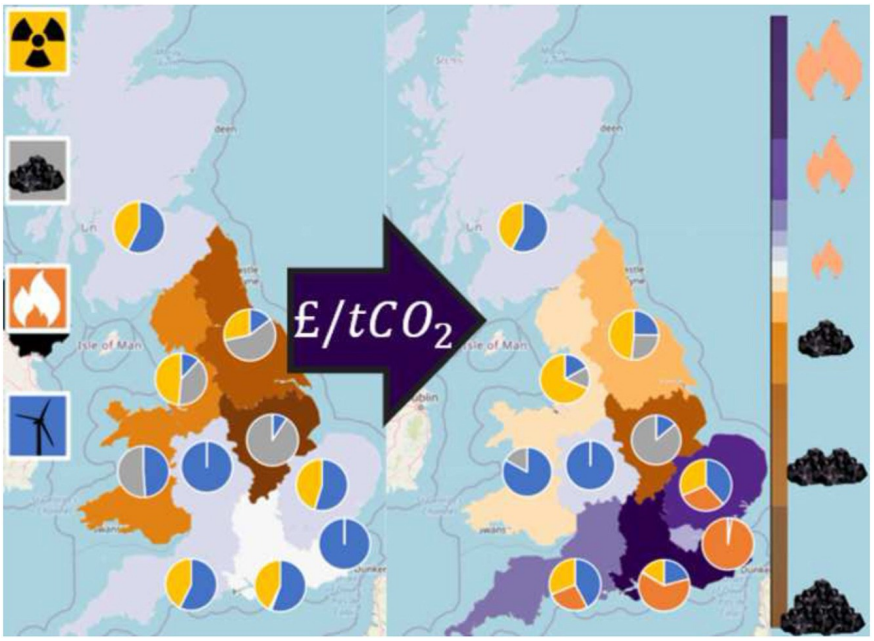
Number of invention and utility model patent applications by domestic and foreign entities in China (2001–2018).

C4T IRP JPS: How does a carbon tax affect Britain's power generation composition?

John Atherton, Wanni Xie, Leonardus Kevin Aditya, Xiaochi Zhou, Gourab Karmakar, Jethro Akroyd, Sebastian Mosbach, Mei Qi Lim and Markus Kraft, *Applied Energy*

DOI: 10.1016/j.apenergy.2021.117117

Abstract: The purpose of this paper is to determine the effect of different carbon tax rates on the power generation composition of Britain. This was accomplished via a regional, geospatial model, accounting for regional loads, transmission losses and generators of Britain's current energy infrastructure. This regional model is also compared to a pure dispatch, nationally aggregated model which considers only costs on the generator side inclusive of the carbon tax, thus allowing the effect of including geospatial conditions to be identified. The effect of this tax (in both the geospatial and nationally aggregated cases) is a transition from coal to combined cycle gas turbine (CCGT) generated power to fulfil demand unmet by nuclear or renewable sources. The more sophisticated regional model, however, differs from the nationally aggregated case by having a significantly larger window of carbon tax rates over which this coal to CCGT transition occurs. Due regional differences in demand and installed capacity technology types it is determined that more than 50% of this transition occurs prior to CCGT becoming more economical than coal from a pure dispatch (nationally aggregated) perspective. Primarily due to CCGT generators typically being closer to larger southern loads than northern coal, transmission losses and the economic disincentive of a carbon tax combine in encouraging this transition. The transition window, therefore, is not only broadened by the consideration of geospatial effects, but furthermore, this broadening significantly and disproportionately occurs by decreasing the lower bound of this transition window. These findings validate the significance of utilising a geospatial model, particularly of regional resolution. They further identify the deployment of current energy infrastructure in Britain under differing carbon tax regimes and by extension, the transition window (found to be from coal to CCGT) an increasing carbon tax rate would create. These results bear not only significance in understanding the UK's currently incrementing (top-up) carbon tax rate, but also shed light on future policies due to the UK's leaving of the EU's Emissions Trading Scheme (ETS), with immediate plans to continue with a domestic carbon tax and trading scheme. Thus, these results hold importance in the understanding the effect of carbon taxation on existing infrastructure, energy modelling and national policy in the UK.

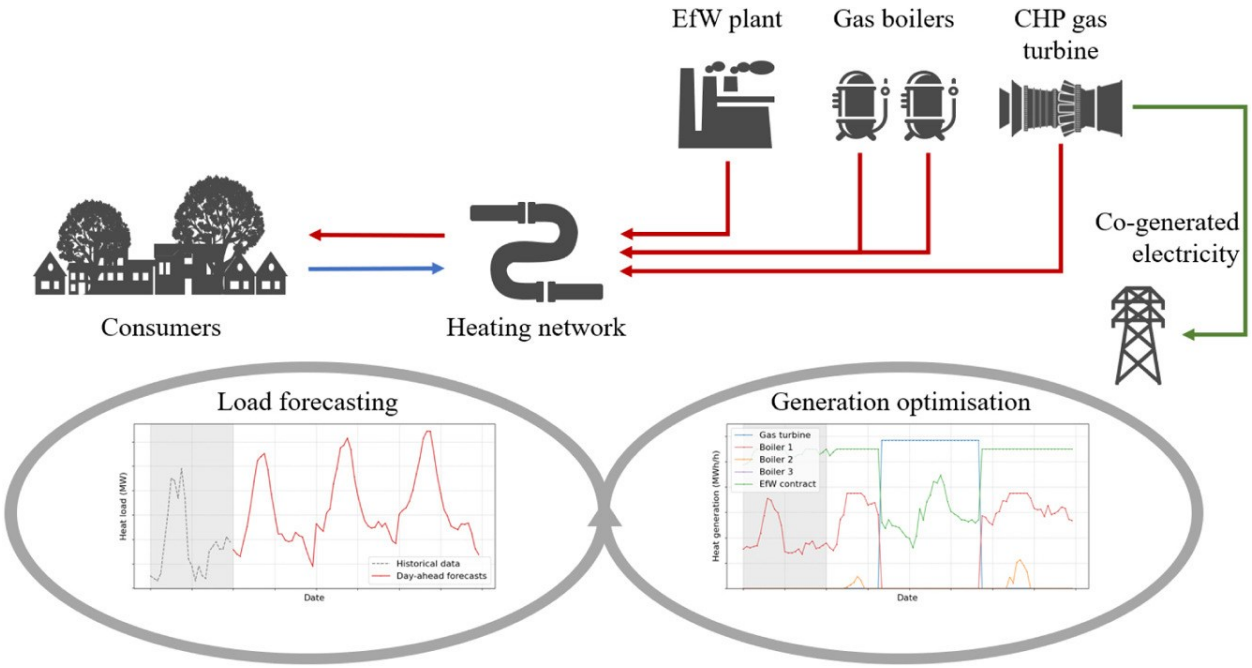


C4T IRP JPS: Resource-optimised generation dispatch strategy for district heating systems using dynamic hierarchical optimisation

Markus Hofmeister, Sebastian Mosbach, Jörg Hammacher, Martin Blum, Gerd Röhrig, Christoph Dörr, Volker Flegel, Amit Bhave, and Markus Kraft, *Applied Energy*

DOI: 10.1016/j.apenergy.2021.117877

Abstract: District heating is expected to play an essential role in the cost-effective decarbonisation strategy of many countries. Resource-optimised management of district heating networks depends on a wide range of factors, including demand forecasting, operational flexibility, and increasingly volatile market conditions. However, traditional operations often still rely on static models and rather simple heuristics, while holistic optimisation requires dynamic cross-domain interoperability to allow the consideration of all these factors. This paper demonstrates a proof-of-concept for a knowledge graph based optimisation problem to minimise total heat generation cost for a district heating provider. The optimisation follows a hierarchical approach based on a merit-order principle and is embedded in a model predictive control framework to allow the system to incorporate most recent information and react to disturbances promptly. A detailed sensitivity study is conducted to identify key model parameters and assess the impact of anticipated changes in regulation and market conditions. Simulation-based optimisation is used to determine the short-term heat generation mix based on data-driven gas consumption models and day-ahead forecasts for the network's energy demand and grid temperatures. Seasonal autoregressive integrated moving average models with exogenous predictor variables are found to be sufficiently accurate and precise. The effectiveness of the approach is demonstrated for a case study of an existing heating network of a midsize town in Germany, where a reduction of approximately 20% and 40% compared to baseline operational data is obtained for operating cost and CO_2 emissions, respectively.

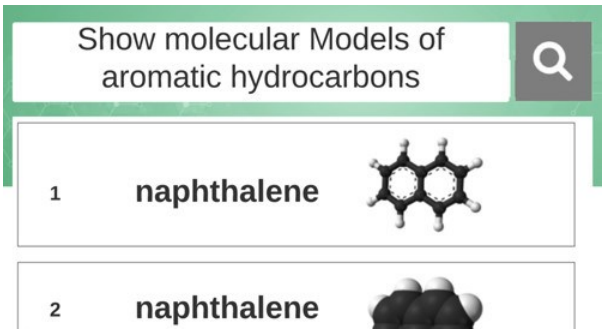


C4T IRP JPS: Question answering system for chemistry

Xiaochi Zhou, Daniel Nurkowski, Sebastian Mosbach, Jethro Akroyd and Markus Kraft, *Journal of Chemical Information and Modelling*

DOI: 10.1021/acs.jcim.1c00275

Abstract: This paper describes the implementation and evaluation of a proof-of-concept Question Answering (QA) system for accessing chemical data from knowledge graphs (KGs) which offer data from chemical kinetics to the chemical and physical properties of species. We trained the question classification and named the entity recognition models that specialize in interpreting chemistry questions. The system has a novel design which applies a topic model to identify the question-to-ontology affiliation to handle ontologies with different structures. The topic model also helps the system to provide answers with a higher quality. Moreover, a new method that automatically generates training questions from ontologies is also implemented. The question set generated for training contains 432,989 questions under 11 types. Such a training set has been proven to be effective for training both the question classification model and the named entity recognition model. We evaluated the system using other KGQA systems as baselines. The system outperforms the chosen KGQA system answering chemistry-related questions. The QA system is also compared to the Google search engine and the WolframAlpha engine. It shows that the QA system can answer certain types of questions better than the search engines.



CLIC: The role of prefrontal cortex in cognitive control and executive function

Naomi P. Friedman and Trevor W. Robbins, *Neuropsychopharmacology*

DOI: 10.1038/s41386-021-01132-0

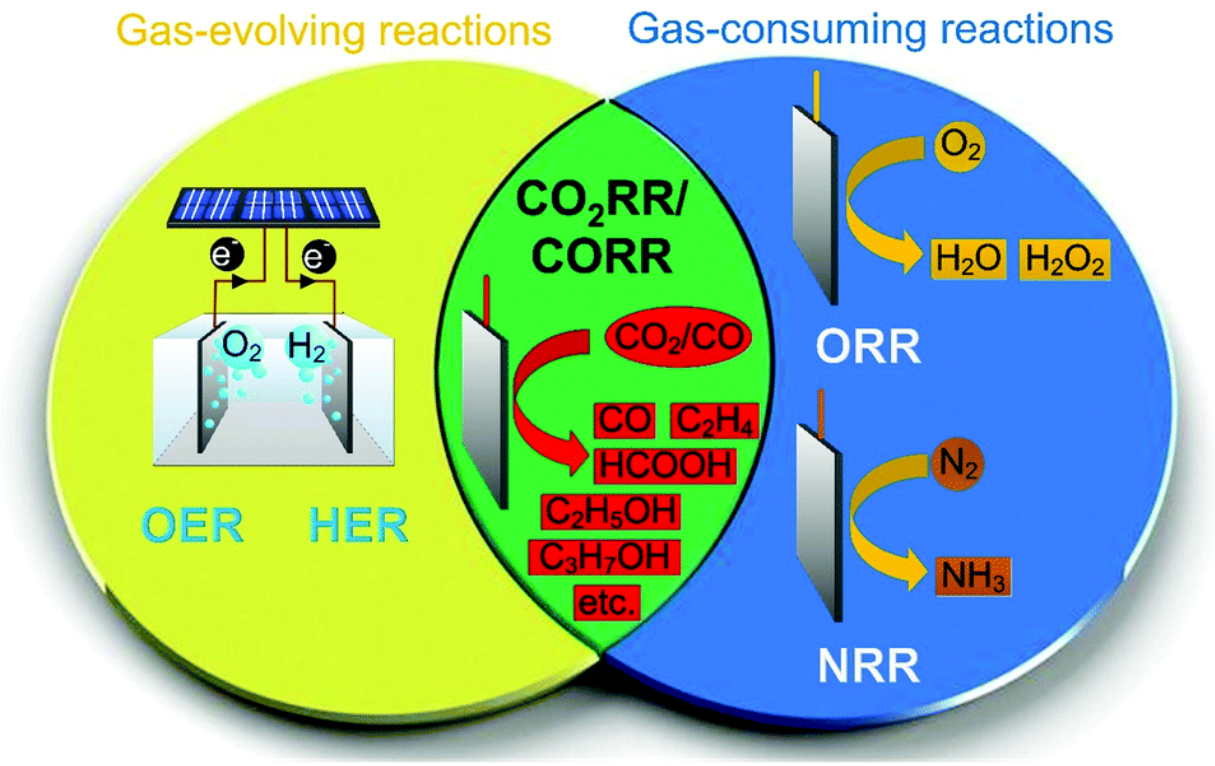
Abstract: Concepts of cognitive control (CC) and executive function (EF) are defined in terms of their relationships with goal-directed behavior versus habits and controlled versus automatic processing, and related to the functions of the prefrontal cortex (PFC) and related regions and networks. A psychometric approach shows unity and diversity in CC constructs, with 3 components in the most commonly studied constructs: general or common CC and components specific to mental set shifting and working memory updating. These constructs are considered against the cellular and systems neurobiology of PFC and what is known of its functional neuroanatomical or network organization based on lesioning, neurochemical, and neuroimaging approaches across species. CC is also considered in the context of motivation, as "cool" and "hot" forms. Its Common CC component is shown to be distinct from general intelligence (*g*) and closely related to response inhibition. Impairments in CC are considered as possible causes of psychiatric symptoms and consequences of disorders. The relationships of CC with the general factor of psychopathology (p) and dimensional constructs such as impulsivity in large scale developmental and adult populations are considered, as well as implications for genetic studies and RDoC approaches to psychiatric classification.

eCO_2EP: Wetting-regulated gas-involving (photo)electrocatalysis: biomimetics in energy conversion

Guanyu Liu, William S. Y. Wong, Markus Kraft, Joel W. Ager, Doris Vollmer and Rong Xu, *Chemical Society Reviews*

DOI: 10.1039/D1CS00258A

Abstract: (Photo)electrolysis of water or gases with water to species serving as industrial feedstocks and energy carriers, such as hydrogen, ammonia, ethylene, propanol, *etc.*, has drawn tremendous attention. Moreover, these processes can often be driven by renewable energy under ambient conditions as a sustainable alternative to traditional high-temperature and high-pressure synthesis methods. In addition to the extensive studies on catalyst development, increasing attention has been paid to the regulation of gas transport/diffusion behaviors during gas-involving (photo)electrocatalytic reactions towards the goal of creating industrially viable catalytic systems with high reaction rates, excellent long-term stabilities and near-unity selectivities. Biomimetic surfaces and systems with special wetting capabilities and structural advantages can shed light on the future design of (photo) electrodes and address long-standing challenges. This article is dedicated to bridging the fields of wetting and catalysis by reviewing the cutting-edge design methodologies of both gas-evolving and gas-consuming (photo)electrocatalytic systems. We first introduce the fundamentals of various in-air/underwater wetting states and their corresponding bioinspired structural properties. The relationship amongst the bubble transport behavior, wettability, and porosity/tortuosity is also discussed. Next, the latest implementations of wetting-related design principles for gas-evolving reactions (*i.e.* the hydrogen evolution reaction and oxygen evolution reaction) and gas-consuming reactions (*i.e.* the oxygen reduction reaction and CO_2 reduction reaction) are summarized. For photoelectrode designs, additional factors are taken into account, such as light absorption and the separation, transport and recombination of photoinduced electrons and holes. The influences of wettability and 3D structuring of (photo)electrodes on the catalytic activity, stability and selectivity are analyzed to reveal the underlying mechanisms. Finally, remaining questions and related future perspectives are outlined.



Categories for (photo)electrocatalytic gas-involving reactions.

IRP 1

SUSTAINABLE REACTION ENGINEERING FOR CARBON NEUTRAL INDUSTRY

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

IRP 1 Principal Investigators:

Professor Alexei LAPKIN
University of Cambridge

Asst Professor Paul LIU Wen
Nanyang Technological University

Professor ZENG Hua Chun
National University of Singapore

OVERVIEW

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

Recent work in IRP 1 has made advances towards a cheaper production process for metal silicates for industrial applications, as well as more effective catalysts for CO_2 conversion. Research into sustainable reaction routes and process chemistry continues with flow chemistry experiments taking place in the lab as well as continued progress on algorithms for more efficient reactions. Nanoparticle synthesis for coatings is also developing, both at the fundamental and commercial levels, with a scale-up platform being tested in Cambridge.

Professor Alexei Lapkin, PI
University of Cambridge

Update on work package 1.1

Design of nano-structured catalysts

There have been extensive studies on the synthesis and application of metal silicates for catalysis and other technological fields. In particular, metal silicates with hollow morphology have demonstrated unique advantages for catalysis applications. Lab scale production of hollow metal silicates usually relies on hydrothermal treatments, producing catalysts from milligram to gram scale and the batch-wise hydrothermal treatment presents a great challenge for scaling up.

For production of metal silicates for industrial applications, it is desirable to design new synthetic methods without the need of hydrothermal conditions, so that the process can be easily translated into flow synthesis using microreactors. Over the past months, **Dr LI Bowen (Research Fellow, NUS)** and **Prof. ZENG Hua Chun (PI, NUS)** have successfully synthesised yolk shell silica@nickel silicate structure under reflux conditions at 80 °C and ambient pressure. The conditions were chosen so that the process could be reproduced with microreactors as flow synthesis or semi-batch process, without the need for costly pressure vessels. In a typical synthesis, Stöber silica spheres were mixed with nickel nitrate solution and sodium hydroxide solution. The reaction time was controlled so that a surface layer of nickel silicate was formed (Figure 1a). This process could be repeated for multiple times to further increase the thickness of nickel silicate layer (Figure 1b-d). Once the desired shell thickness has been obtained, etching with high concentration sodium hydroxide solution will remove the remaining core and give the hollow nickel silicate structure. This work will be later investigated for possible continuous production using microfluidic reactors.

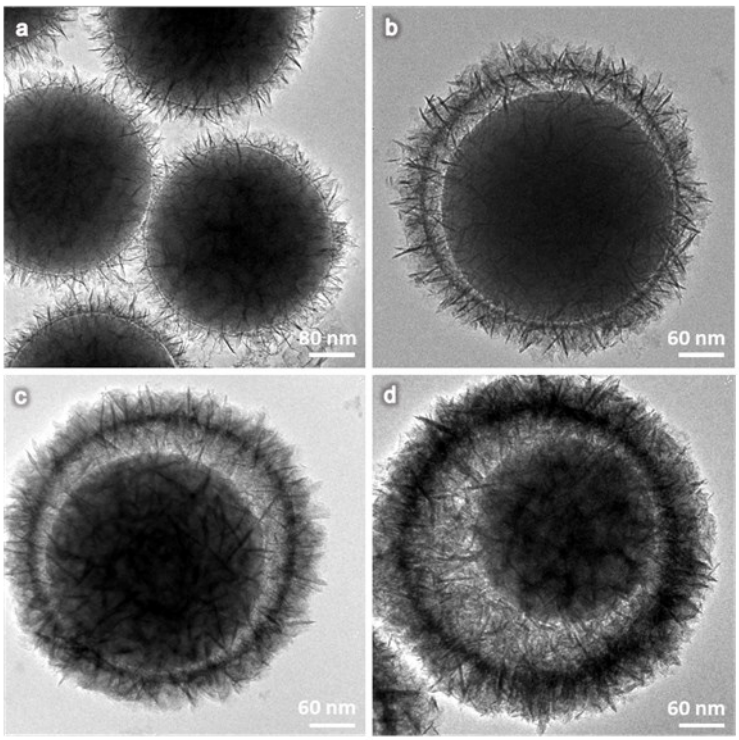


Figure 1.1: Representative TEM images of silica@nickel silicate yolk shell structure after (a) 1, (b) 3, (c) 5 and (d) 7 repeated reactions at 80 °C and ambient pressure.

Dr LI Bowen

Mr Alvin LIM Ming Hao (PhD student, NUS) and **Prof. ZENG Hua Chun** produced three different morphological variations of monodispersed ZnAl-LDH microspheres, with varying degrees of spacing between the nanosheets. The LDH material was calcined into ZnAl-LDO microspheres and loaded with Cu to be used as a catalyst candidate for CO_2 hydrogenation to methanol under high pressure and constant flow. Two different low-cost facile Cu loading methods were also compared, namely wet impregnation and ion exchange. The different morphological variations were then evaluated by CFD simulation (ANSYS Fluent) and experiments of CO_2 hydrogenation to methanol, to explore the effect of nanosheet spacing on catalyst performance in terms of the overall catalytic activity and methanol selectivity. The different loading methods also produced different stability results, where there is a slight drop in performance in incipient wet impregnated catalyst, while the ion exchanged catalyst retains much better over the same period of 40 h. In our preliminary CFD simulation, an increase in the nanosheet spacing improves convection-driven vortices within the wider channels, reaching deeper into the core of the microsphere. The simulated vortex phenomenon explains the higher catalytic activity observed in our experimental results. This work indicates that catalysts with intricate morphological structure engineering would significantly enhance its catalytic activity.

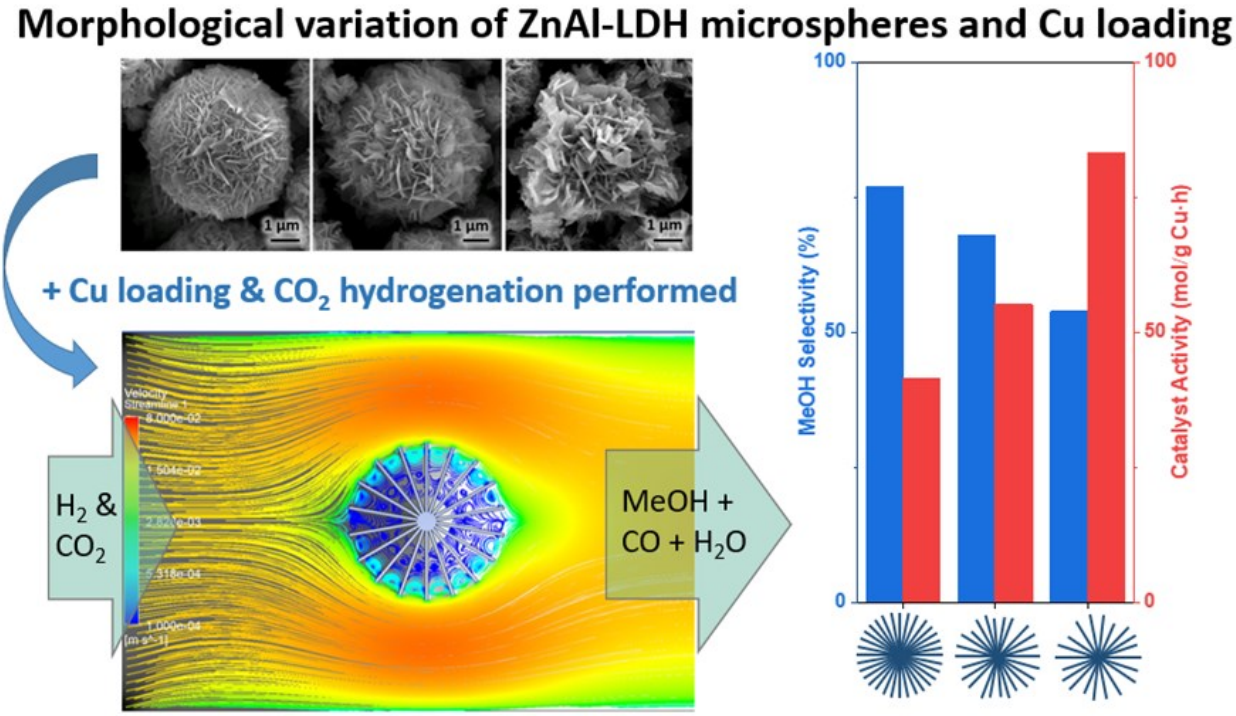


Figure 1.2: Schematic illustration for ZnAl-LDH catalyst morphology variation and corresponding performance for CO_2 hydrogenation to methanol.

Mr Alvin LIM Ming Hao

Update on work package 1.2

Novel reactions and functional molecules

Guided by Prof. Alexei LAPKIN (PI, CAM), **Dr GUO Zhen (Research Fellow, CARES)** continues to work on three research projects: 1) development of new heuristic for chemical route searching based on molecular similarity; 2) guiding PhD candidate Mr Adarsh ARUN on impurity predictions; 3) collaborating with PhD candidate Ms Jana WEBER on a paper regarding roles of digital chemistry on sustainable reaction routes. For the first project, the new similarity-based heuristic has been developed and applied on the reaction route searching. This work has been summarised in a paper which will be submitted after further revisions. An algorithm for generating this similarity-based heuristic was also uploaded to GitHub. The second project is almost complete and impurities, together with the main products, can be predicted by using our prediction systems on the basis of three case studies proposed by Dr Simon SUNG (PIPS C4 project – see page 131). Mr Arun is wrapping up and writing the paper. The third project is complete and a paper on this part of the work has been published in *Chemical Society Reviews*. Dr Guo's next two tasks are: 1) development of an algorithm for long-range search. Searching reaction routes with more than five steps is a challenge due to the "explosion of options" issue. The number of available routes increases exponentially with the number of allowed synthetic routes. To address this issue, we algorithms will be implemented based on expertise knowledge, as well as machine approaches; 2) optimise and formalise current codes to make the system ready for production version.

Mr Perman JORAYEV's (PhD student, CAM) main research focus is on transforming new discoveries into robust processes. This requires (1) prior knowledge generation to identify relevant chemical and physical parameters and (2) using the prior knowledge to optimise the reaction. This would require integrating data extraction and cleaning, descriptor generation and modelling so the entire automated workflow is now complete. To confirm the efficiency of the workflow (i.e. to avoid causation vs correlation issue, the model should be able to extract meaningful knowledge to validate with physical knowledge), several feature engineering methods have been implemented. Overall, the project is mostly complete and now requires end-to-end integration of all individual steps.

On the second half of the project, Mr Jorayev has finalised the optimal hardware setup and reaction conditions (i.e. variable range and reaction concentration). He has carried out 60+ reactions using the automated flow setup to collect the training dataset using Latin Hypercube Sampling in order to initiate the optimisation process. The next step is to sequentially optimise the reaction until a robust model is developed.

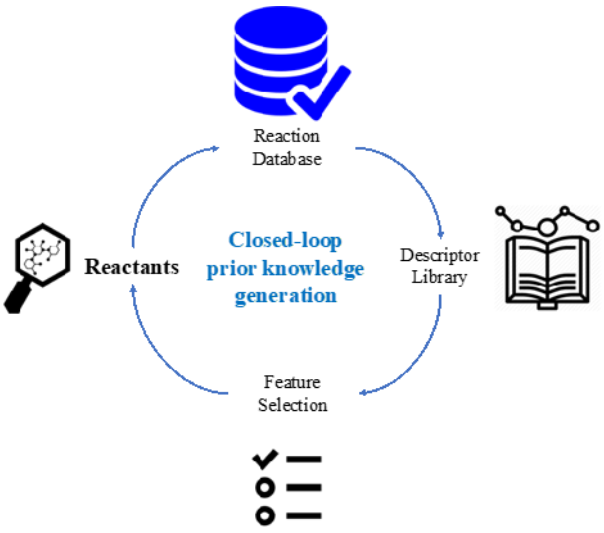


Figure 1.3: Automated prior knowledge generation to select relevant parameters for a given reaction.

Mr Perman JORAYEV

Mr Adarsh ARUN (PhD student, CAM) commenced his PhD in January 2021, and focuses on identifying sustainable routes from biowaste to chemicals using networks.

Recently, he has submitted a paper entitled "Integration of biowaste into chemical reaction networks" outlining a case study of biowaste sources in Singapore, Malaysia and Indonesia, and an exergy analysis of an organosolv (organic solvent) pre-treatment process to yield cellulose, lignin and xylose from Oil Palm Empty Fruit Bunch (EFB). He is currently investigating automated methods to scale up the workflow outlined in the paper across more regions, biowaste sources and pre-treatment methods, creating an integrated network for end-to-end sustainable route selection from raw biowaste sources to high -value platform chemicals.

The other project he is working on involves data mining large chemical databases such as Reaxys to predict impurities and byproducts in chemical reactions, which has the potential to aid early-stage process development. The workflow was successfully tested on three successful case studies, including prediction of impurities from Lersivirine synthesis, which has been performed in the CARES lab under one of the PIPS projects. A paper is currently being written on the workflow and results and will be submitted soon.

Ms Marsha ZAKIR's (Research Engineer, CARES) main research interest is in green electrochemistry. She has been working on improving the lifetime of gas diffusion electrodes for electrochemical CO_2 reduction with **Dr Mikhail KOVALEV (Research Fellow, CARES)**. She is also studying the possibility of C13 enrichment with the electrochemical reduction of CO_2 set up with Dr Kovalev and **Dr Magda BARECKA (Research Fellow, CARES)**.

Ms Kencha SATYA (Research Engineer, CARES) has been focusing on rapid optimisation of nanomaterial production for the now-complete Rapid Industrialization of Next Generation Nanomaterials (RINGs) project, which was funded by the SMART Innovation Centre. Ms Satya's main research interest lies in the studying the properties of Zinc Oxide (ZnO) nanocrystals, in particular the effects of synthesis conditions on their chemical, physical and biological properties. End-use applications lie in protective and catalytic coatings that can reduce reliance on toxic antimicrobials and prolong the lifetimes of buildings and equipment.

Currently she is working on optimisation of zinc oxide nanoparticle synthesis by testing the different variables like pH and precursor salts in order to standardise the antibacterial/antifungal performance of latex/ZnO paint formulations. She is currently developing various methods for measuring and controlling the quality of ZnO nanoparticles using spectroscopic and thermogravimetric analytical techniques. One key result that Ms Satya has found is that the antimicrobial performance is dramatically dependent on the pH of ZnO synthesis using annular microreactor technology. She is now in IRP1, and is currently standardising methods for nanoparticle synthesis in the annular flow microreactor in order to facilitate the future scale up.

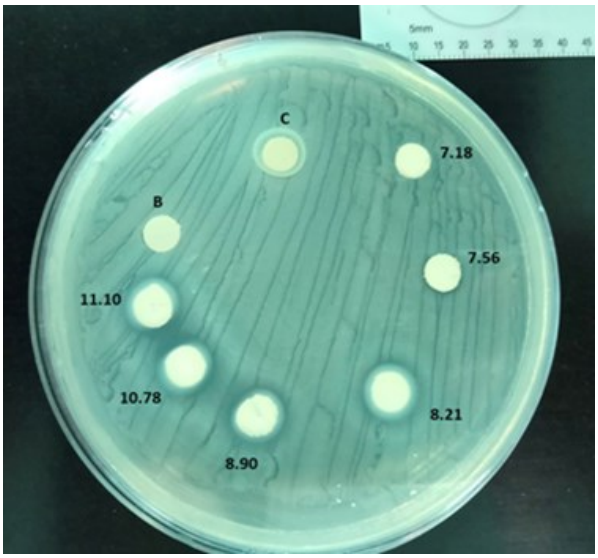


Figure 1.4: Comparing the efficiency of antimicrobial materials in a "disk-diffusion" assay with E. Coli.

Ms Kencha SATYA

Update on work package 1.3

Novel reactors and process technology

Mr FAN Qianwenhao (in-kind PhD student, NTU) has been working on the development of redox active metal oxide nanoparticles with enhanced thermal stability during harsh chemical looping conditions, e.g., a well-defined yolk–shell oxygen carrier, with Fe_2O_3 as the core and ZrO_2 (or Y_2O_3) as the shell. The excellent thermostability of ZrO_2 and Y_2O_3 makes them promising candidates for yolk–shell structures, as it may protect the internal cores from sintering under high temperature, whereas the void can provide space for the volume change of metal oxide core during the redox cycles. The general synthesis route is shown in Figure 1.5a. Uniform Fe_2O_3@SiO_2 spheres (Figure 1.5b) were fabricated according to a modified Stöber method. Recently, Mr Fan has been focusing on the controllable coating of Zr (Y) shell with various morphology and porosity. After careful selection of Zr (Y) metal precursors and reaction conditions applied, Fe_2O_3@void@ZrO_2(Y_2O_3) yolk-shell nanostructures could be obtained and simultaneously well-dispersed, with porous (Figure 1.5c), dense (Figure 1.5d), and pore-expanded (Figure 1.5e) shell morphology. Such morphological architecture of metal oxide shell is currently applied for high temperature chemical looping applications.

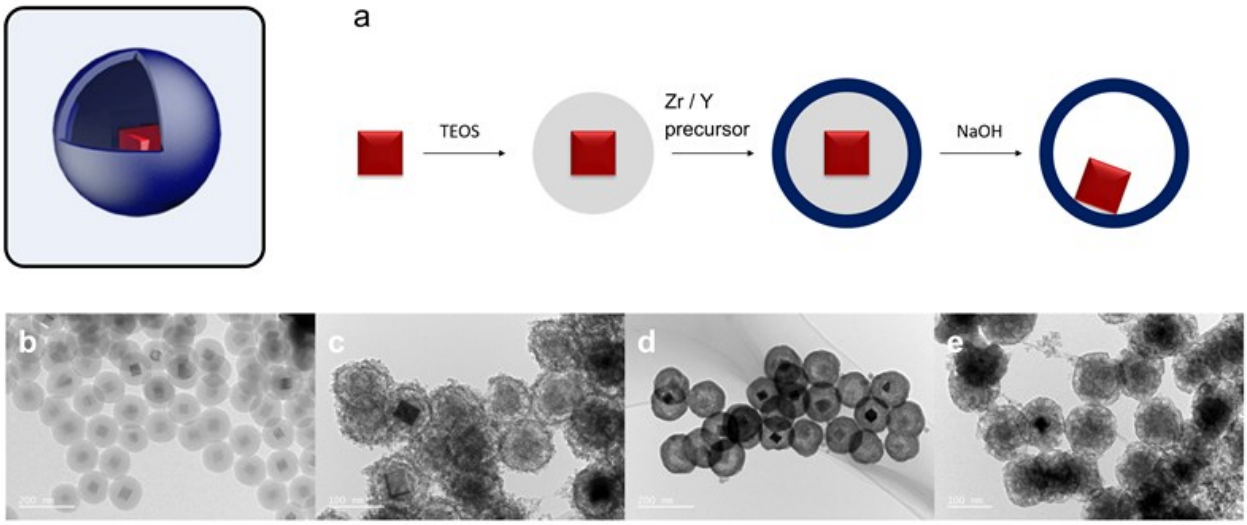


Figure 1.5: Schematic illustration of the synthesis of yolk-shell Fe-based oxygen carriers.

Mr FAN Qianwenhao

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

Scale-up platform: A scale-up platform has been designed and simulated for reactor scale-up via multiplexing, which will accommodate flowrates of up to 1 L/min. This platform is now being calibrated and tested in Cambridge. This platform will be used to scale up hollow shell nickel silicate catalysts previously developed by Dr LI Bowen, in the group of Prof. ZENG Hua Chun.

Simulations: A computational fluid dynamics study has been started to analyse fluid behaviour in annular microreactor technology. This work is being done in collaboration with AWTH Aachen University as the subject of a master's project, which will completed in November. This work will result in a working CFD model for prediction of reactor hydrodynamic behaviour, mixing and reaction kinetics. This is particularly useful in scale-up, in which relatively fewer experiments may be conducted than at the laboratory scale.

Automation: A coding framework for rapid automation of laboratory equipment has been devised and is currently being tested for automating reaction equipment. This framework, *Flab* (standing for Fast, Flexible and Fun) is designed to be experimentalist-friendly with a modular architecture, fast implementation of device drivers and a simple interface. A number of case studies have already been performed on in-house equipment, which provide demonstration of proof of concept. Reporting and documentation on version 1.0 is currently underway.

Mr Syed SAQLINE (PhD student, NTU) has been working on the use of barium ferrites as materials for carbon capture and oxygen storage. Barium ferrites ($Ba_3Fe_2O_6$ and $Ba_5Fe_2O_8$) have been synthesised and tested for their remarkable oxygen carrying capacity and CO_2 absorption properties. Such features of this multifunctional material can be exploited for use as an oxygen carrier material in chemical looping combustion, sorbent in CO_2 looping, and as an air separation agent in chemical looping air separation. Phase identification of the XRD spectra revealed the various phases detected in the samples, as seen in Figure 1.6.

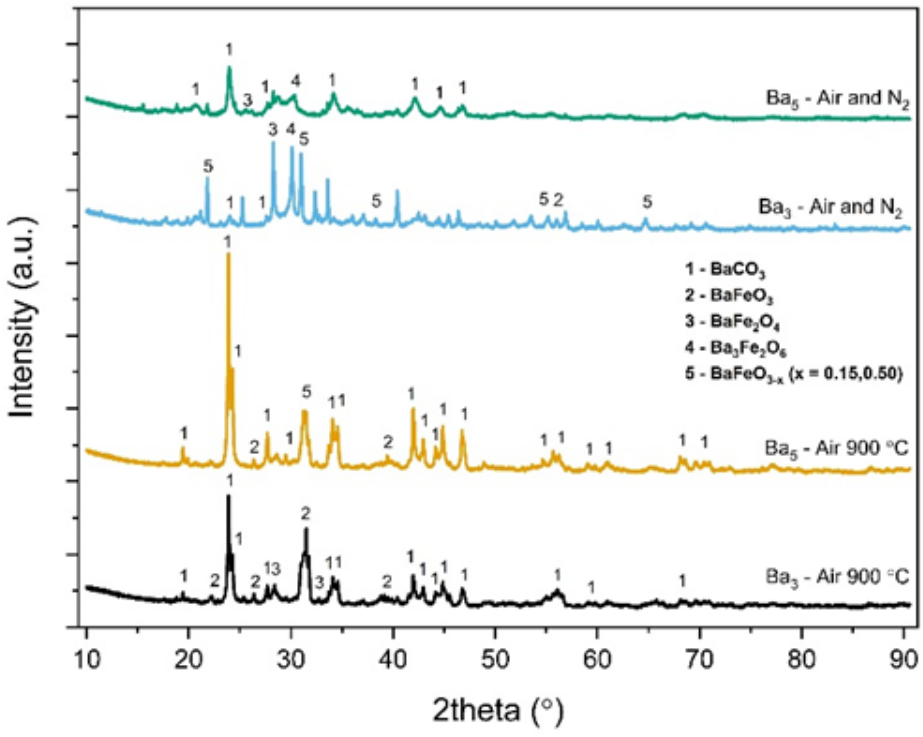


Figure 1.6: XRD pattern of the synthesis barium ferrite materials.

Mr Syed SAQLINE

Scientific output

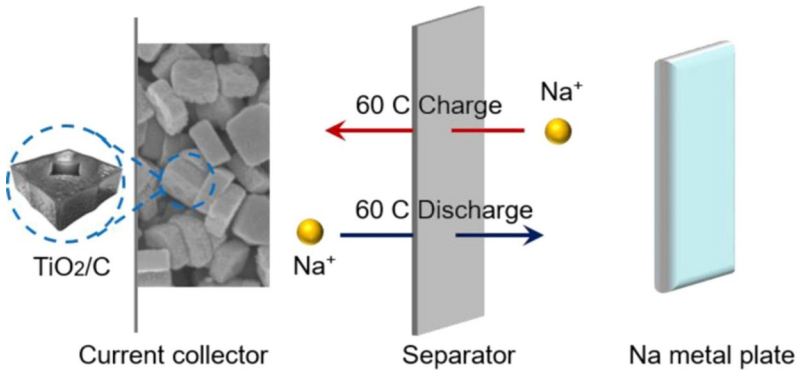
The following are the CREATE-acknowledged publications generated by IRP 1 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

TiO_2/C tetragons with a double-side concave nanostructure and its high rate performance on Na-ion storage

Andi Di, Yu Wang and Hua Chen Zeng, *Applied Surface Science*

DOI: 10.1016/j.apsusc.2021.150756

Abstract: TiO_2 is acting as a low-cost and promising candidate for a high capacity anode material of Na-ion batteries. Its insufficient cyclability and poor capacity utilisation for Na-ion storage can be improved by manipulating its nanostructures. We designed and prepared a carbon-coated TiO_2 (TiO_2/C) material with a double-side concave structure and a large surface area. The as-synthesised TiO_2/C with such special nanostructure, delivered a high capacity of *ca.* 175 mAh g^{-1} at 1 A g^{-1} rate with roughly 100% capacity retention over 1600 cycles and *ca.* 100% Coulombic efficiency. More significantly, TiO_2/C concave tetragons exhibited an outstanding rate capacity of 150 mAh g^{-1} and 60 mAh g^{-1} at 5 A g^{-1} and 20 A g^{-1}, respectively. These results demonstrate the design of the special TiO_2/C concave tetragons allows a sufficiently long cycle life for battery applications, superior reversibility and enhanced rate for the Na-ion storage.



Molecule confined isolated metal sites enable the electrocatalytic synthesis of hydrogen peroxide

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

DOI: 10.1002/adma.202104891

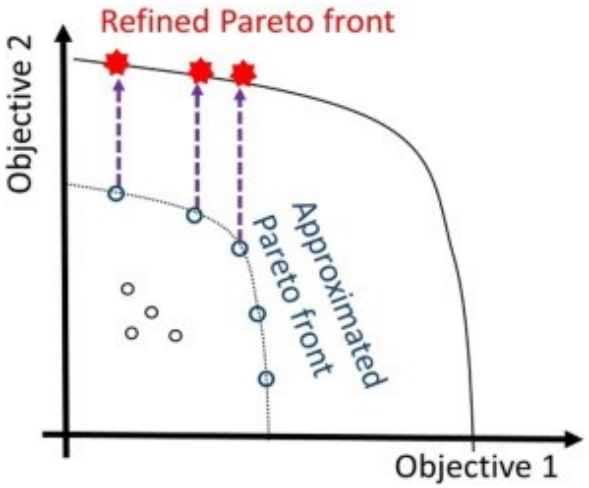
Abstract: The direct synthesis of hydrogen peroxide (H_2O_2) through the two-electron oxygen reduction reaction is a promising alternative to the industrial anthraquinone oxidation process. Selectivity to H_2O_2 is however limited by the four-electron pathway during oxygen reduction. Herein, it is reported 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.

Efficient hybrid multiobjective optimization of pressure swing adsorption

Hao, Zhimian, Adrian Caspari, Artur M. Schweidtmann, Yannic Vaupel, Alexei A. Lapkin and Adel Mhamdi, *Chemical Engineering Journal*

DOI: 10.1016/j.cej.2021.130248

Abstract: Pressure swing adsorption (PSA) is an energy-efficient technology for gas separation, while the multiobjective optimization of PSA is a challenging task. To tackle this, we propose a hybrid optimization framework (TSEMO + DyOS), which integrates two steps. In the first step, a Bayesian stochastic multiobjective optimization algorithm (i.e., TSEMO) searches the entire decision space and identifies an approximated Pareto front within a small number of simulations. Within TSEMO, Gaussian process (GP) surrogate models are trained to approximate the original full process models. In the second step, a gradient -based deterministic algorithm (i.e., DyOS) is initialized at the approximated Pareto front to further refine the solutions until local optimality. Therein, the full process model is used in the optimization. The proposed hybrid framework is efficient, because it benefits from the coarse-to-fine function evaluations and stochastic-to-deterministic searching strategy. When the result is far away from the optima, TSEMO can efficiently approximate a trade-off curve as good as a commonly used evolutional algorithm, i.e., Non-dominated Sorting Genetic Algorithm II (NSGA-II), while TSEMO only uses around 1/16th of CPU time of NSGA-II. This is because the GP-based surrogate model is utilized for function evaluations in the initial coarse search. When the result is near the optima, the searching efficiency of TSEMO dramatically decreases, while DyOS can accelerate the searching efficiency by over 10 times. This is because, in the proximity of optima, the exploitation capacity of DyOS is significantly higher than that of TSEMO.



Single-step production of hydrogen-rich syngas from toluene using multifunctional Ni-dolomite catalysts

Tingting Xu, Xun Wang, Bo Xiao and Wen Liu, *Chemical Engineering Journal*

DOI: 10.1016/j.cej.2021.131522

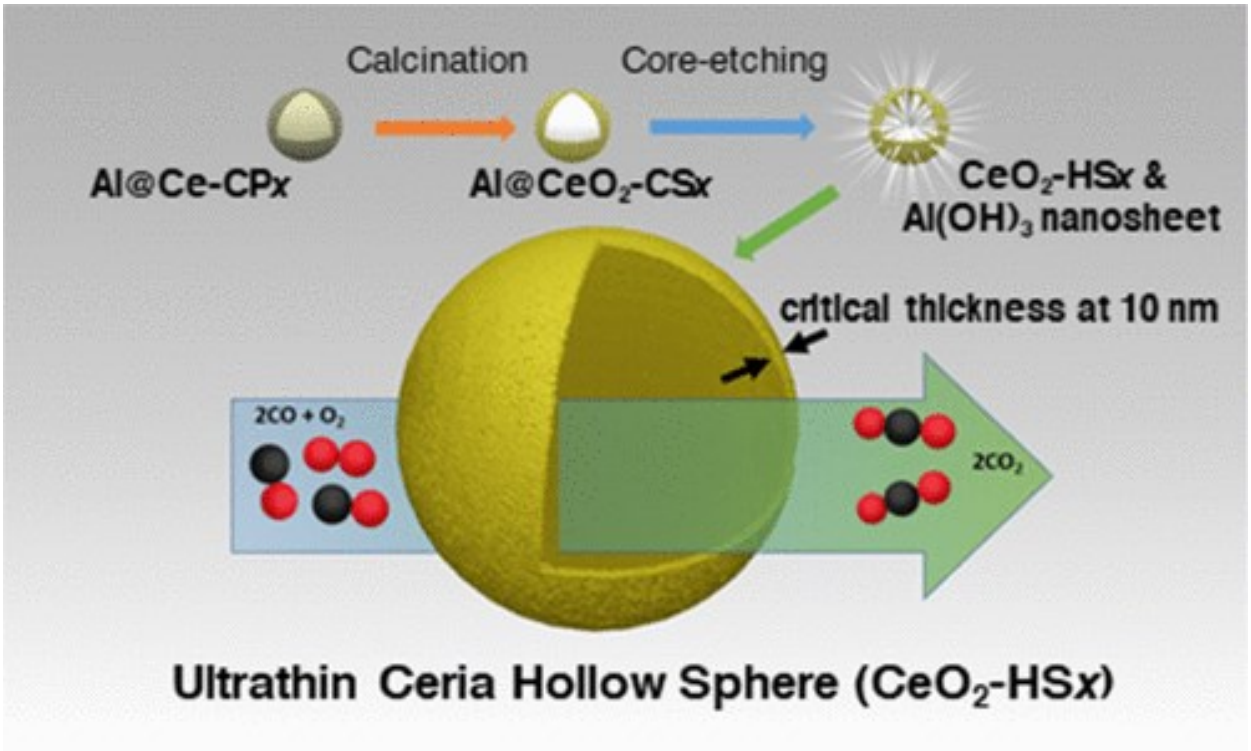
Abstract: Tar compounds such as toluene can be oxidatively converted by reforming, followed by water–gas-shift and CO_2 removal to produce H_2-rich syngas. We report a type of low-cost multifunctional catalysts that are capable of producing hydrogen-rich syngas from toluene in a single reactor. The multifunctional catalysts, derived from Ni-loaded dolomite, also act as oxygen carriers and CO_2 sorbents. When operating under a chemical looping-type scheme at 700 °C, the catalyst containing 15 wt% NiO could produce syngas containing >70% hydrogen, with a cold-gas-efficiency of 90.3%. No sign of deactivation, coking or structural change was observed over 10 consecutive cycles of reforming and regeneration. The remarkable performance is attributed to the promotional effects arising from the formation of the $Mg_xNi_{1-x}O$ solid solution. Additionally, MgO acts as a support and provides sintering resistance to both the Ni catalyst and the CaO-based CO_2 sorbent, making the multifunctional structure highly regenerable over cyclic operation.

Antisolvent route to ultrathin hollow spheres of cerium oxide for enhanced CO oxidation

Alvin M. H. Lim and Hua Chun Zeng, *ACS Applied Materials & Interfaces*

DOI: 10.1021/acsami.1c01320

Abstract: Cerium(IV) oxide (CeO_2), or ceria, is one of the most abundant rare-earth materials that has been extensively investigated for its catalytic properties over the past two decades. However, due to the global scarcity and increasing cost of rare-earth materials, efficient utilization of this class of materials poses a challenging issue for the materials research community. Thus, this work is directed toward an exploration of making ultrathin hollow ceria or other rare-earth metal oxides and mixed rare-earth oxides in general. Such a hollow morphology appears to be attractive, especially when the thickness is trimmed to its limit, so that it can be viewed as a two-dimensional sheet of organized nanoscale crystallites, while remaining three-dimensional spatially. This ensures that both inner and outer shell surfaces can be better utilized in catalytic reactions if the polycrystalline sphere is further endowed with mesoporosity. Herein, we have devised our novel synthetic protocol for making ultrathin mesoporous hollow spheres of ceria or other desired rare-earth oxides with a tunable shell thickness in the region of 10 to 40 nm. Our ceria ultrathin hollow spheres are catalytically active and outperform other reported similar nanostructured ceria for the oxidation reaction of carbon monoxide in terms of fuller utilization of cerium. The versatility of this approach has also been extended to fabricating singular or multicomponent rare-earth metal oxides with the same ultrathin hollow morphology and structural uniformity. Therefore, this approach holds good promise for better utilization of rare-earth metal elements across their various technological applications, not ignoring nano-safety considerations.

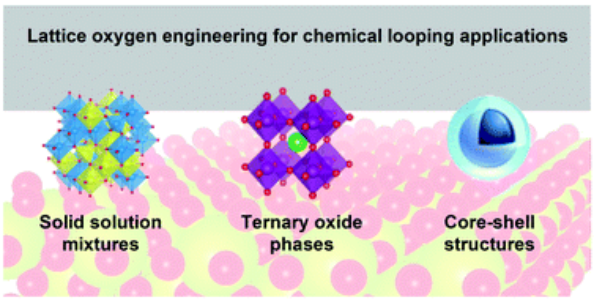


Controlling lattice oxygen activity of oxygen carrier materials by design: a review and perspective

Wen Liu, *Reaction Chemistry & Engineering*

DOI: 10.1039/D1RE00209K

Abstract: Chemical looping is a class of emerging process intensification technologies that enable emission reduction of a wide range of chemical processes. The performance of oxygen carrier materials is critical to the effectiveness of the chemical looping processes. Over the past two decades, understanding of how oxygen carriers behave over chemical looping cycles continued to improve, leading to encouraging advancements in recent years, including several newly developed chemical looping applications showing promise to achieve lower CO_2 footprints compared to conventional reactor technologies. Amongst the key material design considerations, having appropriate lattice oxygen activity is critical for maximising the product yield and selectivity of chemical looping processes. In this mini-review, material design approaches enabling the development of oxygen carriers with well-defined and well-regulated lattice oxygen activity are overviewed and critically assessed. Besides the significant progress made, there remain key knowledge gaps in the area of lattice oxygen engineering. Lastly, the potential roles which computational tools could play in designing oxygen carriers with targeted lattice oxygen activities are discussed.



Coupling chemical looping combustion of solid fuels with advanced steam cycles for CO_2 capture: A process modelling study

Syed Saqline, Zhen Yee Chua and Wen Liu, *Energy Conversion and Management*

DOI: 10.1016/j.enconman.2021.114455

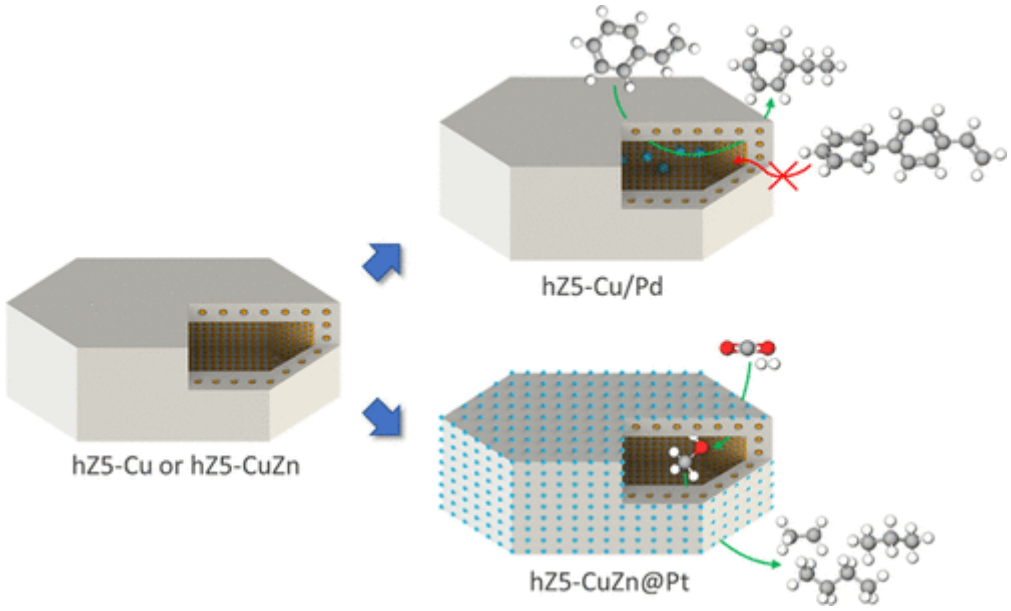
Abstract: Chemical looping combustion is a cost-competitive solution for producing low carbon electricity. In this paper, we investigate by means of a process modelling study, the coupling of chemical looping combustion of solid fuels with advanced steam-based power cycles, viz. supercritical, ultra-supercritical and advanced ultra-supercritical Rankine cycles. The energy and exergy efficiencies of the various chemical looping combustion power plant configurations are compared against the reference plants without carbon capture. Our models incorporate practical considerations for reactor design. With an upper operating temperature limit of 950 °C, the maximum efficiencies achievable by integrated gasification combined cycle chemical looping combustion (IGCC–CLC) and in situ gasification chemical looping combustion power plants (iG-CLC) are 41.3% and 41.5%, respectively. Overall, iG-CLC emerges as the most efficient CLC configuration. Comparing to an integrated gasification combined cycle without carbon capture, the energy efficiency penalties for capturing CO_2 from iG-CLC coupled with subcritical, supercritical, ultra-supercritical or advanced ultra-supercritical steam cycles are 5.1%, 5.0%, 5.2% or 13.0%, respectively. The biomass-fired chemical looping combustion power plants also show low energy efficiency penalties (<2.5%) compared to the reference biomass power plants without CO_2 capture. Our modelling results suggest that chemical looping combustion will remain an attractive carbon capture technology for solid fuel power plants, in a future when supercritical steam turbines become the norm.

Versatile Hollow ZSM-5 Nanoreactors Loaded with Tailorable Metal Catalysts for Selective Hydrogenation Reactions

Bowen Li, Kelvin Mingyao Kwok and Hua Chun Zeng, *ACS Applied Materials & Interfaces*

DOI: 10.1021/acsami.1c01916

Abstract: Zeolites are one of the most commonly used materials in the chemical industry, acting as catalysts or catalyst supports in different applications. Recently, the synthesis and functionalization of hollow zeolites have attracted many research interests, owing to the unique advantages of their hollow morphology. In the development of more sustainable processes, the hollow zeolites are often endowed with additional stability, selectivity, and activity. Herein, we present a stepwise synthetic protocol to prepare a range of complex hollow ZSM-5 catalysts with catalytic nanoparticles. Solid ZSM-5 crystals were first synthesized from Stöber silica spheres. This solid ZSM-5 sample was then loaded with transition metals via the impregnation method. A subsequent hollowing process was carried out in hydrothermal conditions in which hollow ZSM-5 crystals with confined transition metals inside were synthesized. More specifically, after the encapsulation of transition metals inside hollow ZSM-5, two different approaches have been further devised to allow the deposition of noble metals into the interior cavities or onto the exterior surfaces of the hollow ZSM-5. The deposition of Pt on the exterior surface was carried out by mixing the hollow ZSM-5 sample with presynthesized Pt nanoparticles. Loading of Pd in the interior was achieved by the galvanic replacement reaction between the Pd ions and embedded transition metals inside the hollow ZSM-5 sample. The catalytic performance of these reactor-like nanocatalysts has been evaluated with hydrogenation reactions in both liquid and gas phases, and their compositional and structural merits have been illustrated. For the hollow ZSM-5 sample with Pd loaded inside, liquid-phase selective hydrogenation of styrene over 4-vinylbiphenyl has been achieved with the ZSM-5 shell acting as a molecular sieve. The deposition of Pt on the exterior has improved the C_2–C_4 product yield when tested for the gas-phase CO_2 hydrogenation reaction.

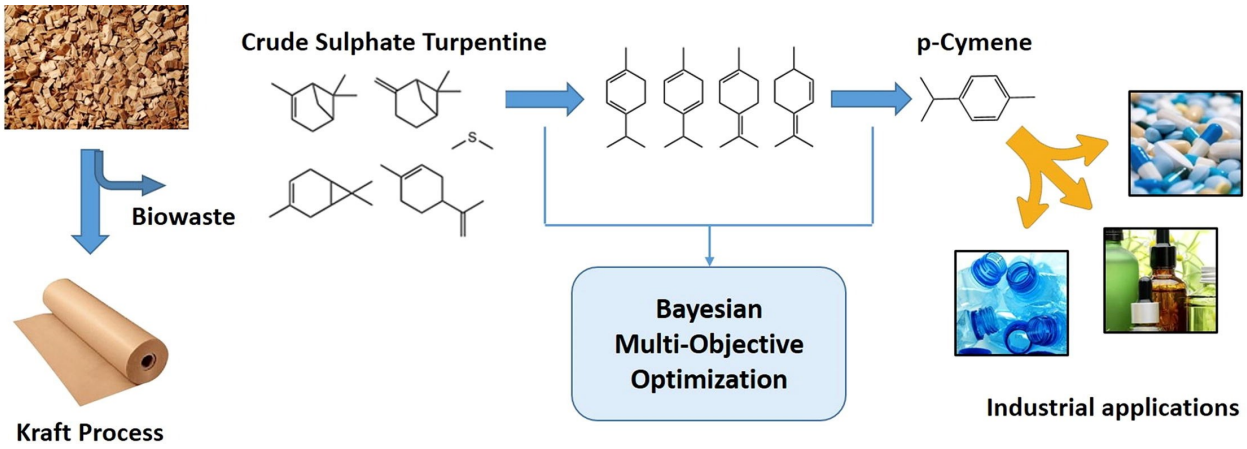


Multi-objective Bayesian optimisation of a two-step synthesis of p-cymene from crude sulphate turpentine

Perman Jorayev, Danilo Russo, Joshua D. Tibbetts, Artur M. Schweidtmann, Paul Deutsch, Steven D. Bull and Alexei A. Lapkin, *Chemical Engineering Science*

DOI: 10.1016/j.ces.2021.116938

Abstract: Production of functional molecules from renewable bio-feedstocks and bio-waste has the potential to significantly reduce the greenhouse gas emissions. However, the development of such processes commonly requires invention and scale-up of highly selective and robust chemistry for complex reaction networks in bio-waste mixtures. We demonstrate an approach to optimising a chemical route for multiple objectives starting from a mixture derived from bio-waste. We optimise the recently developed route from a mixture of waste terpenes to *p*-cymene. In the first reaction step it was not feasible to build a detailed kinetic model. A Bayesian multiple objectives optimisation algorithm TS-EMO was used to optimise the first two steps of reaction for maximum conversion and selectivity. The model suggests a set of very different conditions that result in simultaneous high values of the two outputs.

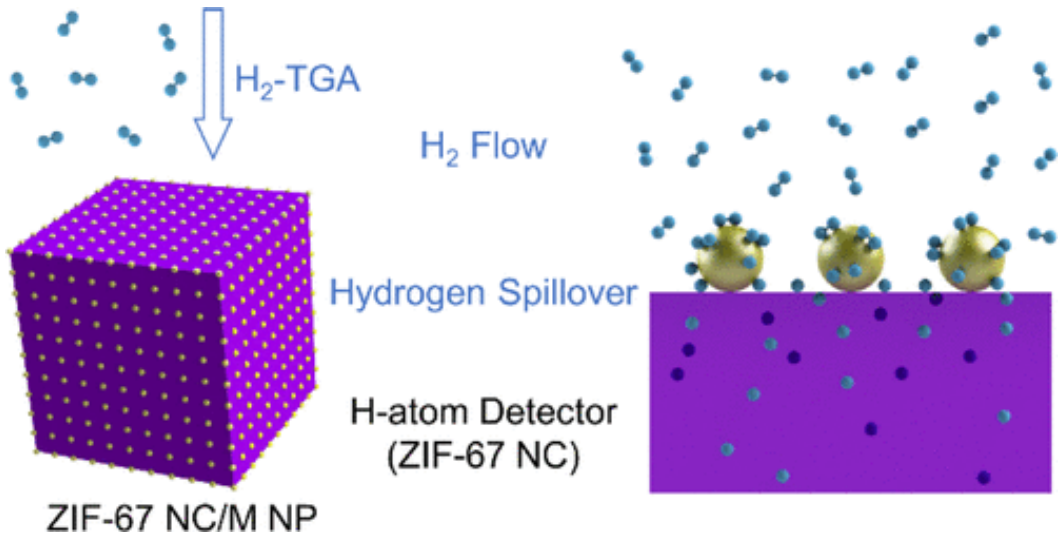


Pt, Ir, Ru, and Rh nanoparticles supported on ZIF-67 nanocubes for evaluation of hydrogen spillover ability of noble metals

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

DOI: 10.1021/acsanm.1c00871

Abstract: The hydrogen spillover phenomenon offers a great potential for enhanced performance in heterogeneous catalysis involving hydrogenation. Despite this, the current applications of hydrogen spillover are usually only for demonstrative purposes and the appropriate metal elements are often chosen by trial-and-error screening. Therefore, herein we systematically study and rigorously compare the hydrogen spillover abilities of various metal nanoparticles (NPs) supported on ZIF-67 nanocubes (NCs) by analyzing the hydrogenolysis of ZIF-67 at elevated temperatures. In this investigation, we make our ultimate efforts to ensure that all factors influencing the hydrogen spillover and thus hydrogenolysis are constant, which is crucial to objectively compare the hydrogen spillover abilities of the studied metals. Finally, a controllable synthetic procedure is devised to anchor presynthesized 2 nm metal NPs onto the exterior surfaces of ZIF-67 NCs. On the basis of this protocol, we have successfully determined the relative ability of hydrogen spillover for a series of 2 nm noble metal NPs: Pt > Ir > Ru > Rh. It is important to recognize that the ZIF-67 NCs serve effectively as a detector (or a receiver) of the dissociated hydrogen, which can measure the amount of hydrogen atoms produced during the hydrogen spillover. Therefore, the findings of this study could guide the rational choice of metal materials in other catalytic hydrogenation reaction systems. Moreover, the hydrogen spillover abilities of a wide variety of metal elements with defined particle sizes can also be determined via devising similar procedures in future investigations.

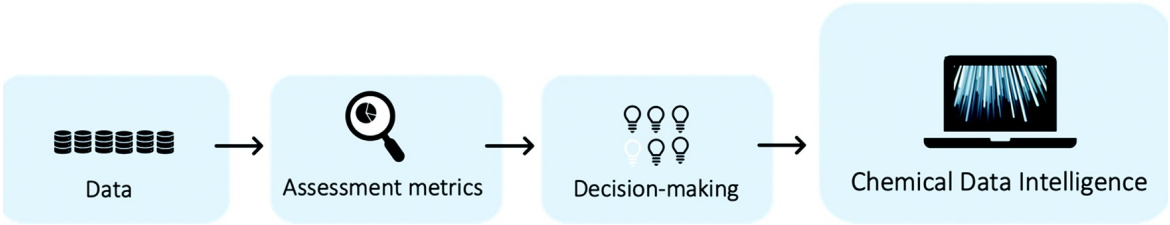


Chemical data intelligence for sustainable chemistry

Jana M. Weber, Zhen Guo, Chonghuan Zhang, Artur M. Schweidtmann, and Alexei A. Lapkin, *ACS Chemical Society Reviews*

DOI: 10.1039/D1CS00477H

Abstract: This study highlights new opportunities for optimal reaction route selection from large chemical databases brought about by the rapid digitalisation of chemical data. The chemical industry requires a transformation towards more sustainable practices, eliminating its dependencies on fossil fuels and limiting its impact on the environment. However, identifying more sustainable process alternatives is, at present, a cumbersome, manual, iterative process, based on chemical intuition and modelling. We give a perspective on methods for automated discovery and assessment of competitive sustainable reaction routes based on renewable or waste feedstocks. Three key areas of transition are outlined and reviewed based on their state-of-the-art as well as bottlenecks: (i) data, (ii) evaluation metrics, and (iii) decision-making. We elucidate their synergies and interfaces since only together these areas can bring about the most benefit. The field of chemical data intelligence offers the opportunity to identify the inherently more sustainable reaction pathways and to identify opportunities for a circular chemical economy. Our review shows that at present the field of data brings about most bottlenecks, such as data completion and data linkage, but also offers the principal opportunity for advancement.



Other activities and achievements

Dr Nicholas JOSE (Research Fellow, CARES) launched Accelerated Materials Ltd, a spin-off to commercialise the innovations made in reactor technology and machine learning for nanomaterials. Accelerated Materials has recently entered the final round of the Cambridge Enterprise Chris Abell Postdoc Business Plan Competition. The grand finale is in November. Accelerated Materials also placed runner-up in the Wolfson Enterprise Pitching competition this summer.

Dr Jose is currently working on a short film commissioned by the Cambridge Centre for Public Engagement on his work in CARES. This film will be animated by two artists (Suzie Hanna and Jude Montague) and screened in the Festival of Social Sciences in Cambridge on 18 November 2021.

Asst Prof Tej CHOKSI (Co-I, NTU) gave an invited talk titled "Tailoring Structure Sensitivity of Metal Nanoparticles on 2D and 3D supports: Insights from Data Driven Approaches" at the *American Chemical Society Fall 2021 Meeting* on 22nd August 2021.

Mr Adarsh ARUN (PhD student, CAM) gave a presentation titled "Towards integration of biowaste into chemical reaction networks: A case study of the waste landscape around Singapore" at the *3rd Sustainable Waste Management Conference AIChE 2021*, 4-6 August 2021.

Ms Lavie REHKI (in-kind PhD student, NTU) presented a poster titled "Quantifying bifunctional perturbations in catalytic descriptors on low-dimensional gold-support heterostructures" at the *SUNCAT Summer Institute, Stanford University* on 18th August 2021.

Ms Rekhi also gave a presentation titled "Breaking the Wall of Materials Space for CO_2 Utilisation" at the final round *Falling Walls Singapore* on 10th September 2021.

IRP 2

ELECTROSYNTHETIC PATHWAYS FOR ADVANCED LOW-CARBON CHEMICAL MANUFACTURING

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

IRP 2 Principal Investigators:

Dr Adrian FISHER
University of Cambridge

Professor WANG Xin
Nanyang Technological University

Professor LEE Jim Yang
National University of Singapore

OVERVIEW

The IRP2 research team have been continuing their activities in the area of advanced low-carbon chemical electrosynthesis methods, with a focus on speciality chemicals. The IRP2 team continue to employ both experimental and computational approaches to optimise synthetic reactor design and identify new configurations for electrosynthetic reactors.

Research by Dr Dai Chencheng and Dr Sun Libo has been exploring the development of heterogeneous molecular catalysts toward electrocatalytic CO_2 reduction and novel MEA structures for use in alkaline water electrolyser environments. These studies have focused on employing microfluidic devices and rapid flow cell technologies designed and then fabricated in the IRP 2 clean room facilities. Studies have focused on the efficient design, modelling and development of novel new gas diffusion electrodes (GDEs). Models developed by Ms Freyja Dagbjartsdóttir have been employed to investigate the performance characteristics and explore the incorporation of these novel approaches within the thin layer microengineered devices.

The work of Ms Dagbjartsdóttir, who is sponsored by our industrial collaboration with Syngenta, has continued to target new numerical approaches and models for the intelligent design of the electrosynthesis plants located in the IRP 2 laboratories. In her recent studies, Freyja has focused on innovative strategies of analysing complex AC voltammetry signals to allow this method to be more widely used and offer the opportunity for the technique to be employed in applications beyond catalyst investigation. Traditionally these signals have been analysed using fast Fourier transforms, but by developing the approaches we have been able to employ machine learning. By using machine learning with superior pattern recognition abilities, process parameters and system changes could be detected and/or extracted with much greater accuracy and speed than current systems. Pre-processing of signals before feeding them to a machine learning algorithm is essential when it comes to developing a fast and efficient algorithm.

The IRP 2 Singapore-based start-up company Datum Electronix (DEX), launched by Dr Kamal Elouarzaki and Prof. Adrian Fisher, has recently begun discussions with a company specialising in green ammonia production. We anticipate the use of the new DEX AI software packages recently brought to market will be employed in this important application of low carbon synthesis technologies.

IRP 2 outreach activities have continued during Covid-19, with a focus on online courses. We have been fortunate to gain funding from Cambridge Africa for a programme (INSPIRE) to develop a specialised outreach activity for children with a range of disabilities. We are currently developing a series of demonstrations of low carbon chemical and biochemical technologies for both virtual and live events.

Dr Adrian Fisher, PI
University of Cambridge

Update on work package 2.1

Advanced electrode architectures

Dr DAI Chencheng (Research Fellow, NTU) has been focusing mainly on alkaline water electrolyser with membrane electrode assembly (MEA-AWE) and MEA-AWE with formate cogeneration from methanol oxidation. The MEA-AWE work compares the oxygen evolution reaction (OER) performances of the commercial IrO_2 catalyst, previously reported NiFeOOH catalyst with the novel pretreated $SmCo/CoO_xH_y$ catalyst. As shown in Figure 2.1, the as-prepared $SmCo/CoO_xH_y$ catalyst shows the best overall performance.

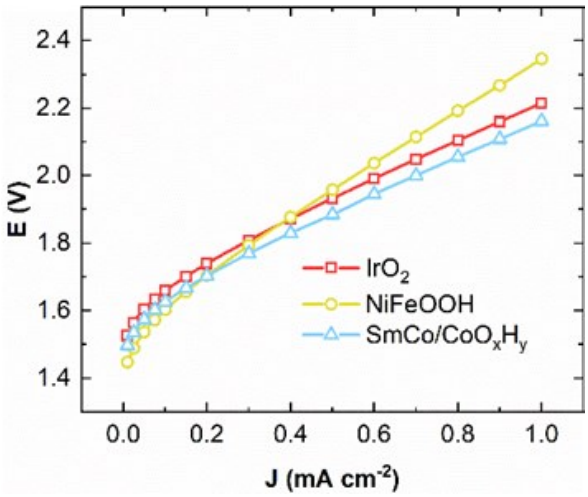


Figure 2.1: Polarisation curves of OER in 1 M KOH electrolyte on various catalysts in the MEA-AWEs.

The MEA-AWE with formate cogeneration from methanol oxidation shows impressive results. Due to the enhanced mass transfer by the flow convection in the flow channels in addition to the diffusion in typical stagnant cell, and the reduced system resistance as a result of the MEA, the current densities and the resulting formate yield rate increase dramatically while the Faradaic efficiency (FE) remains almost the same. For example, at the applied potential of ~1.6 V, the formate yield rate increases from ~0.023 to ~1.5 mol h^{-1} g_{oxide}^{-1}.

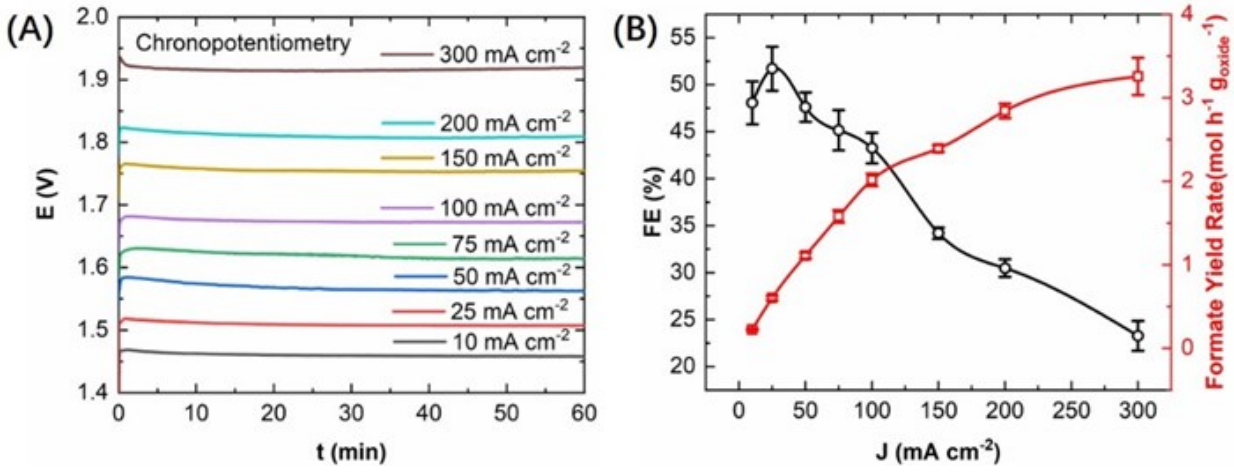


Figure 2.2: (A) Chronopotentiometry under various applied current densities, and (B) formate production from methanol oxidation, in an alkaline water electrolyser integrated with the membrane electrode assembly (MEA) flown with 1 M KOH & 1 M methanol electrolyte.

Dr DAI Chencheng

Update on work package 2.2

Co-generation and electrolytic synthesis reactor engineering

Dr SUN Libo (Research Fellow, NTU) reports that recent years have witnessed the development of heterogeneous molecular catalysts toward electrocatalytic CO_2 reduction. One effective strategy for such heterogenisation is to decorate molecular catalysts directly through axial coordination to functionalised carbon substrates and it will be interesting to elucidate the influence of such functional groups on the activity. Herein, it is demonstrated that among several kinds of N-, O-, and S-derived functional groups-decorated carbon nanotubes, those that are pyridine-based may play the role of a suitable linker and assist in achieving higher activity toward CO_2 reduction by a molecular catalyst. Density functional theory (DFT) calculations are also carried out to support the experimental results. This observation provides more insights into how a substrate can influence the intrinsic catalytic behaviour of molecular catalysts via functional groups without venturing into the complexities involved with the synthesis of novel ligands.

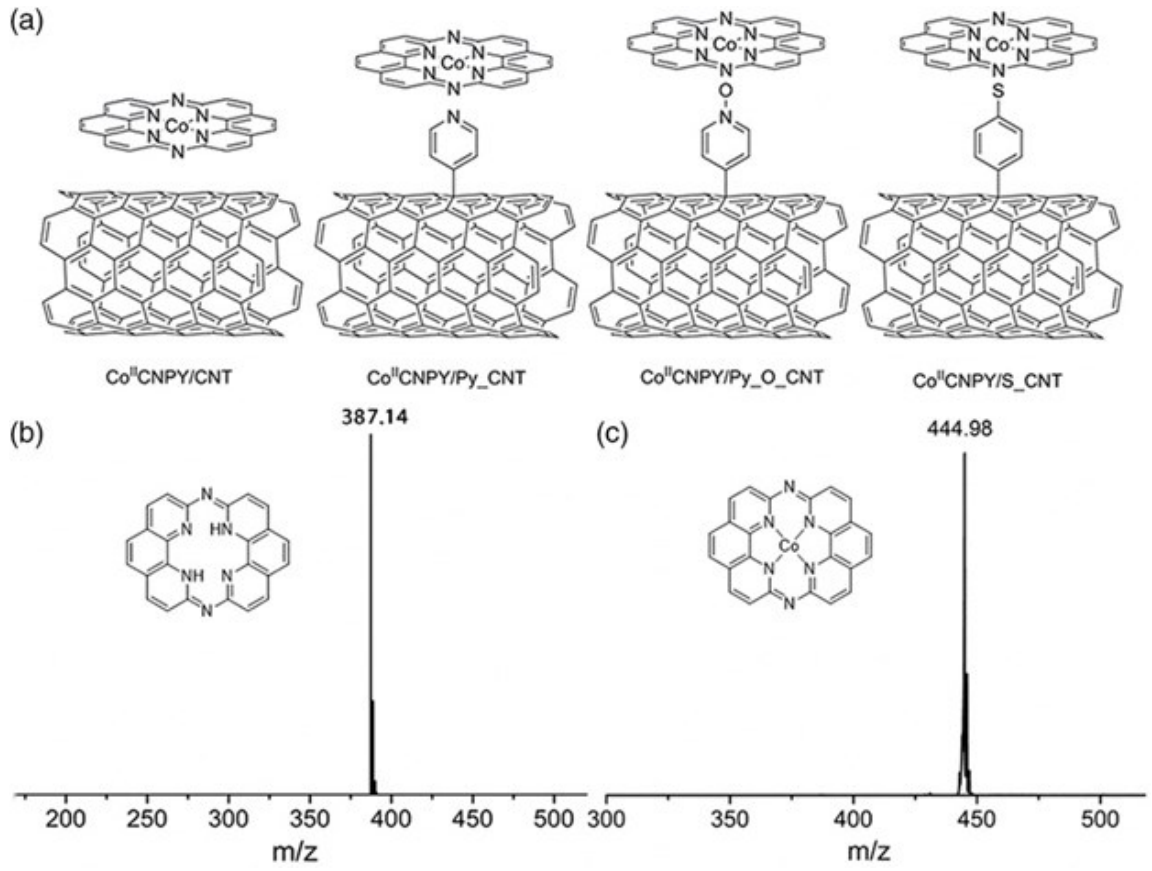


Figure 2.3: (a) The immobilisation of Co^{II}CNPY on to diverse substrates (Co^{II}CNPY/CNT, Co^{II}CNPY/Py_CNT, Co^{II}CNPY/Py_O_CNT, and Co^{II}CNPY/S_CNT). (b) High-resolution mass spectrum for H_2CNPY. (c) MALDI–TOF–MS for Co^{II}CNPY.

Dr SUN Libo

Update on work package 2.3

Micro-variable pressure and temperature electrosynthesis plant

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

Recently her focus has been on innovative ways of analysing large amplitude AC voltammetry signals to make the method more accessible to the user and open up the technique to applications beyond catalyst investigation. These signals are usually analysed using fast Fourier transforms, and the field is progressing into the use of machine learning. By using machine learning with superior pattern recognition abilities, process parameters and system changes could be detected and/or extracted with much greater accuracy and speed than current systems. Pre-processing of signals before feeding them to a machine learning algorithm is essential when it comes to developing a fast and efficient algorithm. This processing is currently done using fast Fourier transforms that do not have any time resolution in the frequency domain, so finding processing methods that yield information simultaneously in the time and frequency domains could move the development of the method further. The initial methods Ms Dagbjartsdóttir investigated, with the help of intern Ms Sophie HALL, are short-time Fourier transforms and continuous wavelet transforms.

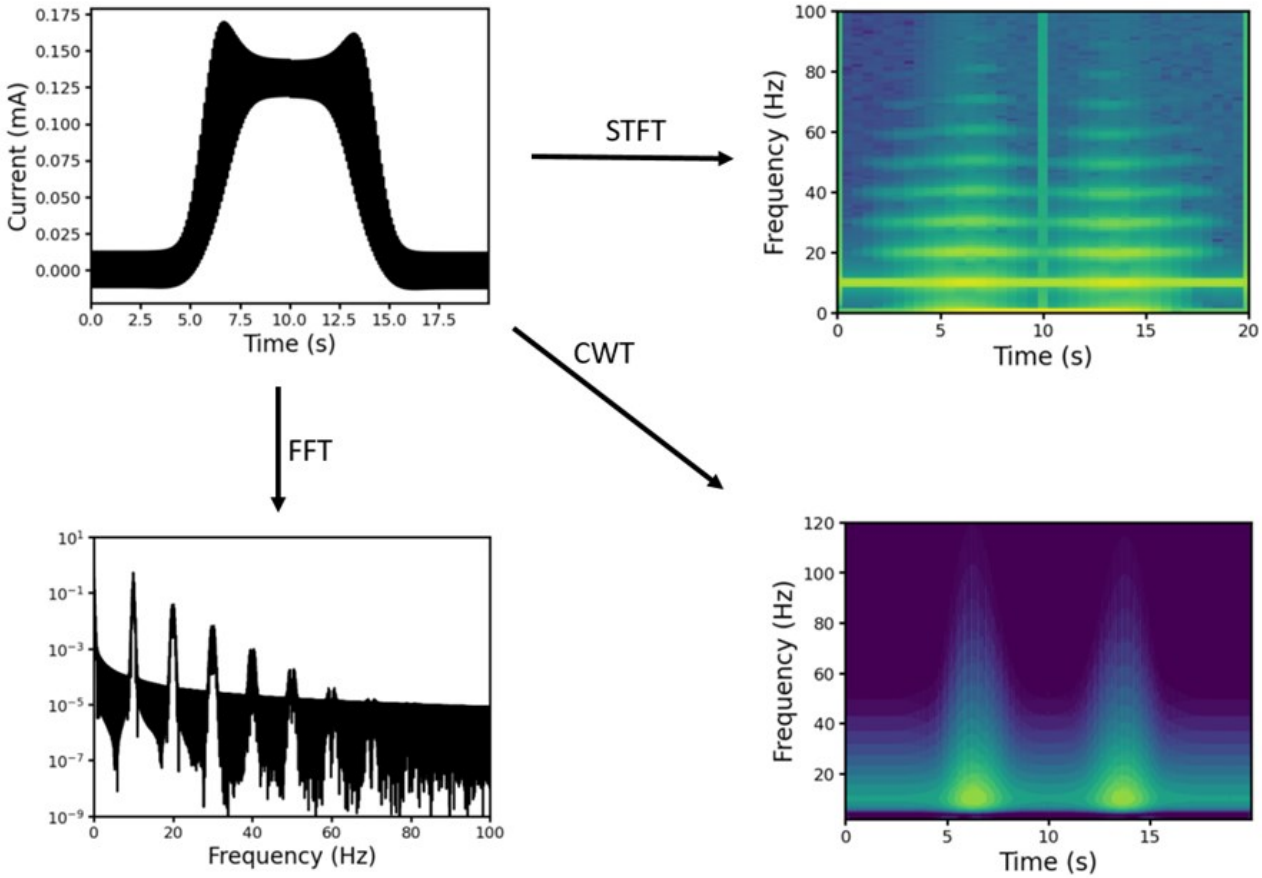


Figure 2.4: A raw large amplitude AC voltammetry signal (top left), same signal after fast Fourier transform (bottom left), same signal after short-time Fourier transform (top right), same signal after continuous wavelet transform (bottom right). The signal was produced using the MECSim software package. [http://www.garethkennedy.net/MECSim.html]

Ms Freyja DAGBJARTSDÓTTIR

Scientific output

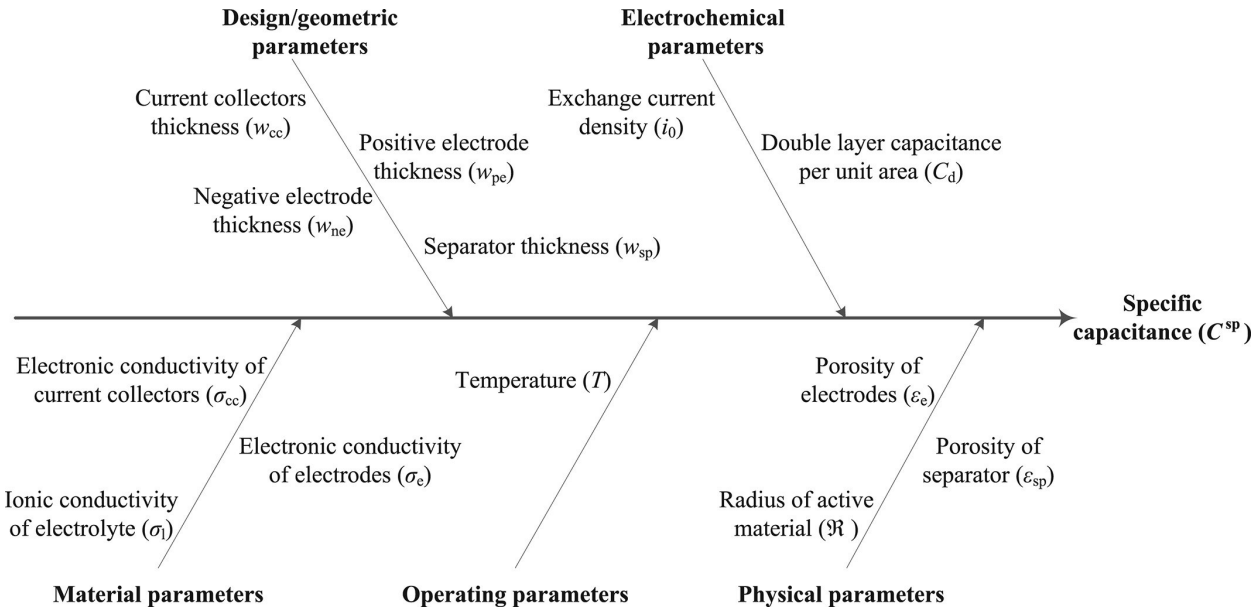
The following are the CREATE-acknowledged publications generated by IRP 2 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Monte Carlo-based sensitivity analysis of an electrochemical capacitor

Vishvak Kannan, Karthik Somasundaram, Adrian Fisher and Erik Birgersson, *International Journal of Energy Research*

DOI: 10.1002/er.6919

Abstract: The efficiency of electrolytic hydrogen production is limited by the slow reaction kinetics of oxygen evolution reaction (OER). Surface reconstructed ferromagnetic (FM) catalysts with spin pinning effect at the FM/oxyhydroxide interface could enhance the spin-dependent OER kinetics. However, in real-life applications electrolyzers are operated under elevated temperature, which may disrupt the spin orientations of FM catalysts and limit their performance. In this work, we prepared surface reconstructed $SmCo_5$/CoO_xH_y, which possesses polarized spins at the FM/oxyhydroxide interface that leads to excellent OER activity. These interfacial polarized spins could be further aligned through a magnetization process, which further enhanced the OER performance. Moreover, the operation temperature was elevated to mimic water electrolyzers' practical operation conditions. It is found that the OER activity enhancement of magnetized $SmCo_5$/CoO_xH_y catalyst can be preserved up to 60 ^oC.



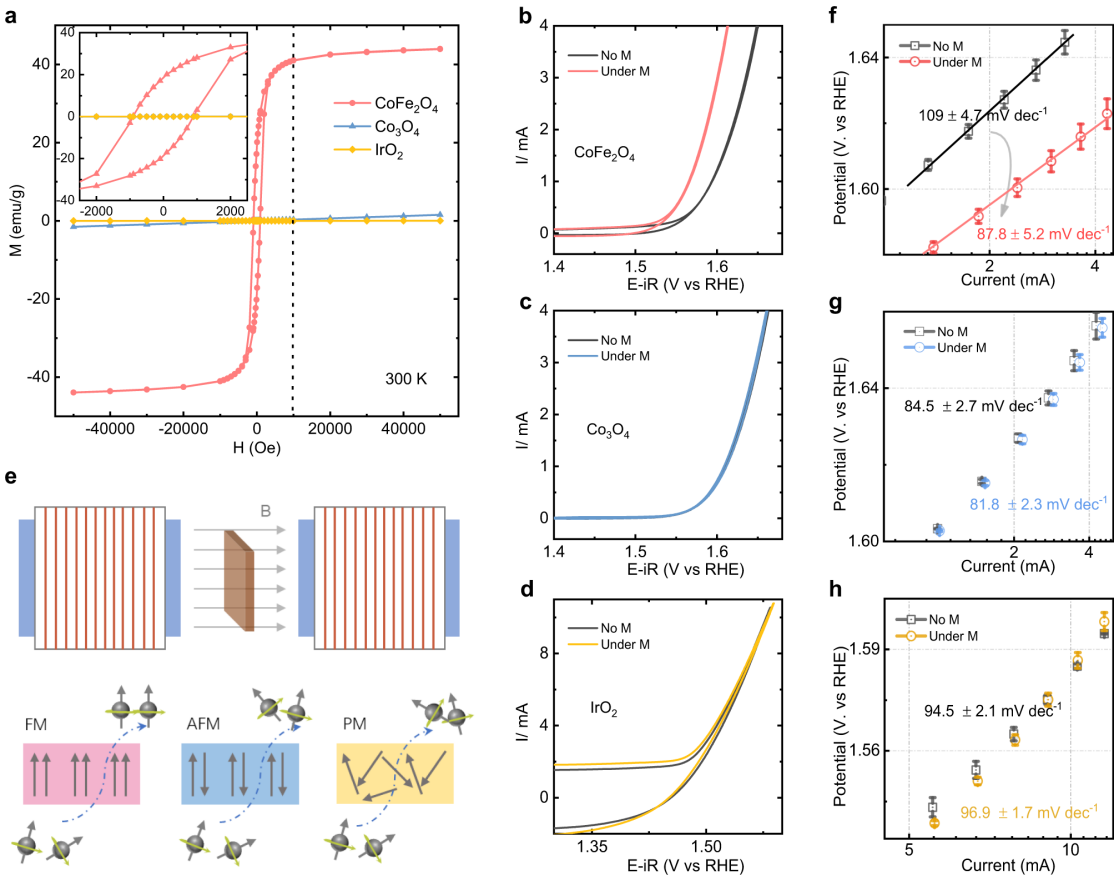
Cause and effect "fish-bone" diagram relating the stochastic input parameters with the response variable.

Spin-polarized oxygen evolution reaction under magnetic field

Ren, Xiao, Tianze Wu, Yuanmiao Sun, Yan Li, Guoyu Xian, Xianhu Liu, Chengmin Shen, Jose Gracia, Hong-Jun Gao, Haitao Yang and Zhichuan J. Xu, *Nature Communications*

DOI: 10.1038/s41467-021-22865-y

Abstract: The oxygen evolution reaction (OER) is the bottleneck that limits the energy efficiency of water-splitting. The process involves four electrons' transfer and the generation of triplet state O_2 from singlet state species (OH^- or H_2O). Recently, explicit spin selection was described as a possible way to promote OER in alkaline conditions, but the specific spin-polarized kinetics remains unclear. Here, we report that by using ferromagnetic ordered catalysts as the spin polarizer for spin selection under a constant magnetic field, the OER can be enhanced. However, it does not applicable to non-ferromagnetic catalysts. We found that the spin polarization occurs at the first electron transfer step in OER, where coherent spin exchange happens between the ferromagnetic catalyst and the adsorbed oxygen species with fast kinetics, under the principle of spin angular momentum conservation. In the next three electron transfer steps, as the adsorbed O species adopt fixed spin direction, the OER electrons need to follow the Hund rule and Pauling exclusion principle, thus to carry out spin polarization spontaneously and finally lead to the generation of triplet state O_2. Here, we showcase spin-polarized kinetics of oxygen evolution reaction, which gives references in the understanding and design of spin-dependent catalysts.



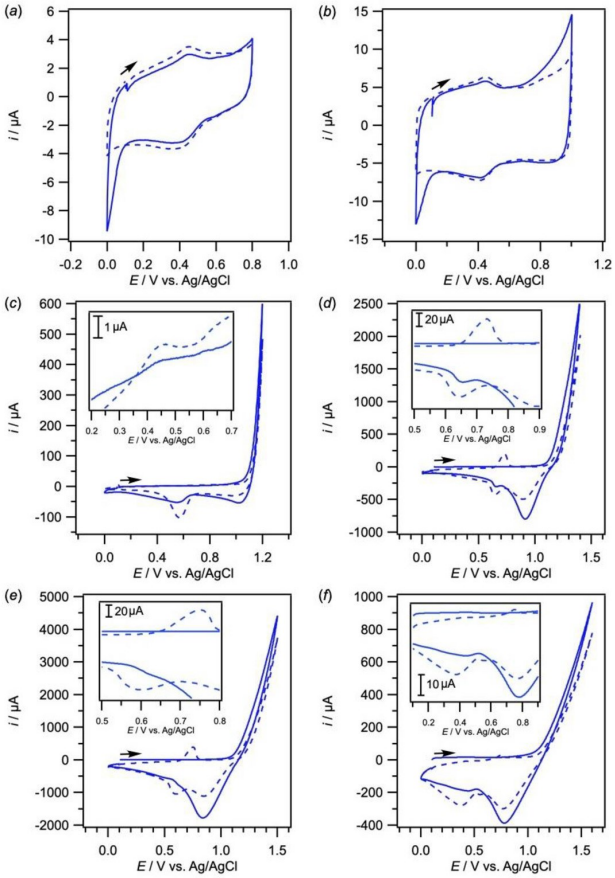
a *Magnetic hysteresis loops of $CoFe_2O_4$, Co_3O_4, and IrO_2 powders at room temperature (300 K) and the magnified graph inset in the top left of this panel. (Here, IrO_2 powder is a commercial catalyst (bulk, Premetek). Cyclic voltammetry (CV) of $CoFe_2O_4$* ***(b)****, Co_3O_4* ***(c)****, and IrO_2* ***(d)*** *catalysts at a scan rate of 10 mV/s in O_2-saturated 1 M KOH with and without a constant magnetic field (10,000 Oe).* ***e*** *The schematic of the generation of the polarized electron under a constant magnetic field. The Tafel plots of $CoFe_2O_4$,* ***(f)*** *Co_3O_4* ***(g)****, and IrO_2* ***(h)*** *catalysts with and without a constant magnetic field (10,000 Oe). The error bar represents three independent tests.*

Properties of electrochemically copolymerized aniline and melamine on functionalized multiwalled-carbon nanotube film electrodes

Guo Xiong Tham, Arnold Subrata, Adrian C. Fisher and Richard D. Webster, *Electrochemical Science Advances*

DOI: 10.1002/elsa.202100021

Abstract: The electrochemical properties of polymerized aniline (PANI) and polymerized melamine (PMEL) that were electrochemical copolymerized (PANIMEL) on a glassy carbon electrode (GCE) that had been coated with functionalized multiwalled carbon nanotubes (fMWCNT) to form a PANIMEL/fMWCNT/GCE film electrode were studied, with an aim toward electrochemical energy storage (EES). A number of factors, such as the choice of working electrode, electrolyte, switching potential, applied scan rate, and type of fMWCNTs, were initially investigated and evaluated during the individual electrochemical polymerization of aniline and melamine via successive potential cycling. The electrochemical copolymerisation of aniline and melamine was then studied with an ideal monomeric ratio of 1:3 that gave an optimal ratio of the voltammetric peak current heights with distinguishable redox peak potentials. Variable scan rate cyclic voltammetry (CV) of the electrosynthesized copolymer film electrode confirmed the dominance of the surface-confined electron transfer process at the electrode. The electrochemical stability of the copolymer film electrode was also assessed and revealed a limited cyclability of the daughter polymeric melamine, which was hypothesized to be due to an excessive nitrogen content combined with a low porosity that led to a poor ion intercalation-deintercalation mechanism. Electrochemical impedance spectroscopy (EIS) was performed to evaluate the electrochemical performance of the copolymerized film electrode with other control electrodes. The corresponding EIS results suggested that the copolymerized film electrode was electrochemically superior to the PMEL/fMWCNT/GCE film electrode but was inferior to the PANI/fMWCNT/GCE film electrode.



Cyclic voltrammetries for the electrochemical polymerization of 2 mM melamine on the surface of a 3-mm diameter fMWCNT/GCE film electrode in 1.0 M HCl solution at a scan rate of 20 mV/s for 20 cycles at 22 (±2)°C. Switching potentials: (a) 0.8 V, (b) 1.0 V, (c) 1.2 V, (d) 1.4 V, (e) 1.5 V and (f) 1.6 V. The solid (––) and dashed (- -) lines represent the 1st and 20th cycle of the potential cycling, respectively.

IRP 3

COMBUSTION FOR CLEANER FUELS AND BETTER CATALYSTS

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

IRP 3 Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor XU Rong
Nanyang Technological University

Assoc Professor YANG Wenming
National University of Singapore

OVERVIEW

In this reporting period, we have further strengthened the links between our molecular modelling efforts and our work on the J-Park Simulator (JPS, theworldavatar.com) in collaboration with IRP JPS. We are in the process of developing a knowledge-graph based framework for automatically fitting reactive force fields for applications in molecular dynamics simulations. For this purpose, we have created an ontology for relaxed potential energy surface scans, which semantically enriches our existing ontological representation of quantum chemical calculations. Building upon this, we have started to develop an autonomous software agent that is capable of finding and retrieving potential energy surface scan results from the knowledge graph and subsequently conducts a reactive force field calibration. In a related effort, we are also extending our ontological description of materials to include metal organic polyhedra, with the aim of predicting as yet unknown members of this exciting class of materials with desirable properties.

Highlights in the lab include our commissioning of a mechanism for the continuous collection of nanoparticles synthesised in a stagnation flame reactor. The mechanism improves both the yield and the reproducibility of the flame-made particles, which is an important step toward the continuous manufacture of large quantities of functional nanomaterials with precisely-tailored characteristics. A patent application has been filed and a journal publication is in progress. We have used the newly developed collection mechanism to flame-synthesise Pt-TiO_2 particles for their application in liquid organic hydrocarbon dehydrogenation catalysis. We then tested the performance of the catalyst in a batch reactor on the dehydrogenation of a promising candidate species for hydrogen storage.

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 ZONG Yichen (Research Fellow, NUS) has been leading the experimental research on future fuels for low emission energy utilisation. The research activities are conducted under the collaboration of NUS and University of Cambridge researchers. The research has continued over the last six months despite the Covid restrictions on working from the office and labs in Singapore. A research paper has been published in *Applied Energy*, which for the first time, reveals the performance of low blending ratios of a poly (oxymethylene) dimethyl ether (PODE) in diesel engines. A conference paper was accepted in the International Conference on Applied Energy focusing on the butanol additive. Dr Zong is also working on engine simulation with CMCL Innovations engineers and air quality monitoring with the collaboration of environmental scientists.

Clifford VO Chi Hung's (PhD student, NUS) main research interest lies in the biological fixation of CO_2 using the archaeon *M. maripaludis* S2. Unlike many other microbes which require organic feedstock, this microorganism can convert CO_2 into CH_4 without any organic carbon input. Mr Vo completed his research work in March 2021. During April – July 2021, he completed and submitted his thesis.

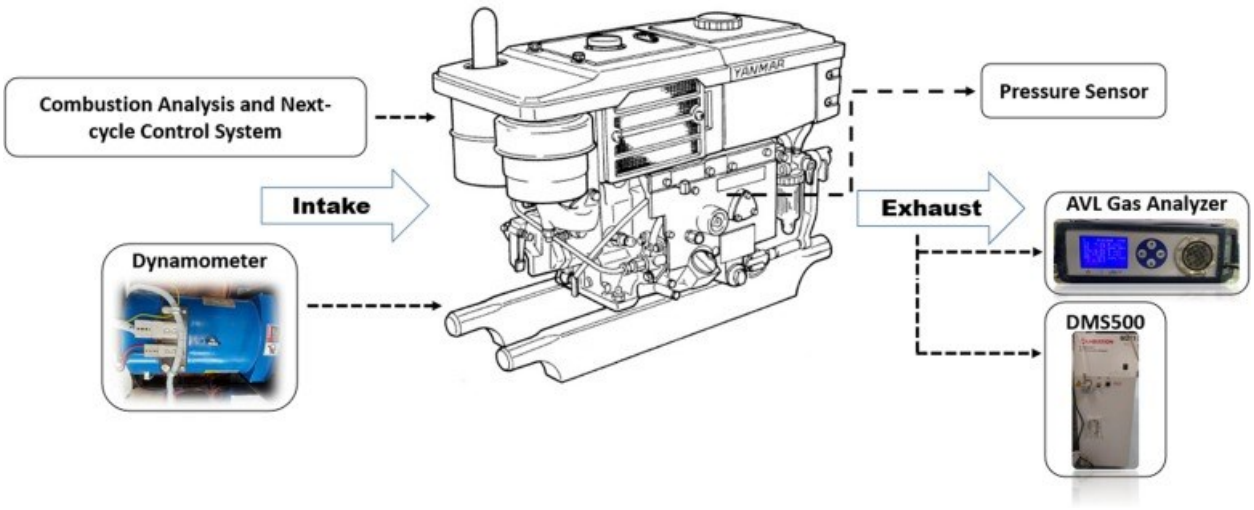


Figure 3.1: Schematic diagram of the experimental setup used to study the effect of diesel-PODE blends.

Dr ZONG Yichen

Mr TAN Yong Ren (PhD student, CAM) is currently investigating the effect of blending oxygenated fuels with Jet A2 fuel on soot formation under the standard ASTM smoke point lamp. The oxygenated fuels that have been chosen are dimethoxymethane (DMM), a poly(oxymethylene) dimethyl ether (PODE3), dimethyl carbonate (DMC) and ethanol (EtOH), which have been identified as promising candidates for sustainable aviation fuels (SAFs). The purpose of the investigation is to measure the sooting tendency of different oxygenated jet fuel A2 blends using the smoke point lamp and to measure, analyse and correlate the corresponding particle size distribution and soot volume fraction of the fuel mixtures. The analysis and correlations of the data will facilitate understanding of the implications of using different oxygenated fuels as SAFs, which could have practical value and relevance to the aviation industry. The sooting tendency of the fuel blends were reported as Oxygen Extended Sooting Index (OESI) from the measurement of smoke point of a smoke point lamp. This method has been used in the aviation industry to evaluate the quality of fuel blends. Figure 3.2 shows that there is a good correlation of the decrease in the OESI with the soot volume fraction and the average particle size of the fuel blends. This is outcome is significant because the aviation industry can use these correlations to support the evaluation of the capability of new SAF blends to meet the particulate matter standards that will be introduced by regulators in the future.

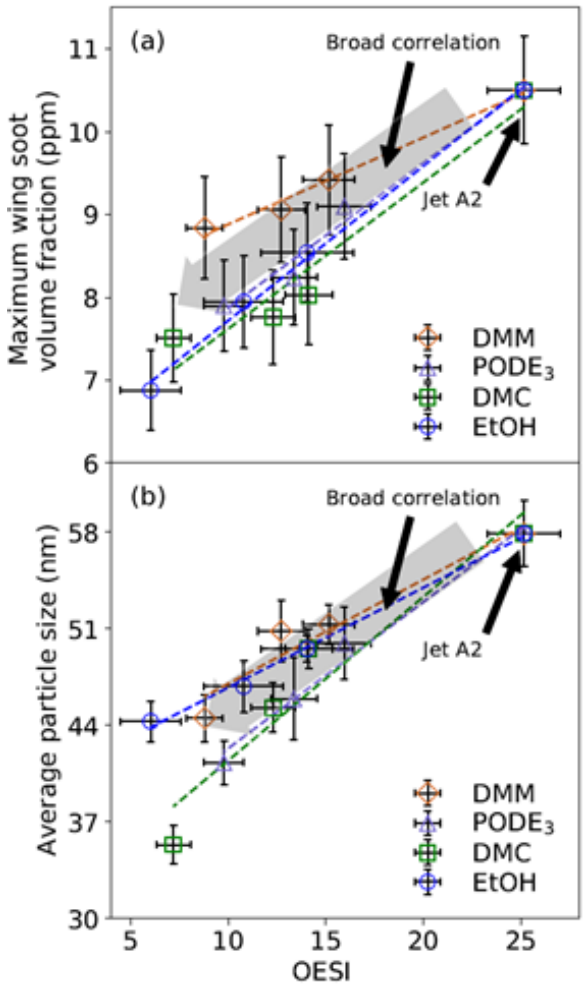


Figure 3.2: (a) The maximum soot volume fraction in the wing of the flame and (b) the average particle size at the tip of the flame versus OESI.

Mr TAN Yong Ren

Update on work package 3.2

Refinery, fuel and engine of the future — modelling

Chemical mechanisms, PAH chemistry, after-treatment

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

Recently, jointly with **Dr Jacob MARTIN (former Research Fellow, CARES)**, she published a paper on the evidence for a triplet π-diradical to fulfil many of the requirements for soot formation using quantum molecular dynamics simulations. The simulations showed that these compounds can provide a chain reaction, bond strongly enough for stability at flame temperature and react rapidly through physically stabilised internal rotors towards soot nanoparticles. Then, given significant concentrations of these species can be demonstrated in the flame, these species could provide a feasible pathway to soot formation.

Currently, Dr Pascazio is working on the development of a knowledge-graph based framework for the automated parameterisation of reactive force fields derived from relaxed potential energy surface (PES) scans. Jointly with **Dr Angiras MENON (Research Associate, CARES)** and CMCL Innovations, an ontological representation for PES scans, OntoPESScan, has been developed that allows for the semantic enrichment of quantum chemical calculations within the J-Park Simulator (JPS, theworldavatar.com). Following this, she is developing a software agent able to perform PES scan result retrieval and reactive force field calibration tasks.

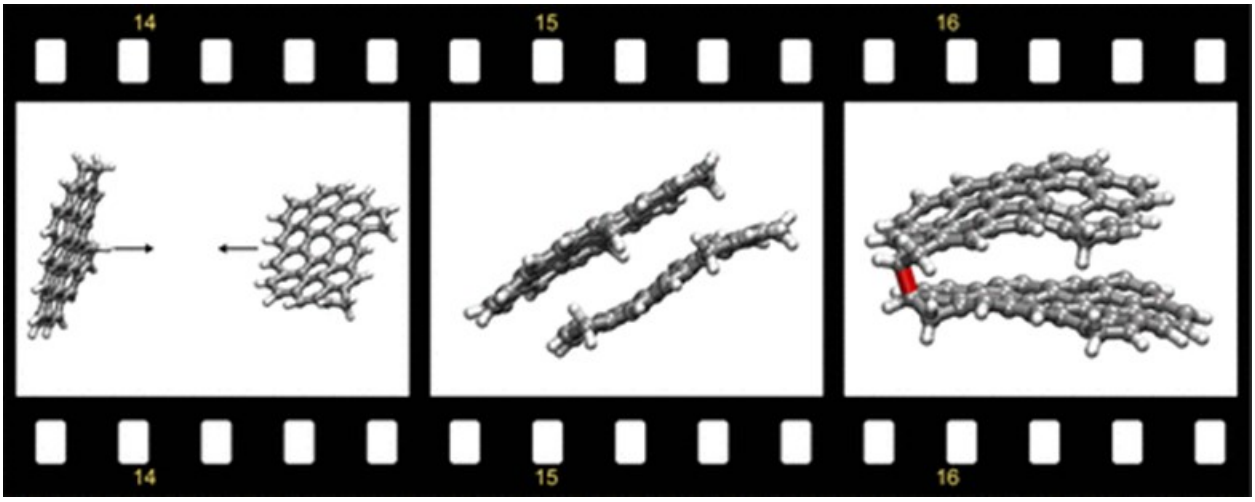


Figure 3.3: Aromatic penta-linked hydrocarbons in soot nanoparticle formation.

Dr Laura PASCAZIO

Dr Angiras MENON's (Research Associate, CAM) work focuses on the intersection of Semantic Web computational chemistry and cheminformatics. The main aim of this project is to aid in the development of ontologies and knowledge graphs that can help facilitate a variety of chemistry projects. A collaborative project between researchers at CARES, University of Cambridge and Sichuan University has been completed and published. This project involved the application of a variety of machine learning techniques to predict the power conversion efficiency of organic photovoltaics from just the SMILES identifier of the organic donor molecule. Whilst computational datasets derived from quantum chemistry calculations could be well predicted by a variety of the machine learning methods, the experimentally measured power conversion efficiencies could not be well predicted by the machine learning methods. This highlighted the need to improve the computational datasets to be more in line with experimental results and to have more standard experimental conditions for synthesising and testing organic solar cells to help machine learning and automated discovery methods.

Otherwise, development of an ontology for potential energy surfaces to help the automated fitting of force fields for molecular dynamics applications is underway in conjunction with **Dr Laura PASCAZIO's (Research Fellow, CAM)** and **Dr Daniel NURKOWSKI**. An ontology for the description and prediction of a novel class of materials, metal organic polyhedra (MOPs), is also in progress in conjunction with Dr Aleksandar KONDINSKI (Research Fellow, CAM) and Dr Nurkowski.

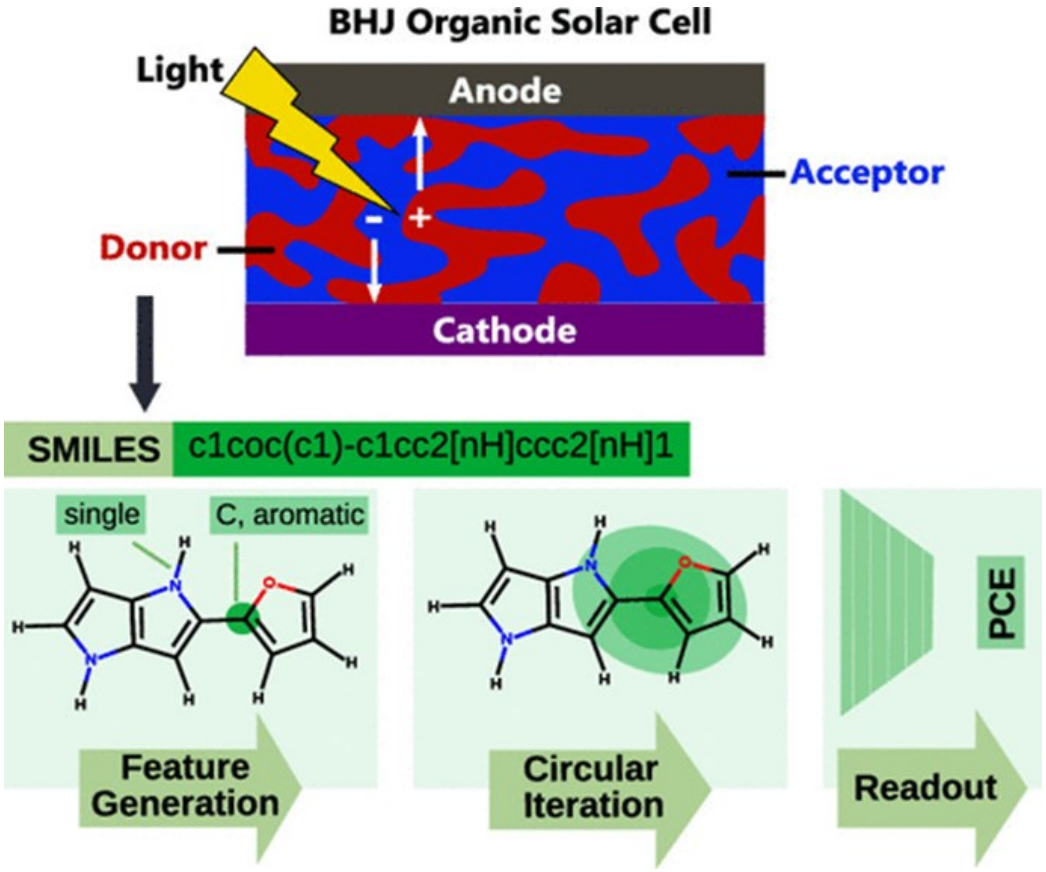


Figure 3.4: Graphical abstract for "Predicting Power Conversion Efficiency of Organic Photovoltaics: Models and Data Analysis". The figure shows the methodology utilised in the paper, by which the performance of an organic solar cell is predicted by taking the graph of the molecular structure of the donor molecule to generate fingerprints for the machine learning model to use. The performance is then predicted by the machine learning models for a variety of different molecular structures.

Dr Angiras MENON

Update on work package 3.3

Better, cheaper, cleaner nanostructures — experimental

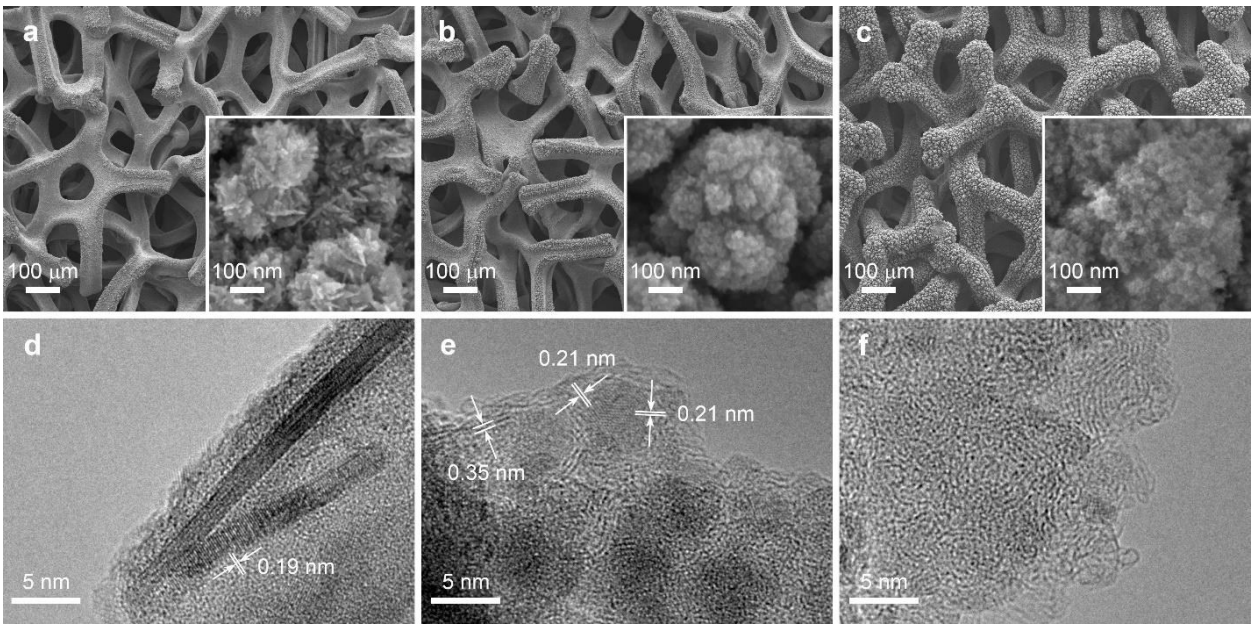
Flame synthesis of thin films of mixed metal oxide nanoparticles

Dr SHENG Yuan (Research Fellow, NTU) has identified a self-refreshing mechanism of NiFe phosphide-carbon composite films that leads to high durability in alkaline water oxidation. The constituent particles of the films detach gradually during electrolysis because of electrochemical removal of the carbon matrix. With optimised phosphide particle size and carbon content, such detachment was found to occur in a controlled manner and continuously refresh the catalytic surface, counteracting surface Fe leaching by the electrolyte to provide stable activity. A manuscript on this study has been prepared.

While working in the eCO_2EP project, Dr Sheng developed a bench-top system for the electrochemical reduction of CO_2 in a continuous flow process (see page 107 for further details). The system is built around a flow cell accepting 100 cm^2 gas diffusion electrodes and includes supporting apparatus for electrolyte recirculation and CO_2 flow/pressure control. Stable performance for >1.5 h has been achieved at a total current of 15 A with the Faradaic efficiency of C_2H_4 exceeding 30%. Test runs at 30 A have also been successful. The scale of the experiments is the largest of its kind in open literature.

Figure 3.5: (a-c) SEM and (d-f) TEM images of (a,d) NiFe-P-1.82, (b,d) NiFe-P-1.88, and (c,f) NiFe-P-1.94.

Dr SHENG Yuan



Update on work package 3.4

Better, cheaper, cleaner nanostructures — modelling

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

Dr Manoel MANUPUTTY (Research Fellow, NTU) has recently worked on developing a continuous particle collection mechanism to be used with the stagnation flame synthesis reactor. The mechanism improves the synthesis yields and the reproducibility of the flame-made materials, allowing their uses in catalytic processes which typically require a large amount of materials. The approach was part of a recent patent submission titled "Non-Stoichiometric Metal Oxides With Tunable Oxygen Vacancies" with **Mr WU Shuyang (former PhD student, NTU)**, **Prof. XU Rong (PI, NTU)**, and **Prof. Markus KRAFT (PI, CAM)**.

A separate journal manuscript is under preparation on the effect of the collection mechanism on oxygen vacancies and the particle characterisation using tandem thermal gravimetry analysis and mass spectrometry (TGA-MS). Further, Dr Manuputty has been using the newly developed particle collection mechanism to prepare flame-made Pt-TiO_2 samples to be used for liquid organic hydrocarbon (LOHC) dehydrogenation catalysts. A batch dehydrogenation reactor was set up for testing the catalyst performance on the dehydrogenation of perhydrodibenzyltoluene (H18-DBT), a promising LOHC candidate for hydrogen storage.

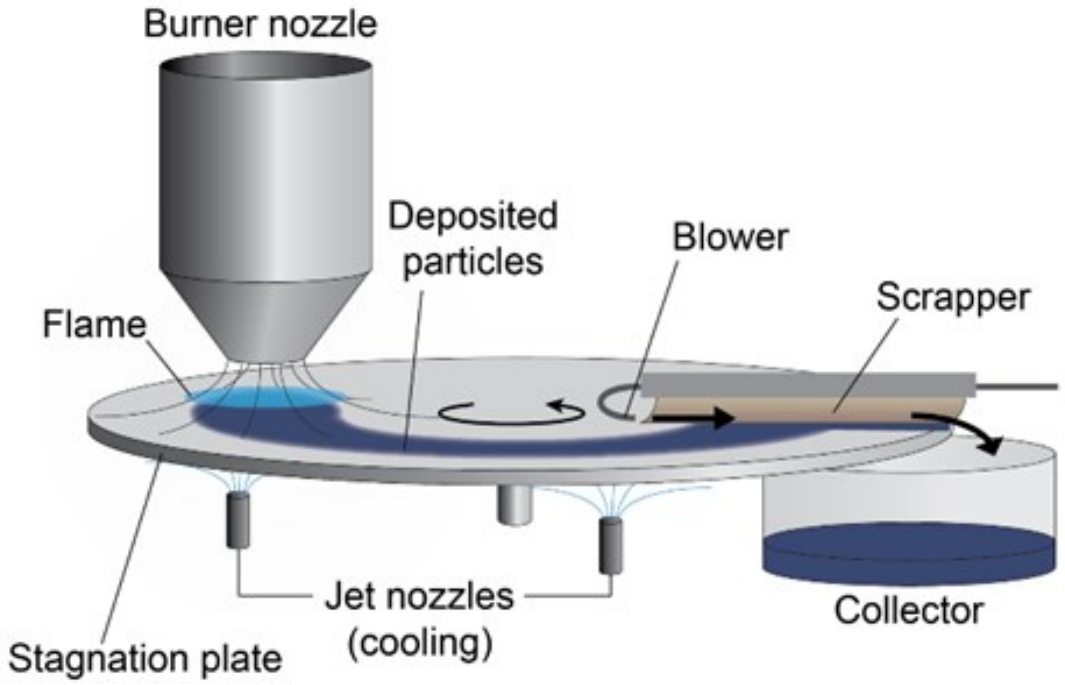


Figure 3.6: The schematic of the continuous particle collection (CPC) mechanism used with stagnation flame synthesis reactor.

Dr Manoel MANUPUTTY

Scientific output

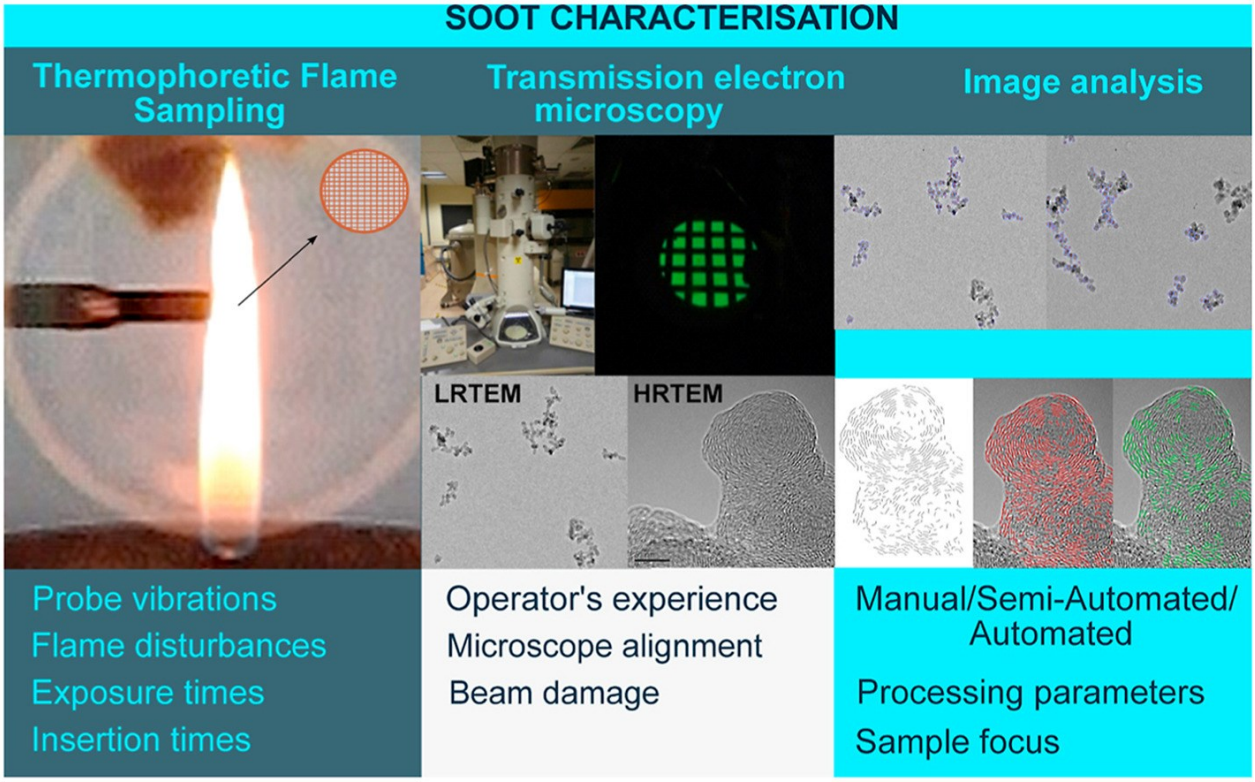
The following are the CREATE-acknowledged publications generated by IRP 3 during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

On the thermophoretic sampling and TEM-based characterisation of soot particles in flames

Maria Botero, Jethro Akroyd, Dongping Chen, Markus Kraft and John R. Agudelo, *Carbon*

DOI: 10.1016/j.carbon.2020.09.074

Abstract: Thermophoretic sampling and TEM imaging are common techniques used to characterise soot particles in flames. In this paper, we present a multi-scale evaluation of operating conditions and methodological aspects of these techniques, and based on our own experimental observations, show how these can influence the characterisation of the particles. Regarding the thermophoretic sampling of soot particles in flames, we evaluated the influence of exposure time, transit times, multiple-insertions, probe design and vibrations in the capture of representative samples, and present a series of recommendations. For the nano-structural characterisation of soot particles using HRTEM combined with fringe analysis we evaluated the influence of microscope alignment and image quality in the mapping of fringes and the calculation of metrics, concluding that the fringe lengths and interfringe spacing are very sensitive to particle focus. Also, the parameters used in the image transformation process are critical and require optimisation for different magnifications and microscopes. Finally, the effect of beam damage was studied, confirming a time of approximately 6 min during which both nascent and mature particles can be imaged without noticeable nanostructural damage. The use of lower microscope electron voltage can further minimise the impact of beam damage.

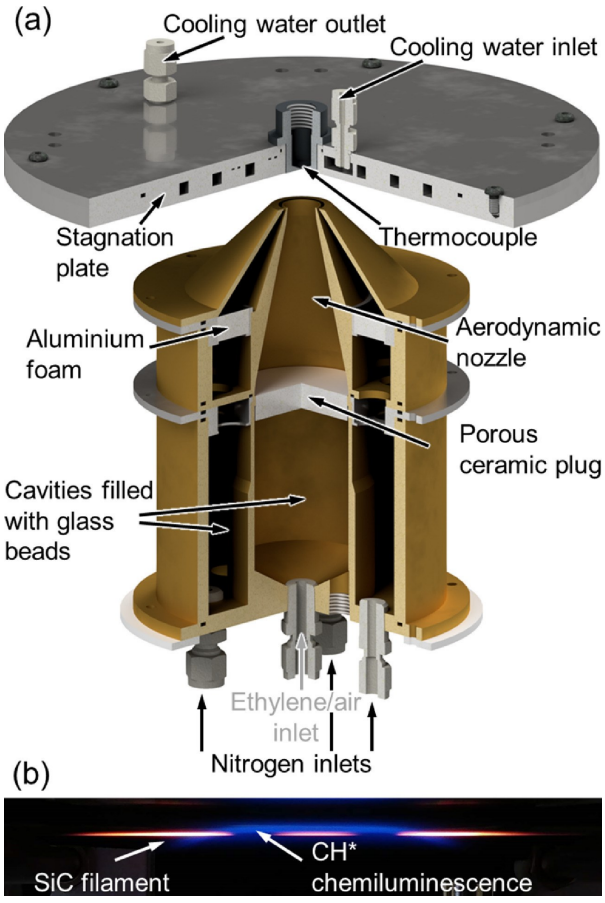


Temperature and CH* measurements and simulations of laminar premixed ethylene jet-wall stagnation flames

Jochen Dreyer, Eric Bringley, Manoel Manuputty, Jethro Akroyd and Markus Kraft, *Proceedings of the Combustion Institute*

DOI: 10.1016/j.proci.2020.06.106

Abstract: New experimental 2D measurements are reported to characterise the flame location, shape and temperature of laminar premixed ethylene jet-wall stagnation flames when the equivalence ratio, exit gas velocity and burner-plate separation distance are varied. Bandpass-filtered optical measurements of the CH* chemiluminescence were used to provide information about the shape and location of the flames. Thin filament pyrometry (TFP) using a 14 µm diameter SiC filament was used to make line measurements of the temperature to reconstruct the full 2D temperature field for the first time in premixed, jet-wall stagnation flames. The comparison of CH* measurements with (intrusive) and without (non-intrusive) the presence of the SiC filament showed that the filament resulted in minimal disturbance of the flame when the filament was placed downstream of the flame front. However, the flame was observed to attach to the filament, resulting in more significant disturbance, when it was placed upstream of the flame front. The flames were simulated using both 1D and 2D models. The 2D simulations were used to provide estimates of the velocity, kinematic viscosity and thermal conductivity required to calculate the gas temperature from the TFP data. The 1D simulations showed excellent agreement with the experimentally observed centreline quantities, but required the strain boundary condition to be fitted in order to match the experimentally observed flame location. The 2D simulations showed excellent agreement without the need for any fitting, and correctly predicted the flame shape, location and temperature as the experimental conditions were varied. A comparison of the set of simulated temperature-residence times along different streamlines showed relatively uniform distributions within each flame. However, the most uniform set of temperature-residence time distributions did not correlate with the flattest flame.

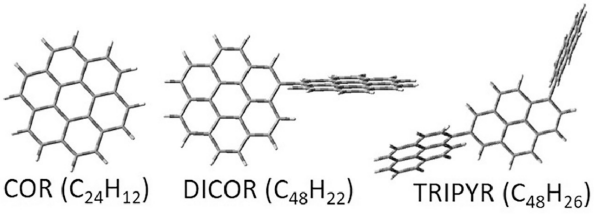


Atomic insights into the sintering process of polycyclic aromatic hydrocarbon clusters

Dingyu Hou, Qingzhao Chu, Dongping Chen, Laura Pascazio, Markus Kraft and Xiaoqing You,
Proceedings of the Combustion Institute

DOI: 10.1016/j.proci.2020.06.368

Abstract: In this work, we studied the sintering process of two homogeneous polycyclic aromatic hydrocarbon (PAH) clusters with diameters in the range of 3–6 nm using molecular dynamics (MD) simulations. The sintering process was quantified through monitoring the solvent accessible surface area (SASA) and the distance between the center of mass (COM) of the two PAH clusters. The effect of temperature and crosslinking level of PAH clusters on sintering was investigated. The results show that the sintering rate of two PAH clusters at a certain temperature T is largely dependent on the melting point (T_{MP}) of the PAH cluster. When T is higher than T_{MP}, the characteristic sintering time (τ_s) is around 10−2 ns and sintering is not affected by the crosslinking level as the PAH clusters are liquid-like. In contrast, when T is much lower than T_{MP}, the PAH clusters sinter rather slowly with $\tau_s > 5$ ns, and the sintering process is hindered by the crosslinks between PAH molecules within solid-like PAH clusters due to the enhanced steric effect.



Monomers of the PAH clusters.

Reactive localized π-radicals on rim-based pentagonal rings: Properties and concentration in flames

Angiras Menon, Jacob W. Martin, Gustavo Leon, Dingyu Hou, Laura Pascazio Xiaoqing You and Markus Kraft,
Proceedings of the Combustion Institute

DOI: 10.1016/j.proci.2020.07.042

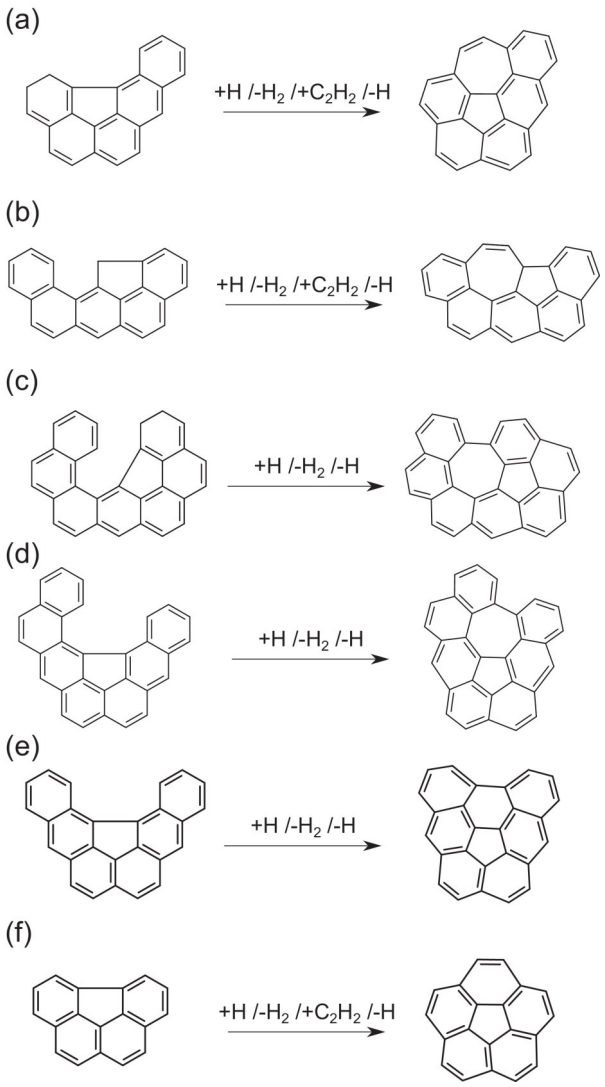
The impact of localized π-radicals on soot formation is explored by considering their electronic structure and computing their relative concentrations in flame conditions. Electronic structure calculations reveal that the presence of localized π-radicals on rim-based pentagonal rings is due to aromaticity. We further calculated a complete mechanism for the formation and elimination of the site from hydrogen additions and abstractions. A batch reactor with flame concentrations of $H^{\bullet}$ and H_2 was used to determine the time-dependent concentration of localized π-radicals. Low temperatures (< 1000 K) favored the fully saturated rim-based pentagonal ring. Soot nucleation temperatures (1000–1500 K) give way to unsaturated rim-based pentagons being favored. Localized π-radicals on rim-based pentagonal rings are found to be in higher concentration than the aryl-type σ-radical on the rim-based pentagon (mole fractions of 10−6–10−7) in below < 1500 K, consistent with recent experimental observations. Higher temperatures favor the σ-radical and the concentration of the localized π-radical on rim-based pentagons becomes negligible. A kinetic Monte Carlo treatment of multiple sites indicates that multiple localized π-radicals are possible on a single molecule. These results reveal the importance of localized π-radicals on rim-based pentagonal rings for PAH chemistry leading to formation of soot nanoparticles in flames involving aromatic rim-linked hydrocarbons (ARLH).

Kinetic Monte Carlo statistics of curvature integration by HACA growth and bay closure reactions for PAH growth in a counterflow diffusion flame

Gustavo Leon, Angiras Menon, Laura Pascazio, Eric Bringley, Jethro Akroyd and Markus Kraft, *Proceedings of the Combustion Institute*

DOI: 10.1016/j.proci.2020.06.352

Abstract: This paper uses a Kinetic Monte Carlo model that includes processes to integrate curvature due to the formation of five- and seven-member rings to simulate polycyclic aromatic hydrocarbons (PAHs) growing in lightly sooting ethylene and acetylene counterflow diffusion flames. The model includes new processes to form seven-member rings via hydrogen-abstraction-acetylene-addition and bay closure reactions on sites containing partially embedded five-member rings. The model additionally includes bay closure and HACA bay capping reactions for the integration of five-member rings. The mass spectra of PAHs predicted by the model are assessed against experimental data, and the distribution of embedded five-member rings and seven-member rings is studied as a function of spatial location, molecule size and frequency of events sampled in the simulation. The simulations show that the formation of seven-member rings and the embedding of five-member rings is a competitive process. Both types of rings are observed more frequently as the simulation proceeds from the fuel outlet towards the stagnation plane. Approximately 15% of the events that integrate curvature resulted in the formation of a seven-member ring coupled to an embedded five-member ring, and the remaining 85% of events embedded five-member rings via the formation of six-member rings. The proportion of PAHs containing embedded five-member rings and/or seven-member rings is observed to be a function of PAH size, passing through a maximum for PAHs containing 15–20 six-member rings. However, the proportion of PAHs containing both types of ring increases with PAH size, where upwards of 10% of PAHs containing at least one five-member ring and 15 or more six-member rings also contain a seven-member ring.



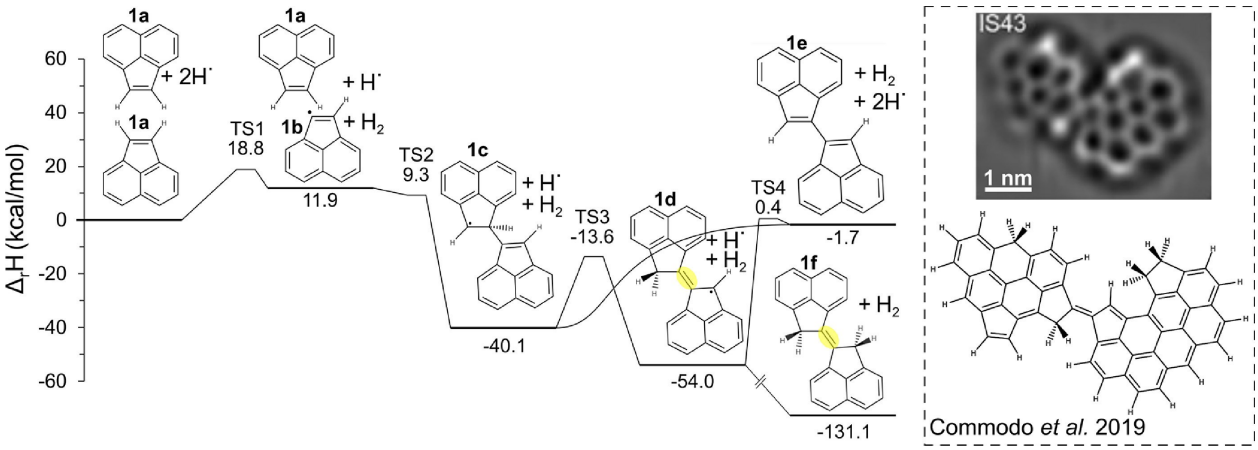
Curvature integration jump processes.

Aromatic penta-linked hydrocarbons in soot nanoparticle formation

Laura Pascazio, Jacob W. Martin, Angiras Menon, Dingyu Hou, Xiaoqing You and Markus Kraft,
Proceedings of the Combustion Institute

DOI: 10.1016/j.proci.2020.09.029

Abstract: A new crosslinking reaction between two pentagonal rings around the periphery of planar pericondensed aromatic molecules is proposed and its impact on soot nanoparticle formation explored. The reaction mechanism was computed, using density functional theory, between an aryl-type σ-radical on a rim-based pentagonal ring attacking another rim-based pentagonal ring. A hydrogen migration allowed for the formation of a double bond forming a planar aromatic penta-linked hydrocarbon (APLH) complex, recently experimentally observed. The clustering of this planar species is compared with a pericondensed polyaromatic hydrocarbon (PCAH) and an aromatic aryl-linked hydrocarbon (AALH) using molecular dynamics and metadynamics. Similar clustering is found for the investigated species compared with a pericondensed structure of similar mass indicating enhanced physical interactions after forming the crosslink. Finally, a further crosslink is possible between the unsaturated pentagonal ring sites forming an aromatic rim-linked hydrocarbon (ARLH) complex of considerable stability. This was confirmed by simulating the stable molecular dynamics of such a complex with on-the-fly quantum forces from a quantum semi-empirical method, revealing possible reactions under flame conditions that might play a role in soot nucleation.



Potential energy diagram for the formation of a planar crosslinked aromatic molecule with a double bond (highlighted) connecting rim-based pentagonal rings of the aromatic subunits at 0 K. A similar species observed experimentally has been also reported for comparison:

Commodo, Mario, Katharina Kaiser, Gianluigi De Falco, Patrizia Minutolo, Fabian Schulz, Andrea D'Anna, and Leo Gross. 2019. 'On the Early Stages of Soot Formation: Molecular Structure Elucidation by High-Resolution Atomic Force Microscopy'. Combustion and Flame *205 (July): 154–64. https://doi.org/10.1016/j.combustflame.2019.03.042. Used with permission CC BY-NC-ND 4.0.*

Other activities and achievements

Dr ZONG Yichen (Research Fellow, CARES) has had a paper titled "Evaluating the effect of n-butanol additive in a common-rail diesel engine" accepted for the *International Conference on Applied Energy 2021*, 29 November – 2 December 2021. Other authors on the paper are Qiren Zhu, Wenming Yang and Markus Kraft.

The NUS Engine Lab received the NUS Green Lab Award in June for its continuous improvement in minimising the environmental impact of its operations.

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

IRP 4

BETTER, CLEANER HEAT USAGE

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

IRP 4 Principal Investigators:

Professor Epaminondas MASTORAKOS
University of Cambridge

Professor Alessandro ROMAGNOLI
Nanyang Technological University

Professor LEE Poh Seng
National University of Singapore

OVERVIEW

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

During the reporting period, some personnel left and so some work packages made only little progress until new researchers could be employed. The engine modelling work advanced well and resulted in a paper in one of the top conferences in the field, organised by SAE. In addition, we saw the culmination of years of effort building the particulate-matter sensors on the CARES drone, with a field trip at a port with passenger ferries. The data are very useful and demonstrate the pattern of the pollutant-carrying plume close to ships, which is important information for modelling pollutant dispersion from ships in ports and coastal areas.

Professor Epaminondas Mastorakos, PI
University of Cambridge

Update on work package 4.1

Engine combustion — best fuel, best operating condition

In the previous report, the advanced simulations of a heavy-duty MTU396 research engine using STARCD + CMC were presented, showing excellent agreement with the measurement data in terms of pressure trace. The soot and NOx trends for variations in the start of injection (SOI) are shown in Figure 4.1. Soot mass fraction was evaluated using the 2-equation soot model. (SOI1 case = SOI at -6° CA; reference case = SOI at -10° CA; SOI2 case = SOI at -14° CA).

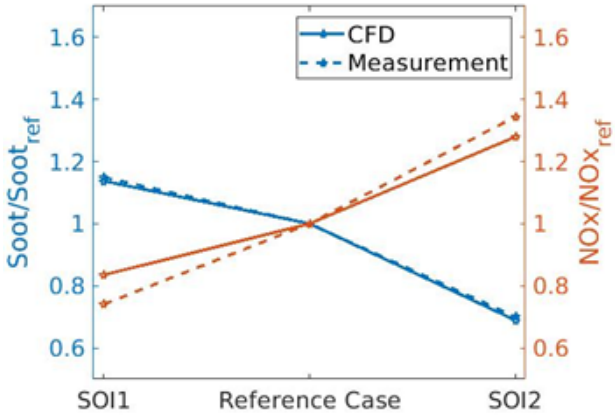


Figure 4.1: Soot and NOx trends for the SOI variation cases. The soot and NOx mass fractions are normalised by the corresponding reference case value (SOI = -10° CA) for experiments (dotted lines) and simulations (solid lines).

Dr Shrey TRIVEDI (Research Associate, CAM) has developed a postprocessing tool based on the Incompletely Stirred Reactor (ISR) concept to estimate soot mass fraction at a fraction of the computational cost. It takes the core-volume averaged frozen flow field from an existing CFD solution and is capable of applying more detailed chemistry and soot-models. Results for soot mass fraction using the 2-equation model with C_7H_{16} chemistry as well as more advanced Napoli sectional soot model (NAPS model) [1] coupled with Kerosene based HyChem mechanism [2] are presented in Figure 4.2. These are also compared with the CFD+CMC results.

The NAPS model can also be used to predict the soot particle size distribution (PSD) and the results are shown in Figure 4.3 and are compared with the measurement data. For the ISR simulations, the PSDs are evaluated at 40 ° CA after start of injection (aSOI). The overprediction shown by the ISR results both for soot mass fraction and for the PSDs is under investigation but is likely because of underrepresentation of mixing in a core-volume averaged data entered into ISR. More improved mixing models and using a network of ISRs (ISRN method) [3] will improve these results.

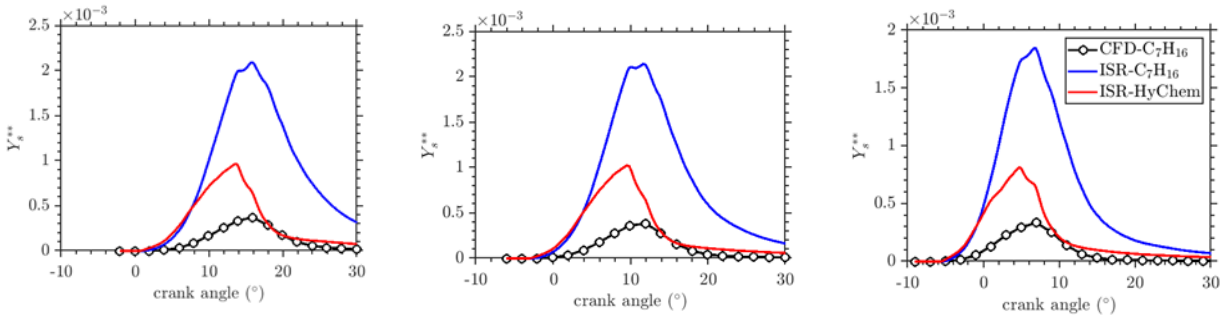
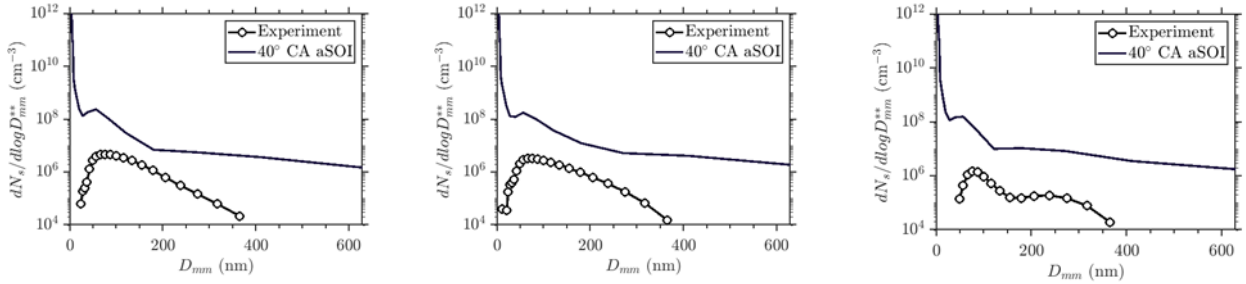


Figure 4.2: Soot mass fraction obtained from postprocessing using the ISR strategy and compared with the CFD results.

Furthermore, an improved LIBSC CMC version is also being implemented into STAR-CD. This version allows us to use more advanced chemical mechanisms, which further allow us to use improved soot models through CFD+CMC as well.



SOI1 Reference case SOI2

Figure 4.3: Soot particle size distribution (PSD) obtained from postprocessing using the ISR strategy and compared with the measurement data.

Dr Shrey TRIVEDI

[1] H. Wang, R. Xu, K. Wang, C. T. Bowman, R. K. Hanson, D. F. Davidson, K. Brezinsky and F. N. Egolfopoulos. A physics-based approach to modeling real-fuel combustion chemistry - I. Evidence from experiments,and thermodynamic, chemical kinetic and statistical considerations. Combustion and Flame,193:502–519, July 2018.

[2] S. Gkantonas, M. Sirignano, A. Giusti, A. D'Anna, and E. Mastorakos. Comprehensive soot particle size distribution modelling of a model rich-quench-lean burner. Fuel, 270:117483, June 2020.

[3] S. Gkantonas, J. M. Foale, A. Giusti, and E. Mastorakos. Soot Emission Simulations of a Single Sector Model Combustor Using Incompletely Stirred Reactor Network Modeling. Journal of Engineering for Gas Turbines and Power, 142(10):101007, September 2020.

Update on work package 4.2

Closed power cycles—selection and analysis

Update on work package 4.3

High-efficiency heat exchanger

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

Update on work package 4.4

Process system model for the J-Park Simulator

Dr Molly HAUGEN, Dr Savvas GKANTONAS, Dr Ingrid El HELOU, Mr Rohit PATHANIA, Dr Adam BOIES and **Prof. Epaminondas MASTORAKOS** (all University of Cambridge) have contributed to acquiring the required equipment necessary for the field campaign in Greece, as well as making custom adjustments to ensure its success. In Cambridge, the team developed and manufactured a platform for all particle sensors to be attached under the drone. This included distributing the sensors' weight below the drone, eliminating vibration and swaying effects, and a failsafe mechanism that would keep all sensors attached to the drone. It is pictured in Figure 4.4 with the particle sensors attached to the drone at the pier take-off location in Rafina, Greece.

The drone measurements were successful in measuring plumes from ferries sitting idle in the port as well as ferries that were departing and arriving. Figure 4.5 shows the drone-based measurement locations. There were three sensors on the ground on the pier at approximately personal exposure level (~1.5 m, red dot) and identical sensors on the drone, which was flown between the pier and the ferries (purple and yellow Xs). The drone location also had a vertical element, which is noted in the sub-figures, going from 5 m up to 40 m and back down. The probe on the drone was pointed in the direction of the wind and the drone was positioned directly downwind of the ferries. Figure 4.6 shows the view from the drone. The three sub-figures in Figure 4.5 are the three sensors that were on the drone and at the pier; an AethLab Aethalometer that measures black carbon, a TSI P-Trak that measures the number of particles in a given sample volume and a Naneos Partector that determines Lung Deposited Surface Area (LDSA).

Figure 4.4: Drone with instrument platform ready for take-off.

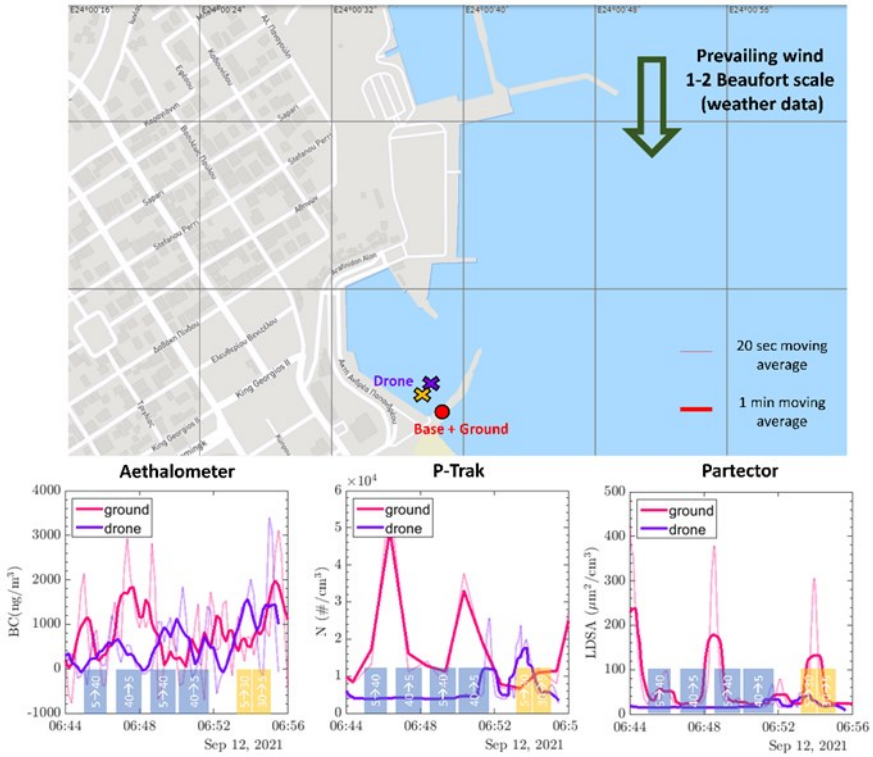


Figure 4.5: Preliminary data from three particle sensors on the drone at locations within the port (purple lines) compared to data from sensors on the ground (pink lines).

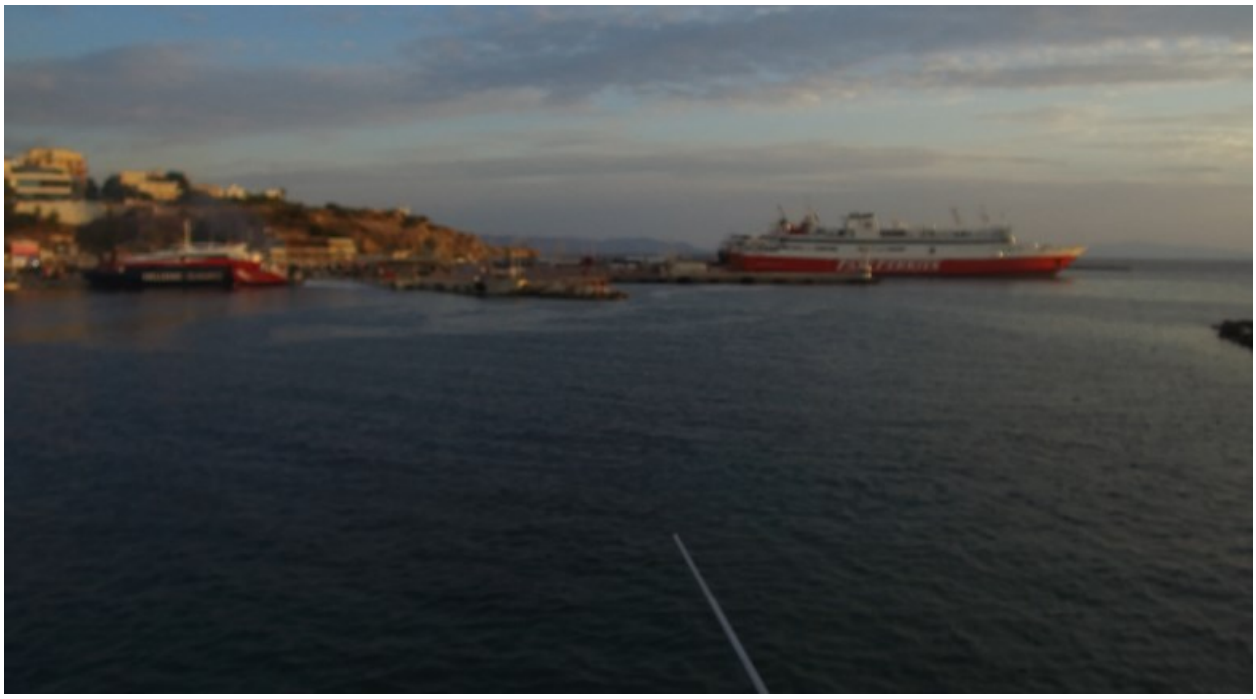


Figure 4.6: Drone view during sampling.

The data presented here requires post-processing to fully understand the relevance as there are many variables that must be considered to accurately interpret the raw data. These variables include wind speed, wind direction, ferry location, ferry speed, exhaust plume dispersion dynamics, drone location, drone speed, instrument delay times and dilution rates. Therefore, Figure 4.5 shows the preliminary results for the drone component of this campaign. Additionally, and importantly, this portion of the field work highlighted a number of improvements that must be made and reported for further work in this area. By conducting this field campaign, the group will be able to contribute to a more robust at-sea measurement technique useful to the drone community, emission modelling communities and the public health sector.

The second part of the campaign focused on land-based measurements to explore the dispersion of ferry plumes within the port as a whole. Figure 4.7 is an example of one day (8th September, 2021) where multiple particle sensors were dispersed around the port, with the docked ferry locations shown. During the time of sampling, all ferries departed the port (indicated by the yellow and blue vertical bars within each sub-figure). With this data, we will be able to validate and add to plume dispersion models for ferry exhaust plumes. The different sensors measure a different characteristic of the particles, such as LDSA, black carbon and particle number. The data collected in the land-based measurements will be useful to understand how plumes disperse, as well as how the particle characteristics change as the plume ages.

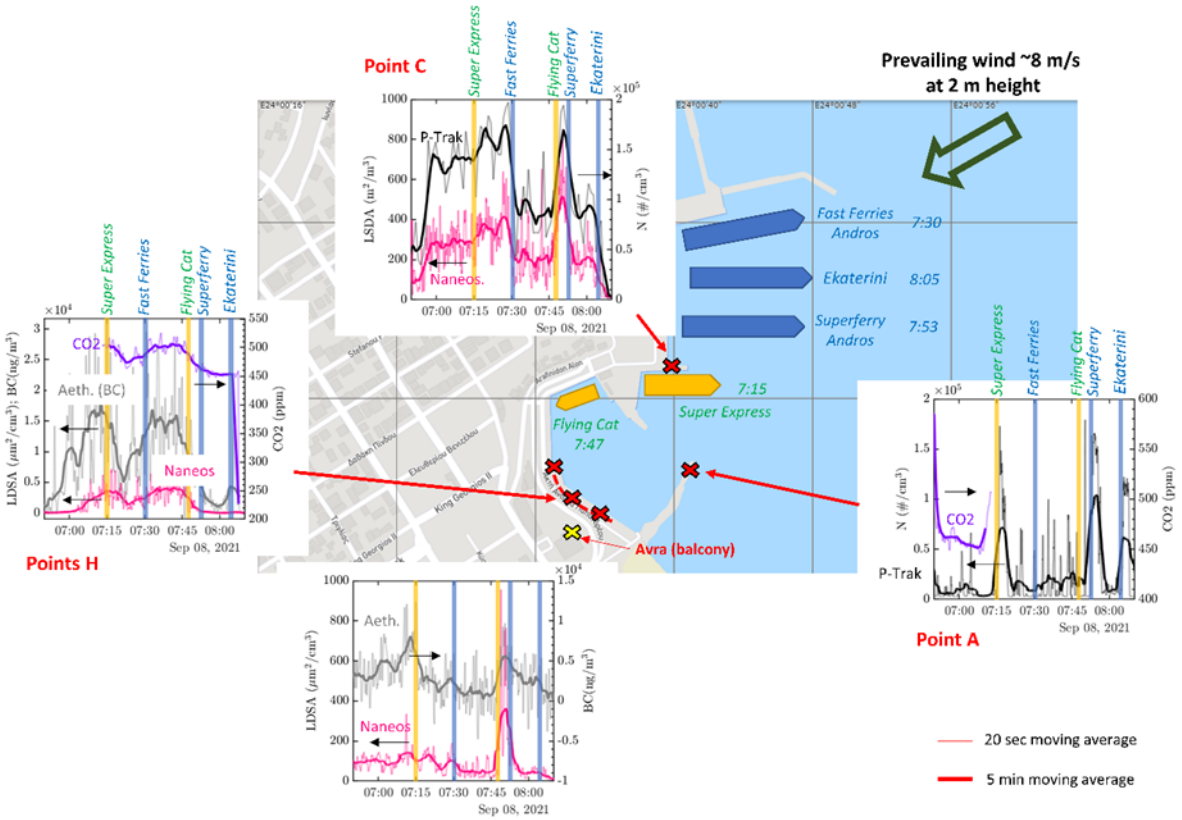


Figure 4.7: Preliminary land-based data collected on one day from various locations around the port as the ferries departed.

Other activities and achievements

Dr Shrey TRIVEDI (Research Associate, CAM) presented a technical paper titled "Conditional Moment Closure Approaches for Simulating Soot and NOx in a Heavy-Duty Diesel Engine" at the *SAE 15th International Conference on Engines and Vehicles* in Naples, Italy, 12-16 September 2021.

Using a drone to sample shipping emissions may help us to better understand the effects of the shipping industry on air quality in Singapore.

IRP BB

BETTER BUSINESS: PATHWAYS TO INDUSTRIAL DECARBONISATION

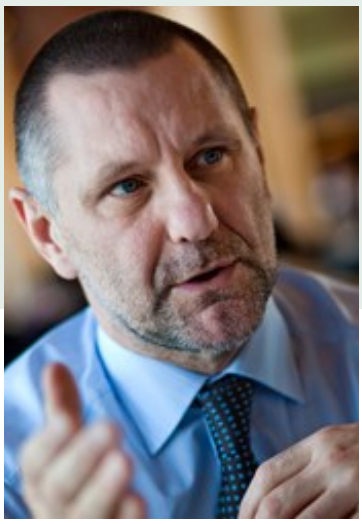
The Better Business IRP acts as an incubator for ideas from all other IRPs and will support the acceleration and scaling of the technology outputs from the programme. It will examine different possible business models and compare the situation in Singapore with other important chemical clusters worldwide,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

IRP BB Principal Investigators:

Professor Steve EVANS
University of Cambridge

Professor S. VISWANATHAN
Nanyang Technological University

Assoc Professor Kenneth HUANG Guang-Lih
National University of Singapore



OVERVIEW

Over the past six months, we welcomed two new Research Fellows to IRP BB. Dr Lemy Martin is a PhD from Nanyang Technological University. He is working with Prof. Viswanathan since August 2021. We also welcomed Dr Xiaomin (Michelle) Fan. She has earned her PhD from Fudan University (in Shanghai, China). She will be working with Prof Kenneth Huang at NUS starting October 2021.

We have been working on several research fronts related to our work packages in the last six months. Our survey study field work was completed in June 2021 and we will be aiming to submit the manuscript to relevant journals based on the survey analysis and theoretical interpretation. We recently procured the Trucost datasets. The datasets will be used for the comparison of the environmental profiles of the oil and gas, chemical and steel sector that we are currently focusing on. The research is ongoing and has given some initial insights which will be elaborated in the subsequent reports. In our research on business model innovation related to solar energy adoption, we are working on finishing the generalisation from two to N heterogeneous customers, which should complete the current study and will be written into a manuscript.

In the research work on impact of policies, we are exploring new areas to see possible correlations between organisation level pollution data after the climate change agreements. We are also starting a new research project analysing venture capitalists' investment behaviour related to clean technology in the context of Singapore and China. We will continue working on the decarbonisation road-mapping activity and collaborations with other IRPs for commercialisation potential evaluations.

Professor Steve Evans, PI
University of Cambridge

Update on work package BB.1

Business model innovation potentials

Work continues on business model innovations for adopting sustainable innovations and technologies. This work was halted temporarily following the departure of a Research Fellow but has now been taken up by Dr Lemy MARTIN.

Previously, the Stackelberg game was solved via backward induction for each business model (sales, leasing, and power purchasing agreement) to obtain the optimal pricing and O&M strategy for the monopolistic firm and/or consumer. To constrain the firm's theoretically unbounded profit maximising objective and incorporate a consumer incentive to switch to solar energy, the BB team introduced an equal system cost savings sharing constraint when identifying the optimal strategies under each model. This is now generalised for any proportion of system cost saving sharing, along with a generalisation of several other parameter assumptions, and find that the previous results continue to hold with some slight algebraic modifications, particularly in the leasing business model. Most of the insights for a representative (homogeneous) customer continue to hold. The team is now working on finishing this generalisation for two to N heterogeneous customers, which should complete the paper for submission. It is hoped to complete the manuscript of the paper and submit it for review within the next few months.

Update on work package BB.2

Policy formulation, customer and industry perceptions

In this work package, work continues to quantify the effect of international policies on clean technology innovation. The fieldwork for the survey was completed in June 2021.

For the research on policy impact on industry and company's low-carbon footprint, the BB researchers further validated the preliminary conclusion by adding empirical analysis and modelling. The assumption was verified in different contexts. The focus is currently more on clean technology innovation. Pollutant emission data was collected from listed companies in order to evaluate the impact on pollution. Thus, through this, the new research angle being explored is to add the analysis regarding how climate change agreement will have an impact on the company's energy consumption and emissions.

New Research Fellow **Dr Michelle FAN (NUS)**, will explore venture capitalists' (VCs) investment in clean/renewable technologies or technologies to reduce carbon emissions and their impacts. She plans to conduct comparative analysis about VC investment behaviour related to the clean technology industries in Singapore and China.

For the survey study, aiming to understand the attitudes and perceptions towards adoption of clean technology, the field study finished in June 2021. Several checks on data quality followed by data analysis were completed. Manuscript preparation has begun; it is 70% complete and will be submitted before December 2021 to a relevant journal. Several interesting insights are revealed in the paper, including some which highlight commonalities across sectors, and some very sector-specific differences. The theoretical work has also been expanded to adapt the Belief-Action-Outcome model in context of the clean technology adoption considering the specific constraints and variables related to it, like lack of measurable outcomes, correlation of belief with expected and actual outcomes, etc.

One of the findings from sectoral comparison is shown in Figure 1 and Figure 2. It can be seen that governments as well as large organizations want to adopt clean technology with a long-term view of mitigating climate change and see cost as a major barrier for adoption. However, financial institutions which are directly facing the pressure, in terms of providing green finance and pulling out of coal and other fossil investments, in the current context, have demonstration of climate consciousness as their current and biggest motivator, so that the stakeholders have trust in their actions. The barriers faced by them are also tangible and immediate, in terms of uncertainty of regulations, cost and uncertainty in technology evolution. Such and various other findings will be reported in the manuscript.

As part of the second phase of the survey study, we would be selecting a subset of big industry participants for targeted study to understand adoption of CO2 emission reduction efforts through surveys and possibly interviews. We will be reaching out to potential industry partners for such a study in Q2 of 2022.

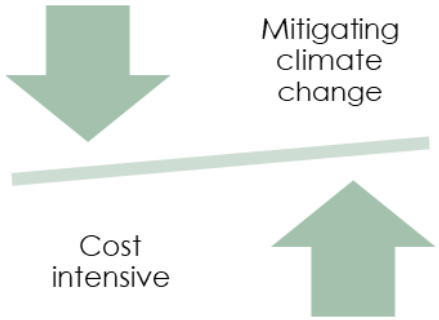


Figure 5.1: Motivations for large organisations and government organisations to adopt green technology.

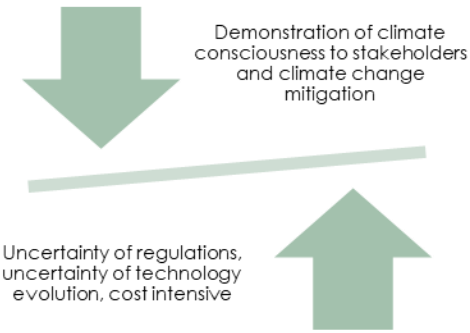


Figure 5.2: Motivations for financial organisations to adopt green technology.

Update on work package BB.3

Future roadmap for industrial decarbonisation, including international comparisons

For WP3, IRP BB continues to work closely with the technology IRPs, including meetings with emerging (and potential) spin-outs from IRPs 1, 2 and 3. The BB team has worked with two spin-outs under Prof. Alexei LAPKIN (IRP1 PI, CAM) to further explore their business models and technology roadmaps and have made multiple introductions to potential future customers. In general, this research has been slowed by lack of face -to-face interactions. BB has also worked with Dr Adrian FISHER (IRP2 PI, CAM) to identify key theories that can inform his technology roadmap through a new PhD.

Due to Covid-19 travel restrictions, **Prof. Steve EVANS (PI, CAM)** has been unable to complete planned travel to Singapore and in-person meetings and workshops with the different IRPs have been challenging. However, work is continuing online where feasible. The researchers are benefitting from parallel work conducted for UKRI in developing their 'Sustainable and Digital Future Roadmap'.

BB is also exploring Life Cycle Analysis (LCA) to address a different facet of road mapping research. Singapore's roadmap to decarbonisation may involve the hydrogen economy as a component. And through LCA, it is planned to uncover and compare some configurations which will help evaluate the environmental impacts of these configurations. Evaluation of a specific waste-to-hydrogen technology has begun, as a first case study for this research interest.

Scientific output

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

"Towards Industry 4.0: Efficient and Sustainable Manufacturing Leveraging MTEF – MTEF-MAESTRI Total Efficiency Framework" in Technological Developments in Industry 4.0 for Business Applications

Emil Lezak, Enrico Ferrera and Steve Evans, *IGI Global*

DOI: 10.4018/978-1-5225-4936-9

Abstract: An overview of the work under development within the EU-funded collaborative project MAESTRI is presented in this chapter. The project provides a framework of new Industrial methodology, integrating several tools and methods, to help industries facing the fourth industrial revolution. This concept, called the MAESTRI Total Efficiency Framework (MTEF), aims to advance the sustainability of manufacturing and process industries by providing a management system in the form of a flexible and scalable platform and methodology. The MTEF is based on four pillars: a) an effective management system targeted at continuous process improvement; b) Efficiency assessment tools to support improvements, optimization strategies and decision-making support; c) Industrial Symbiosis paradigm to gain value from waste and energy exchange; d) an Internet-of-Things infrastructure to support easy integration and data exchange among shop-floor, business systems and MAESTRI tools.

Other activities and achievements

Prof. S. VISWANATHAN's (PI, NTU) course on Corporate Sustainability in Nanyang Business School is now being offered across all MBA disciplines including the Professional MBA (PMBA) and the Executive MBA (EMBA) streams.

Prof. Kenneth HUANG (PI, NUS) has been appointed as the Advisory Board Member of the Economist Intelligence Unit (research and analysis division of the Economist Group) starting 2021.

Prof. Huang has also been appointed as the Senior Editor of *Management and Organization Review*, which is one of the Cambridge Core journals and a premier journal for ground-breaking insights about management and organisations in China and global comparative contexts. He continues to serve on the editorial board of top-tier journals such as the *Academy of Management Journal*, *Strategic Management Journal* and *Journal of International Business Studies*.

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 utilises 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. A main focus is to create superstructures of models contained within the developed ontologies for industrial parks to provide an accurate and fast-to-evaluate approximation of computationally expensive mathematical models for process industry plants in high dimensions.

IRP JPS Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Assoc Professor Raymond LAU Wai Man
Nanyang Technological University

Professor Iftekhar KARIMI
National University of Singapore

OVERVIEW

Over the past six months, the J-Park Simulator (JPS) has progressed on several fronts with regard to developing new functionalities to demonstrate its multi-domain capabilities, and to augment its degree of autonomy and connectivity to the physical world. For instance, we have been working on the development of ontologies for purchase requisition processes, electrical devices and sensors. This work will allow us to describe and store various domain information about a device in the knowledge graph. Furthermore, in order to increase JPS' connectivity to the physical world, we are working on the design of a multi-purpose smart meter that is able to measure the temperature and humidity of the surroundings, as well as the electricity consumption of appliances/devices. These measurements will eventually be integrated into the knowledge graph. We are also in the process of designing a Radio-Frequency Identification (RFID) based system that is able to track assets within the CARES laboratory. In the first instance, this will involve tracking of chemical bottles going in and out of a cabinet located in the laboratory. A time-based trigger function can then be implemented in the knowledge graph such that when the bottles are not returned back after a certain period of time, an email will be sent to the relevant lab personnel to alert them of the situation.

In addition, we have been working on improving the technology agnostic store router with the instantiation of an ontology called OntoKGRouter developed for describing routing information in the form of triples in a routing table. We have also enhanced the JPS architecture by greatly simplifying SPARQL access for the agents with a new AccessAgent which provides abstracted SPARQL access to the knowledge graph in a store technology agnostic manner.

Moreover, we have extended both the OntoAgent ontology and Marie, a Question and Answering system, for automated agent discovery and agent invocation. The OntoAgent ontology is extended such that any new agent described using it can be automatically included into Marie. The mechanism for Marie to train its Natural Language Processing models based on ontologies was also further improved. This will allow Marie to evolve along with the growth of the knowledge graph, in particular with the inclusion of new agents.

Professor Markus Kraft, PI
University of Cambridge

Update on work package JPS.1

Big data — sensors and data modelling

Dr Niklas KASENBURG (Senior Software Developer, CARES) has been working on the development of ontologies for purchase requisition processes, electrical devices and sensors. This involves evaluating various existing ontologies such as schema.org and the Funding, Research Administration and Projects Ontology (FRAPO) for the purchase requisition processes, and the Smart Applications Reference (SAREF), Sensor Model Language (SensorML) and Semantic Sensor Network (SSN) ontologies for the sensors. The preliminary findings were disseminated within the group and will be further developed or adapted in various research activities. In order to describe and store the time series measurement data of the devices, Dr Kasenburg, in close collaboration with **Mr Markus HOFMEISTER (PhD student, CAM)**, has developed a functionality which allows time series information retrieved from different sources such as Application Programming Interfaces (APIs) or files, to be connected to the knowledge graph. This functionality has been demonstrated in an example agent that retrieves and stores data from AQMesh, a small-sensor air quality monitoring system that offers real-time localised outdoor weather and air quality information.

Mr Wilson ANG (Software Developer, CARES), in close collaboration with Dr Kasenburg and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, has been working on the design of a multi-purpose smart meter that is able to measure the temperature and humidity of the surroundings, as well as the electricity consumption of appliances/devices. These measurements are being sent to an online cloud server or IoT platform. The components of the smart meter include a DHT22 for measuring temperature and humidity, an electronic module (PZEM004T) with a current sensor for measuring current, voltage and power, an AC Line Splitter that allows measurement to be conducted in a non-invasive manner, an Arduino UNO microcontroller, a 20x4 LCD Display module for offline display of measurements, and an ESP8266 Wi-Fi module that allows the Arduino UNO to send the measurement data to an online cloud server or IoT platform via Wi-Fi and APIs. The measurement data will be integrated into the knowledge graph via the above-mentioned time series functionality. The overall layout of the multi-purpose smart meter is shown in Figure 6.2.

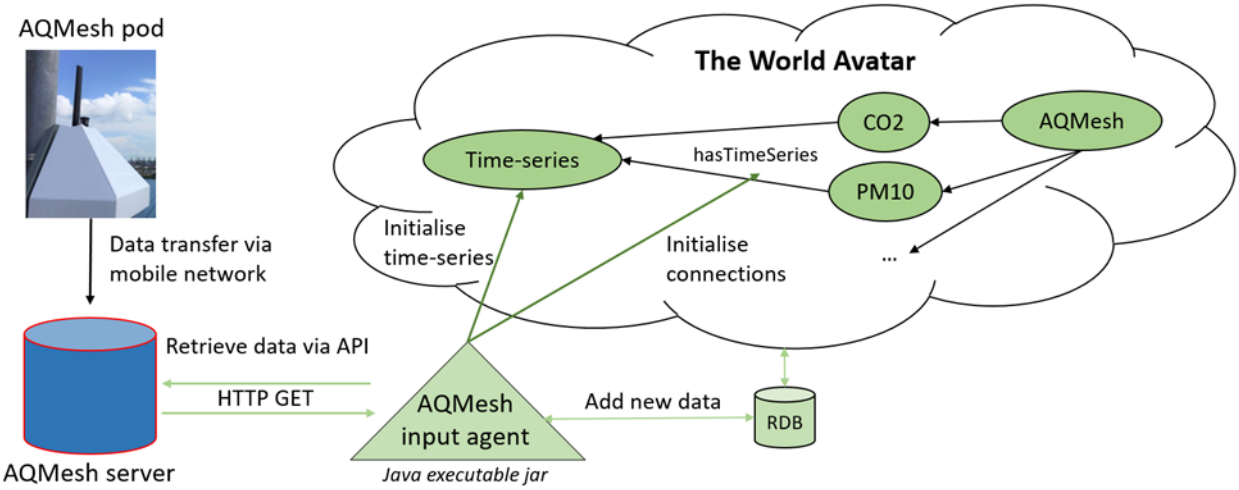


Figure 6.1: Diagram of the implementation of the time series data functionality for the AQMesh agent.

In addition, Mr Ang together with Mr Chadzynski, is also designing a Radio-Frequency Identification (RFID) based system that is able to track assets within the CARES laboratory. In the first instance, as a proof of concept, the system will be designed to track chemical bottles going in and out of a cabinet located in the laboratory. The RFID system includes an Android O.S based reader, a directional antenna and a few RFID label tags for tagging the assets (chemical bottles). The system uses an antenna placed at the entrance of the cabinet to scan the tagged bottles. The operation of the reader, data collection and transmission will be controlled by an Android application developed in either Android Studio or Eclipse. The data will be sent to a database such as PostgreSQL, either via Wi-Fi, or using an API such as MQTT. The data will also be integrated into the knowledge graph via the above-mentioned time series functionality to create a list that indicates which chemical bottles were removed from the cabinet, their times of removal and return to the cabinet. Furthermore, a time-based trigger function can also be implemented in the knowledge graph such that when the bottles are not returned back after a certain period of time, an email will be sent to the relevant lab personnel to alert them of the situation. The overall layout of the RFID based system for asset tracking is shown in Figure 6.3.

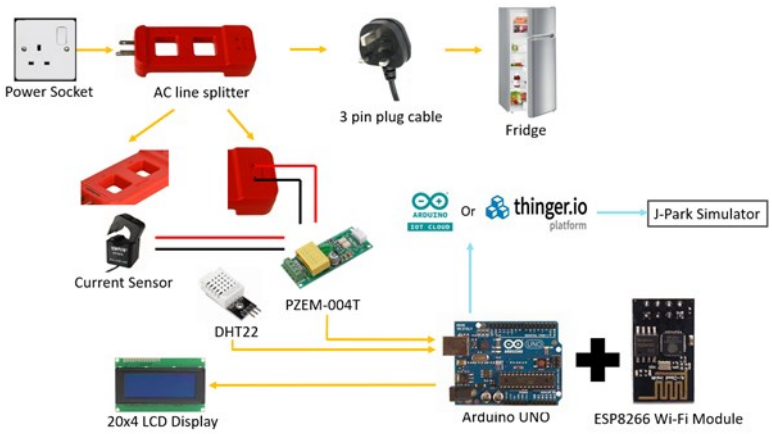


Figure 6.2: Overall layout of the multi-purpose smart meter system.

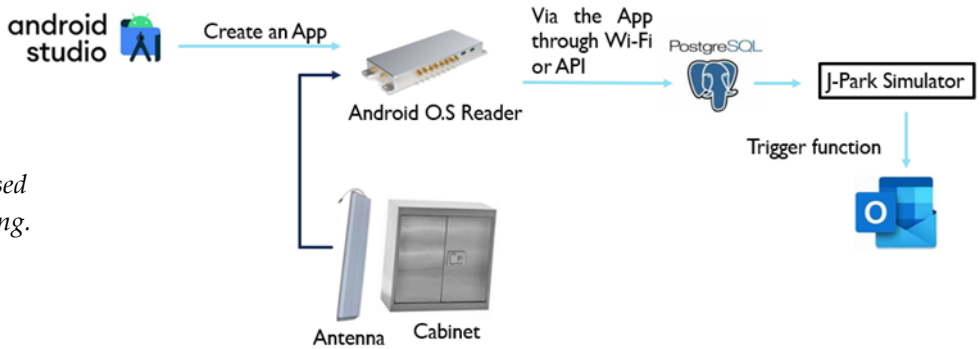


Figure 6.3: Overall layout of the RFID based system for asset tracking.

Dr Jethro AKROYD (Senior Research Fellow, CARES), **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, **Dr Feroz FARAZI (Research Associate, CAM)**, **Dr Angiras MENON (Research Associate, CAM)** and **Dr Aleksandar KONDINSKI (Research Associate, CAM)** have been working on the extension of both the OntoSpecies and OntoKin ontologies that are used for describing the 3D geometry of each atom in a species and in different phases (solid or liquid phases), respectively. In addition, a new ontology called OntoPESScan has been developed to represent potential energy surface scans.

Update on work package JPS.2

Surrogate models, superstructure and architecture development

Dr Jethro AKROYD (Senior Research Fellow, CARES), **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, **Dr Feroz FARAZI (Research Associate, CAM)** and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)** have continued to drive forward the overall JPS architecture. For instance, to enable agents to operate on classes, properties, instances and data collated from multiple domains and represented in the knowledge graph that is distributed over several servers, along with the possibility of migrating to new servers due to ever-increasing demand for performance and storage capacity, a server agnostic approach is implemented for accessing the knowledge graph. To this end, a technology agnostic store router has been optimised with the instantiation of an ontology called OntoKGRouter developed for describing routing information in the form of triples in a routing table consisting of subject, predicate and object columns. The subject refers to the relative Uniform Resource Identifier (URI) of a domain, while the object refers to the absolute URI, and the predicate links the subject and object. As shown in Figure 6.4, when the store router receives a request from an agent with the relative URI of a triple store or the absolute URI of an RDF/OWL file to establish access, the store router validates the request and detects the corresponding store type. Any request targeting a triple store or an RDF/OWL file invokes the query builder to form a query to retrieve the available, absolute URI of the triple store endpoint or base URI of the file store from the KG routing table. By combining the base URI and the absolute URI of a file, the absolute file path is formulated, which is indispensable for executing update operations on a file. Finally, the store router generates a StoreClientInterface type object and returns it to the requesting agent for querying or updating the

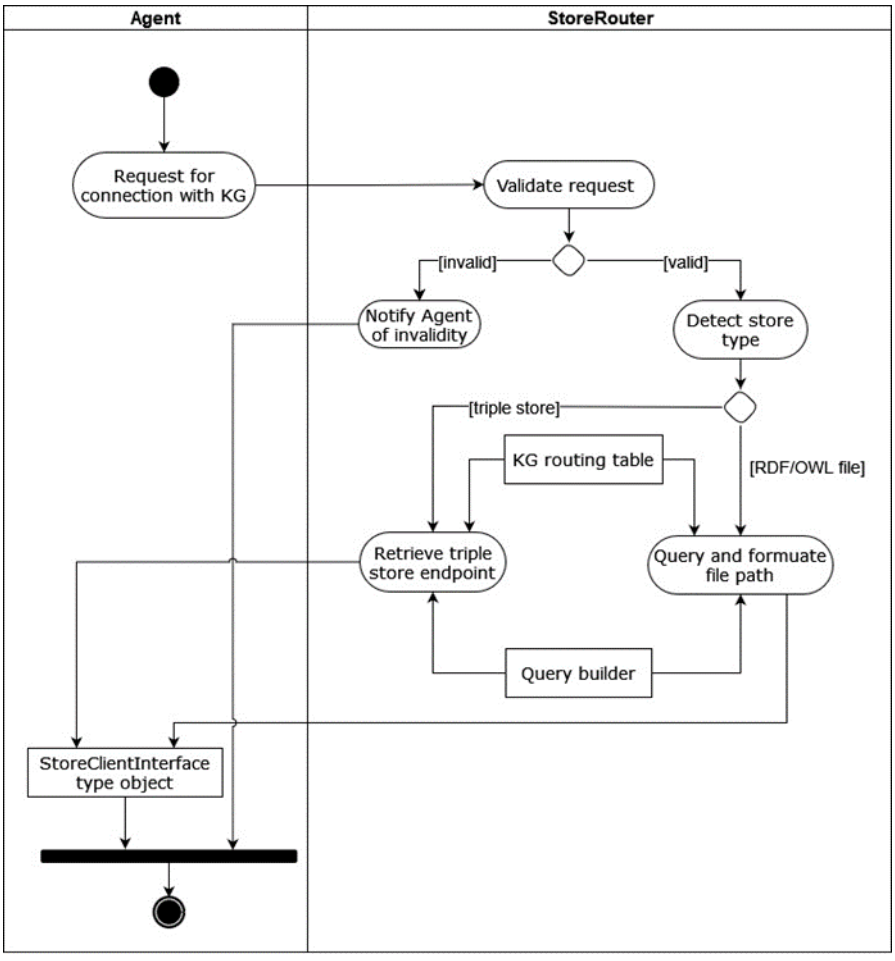


Figure 6.4: An activity diagram of the optimised StoreRouter demonstrating the application of an ontology-based routing table and query builder.

target resource within the knowledge graph. An agent can send multiple requests to set up combined access to different domains stored either in triple stores or files, or both.

In addition, together with **Dr Casper LINDBERG (Research Fellow, CARES)**, Dr Akroyd, Dr Mosbach, Dr Farazi and Mr Chadzynski, have enhanced the JPS architecture by greatly simplifying SPARQL access for JPS agents. Dr Lindberg has developed a new AccessAgent which provides the JPS agents with abstracted SPARQL access to the knowledge graph. The AccessAgent extends the previously implemented storage abstraction to provide a point of access over HTTP for querying or updating RDF data in the knowledge graph in a store technology agnostic manner. The AccessAgent utilises the StoreRouter class together with the OntoKGRouter triple store to retrieve the SPARQL endpoint or file path for a requested resource. Depending on the type of the requested resource, it then instantiates a RemoteStoreClient or FileBasedStoreClient, corresponding to connection to a triple store or OWL file, respectively. In order to create and send HTTP requests to the new AccessAgent, Dr Lindberg also developed an AccessAgentCaller class. This class is wrapped into the JPSAgent framework and provides agents within the framework with simple methods to execute SPARQL queries or perform update operations on data in the knowledge graph.

Furthermore, Dr Lindberg has implemented the new abstracted store clients within the existing ScenarioAccessAgent. Dr Lindberg has also reviewed the naming conventions used in the aforementioned classes and established clearer names and consistency across the JPS Base Library.

Mr Chadzynski is also heavily involved in training, supporting and providing guidance especially to new members of the team concerning documentation, questions on software design, agent development and non-functional requirements such as performance and scalability.

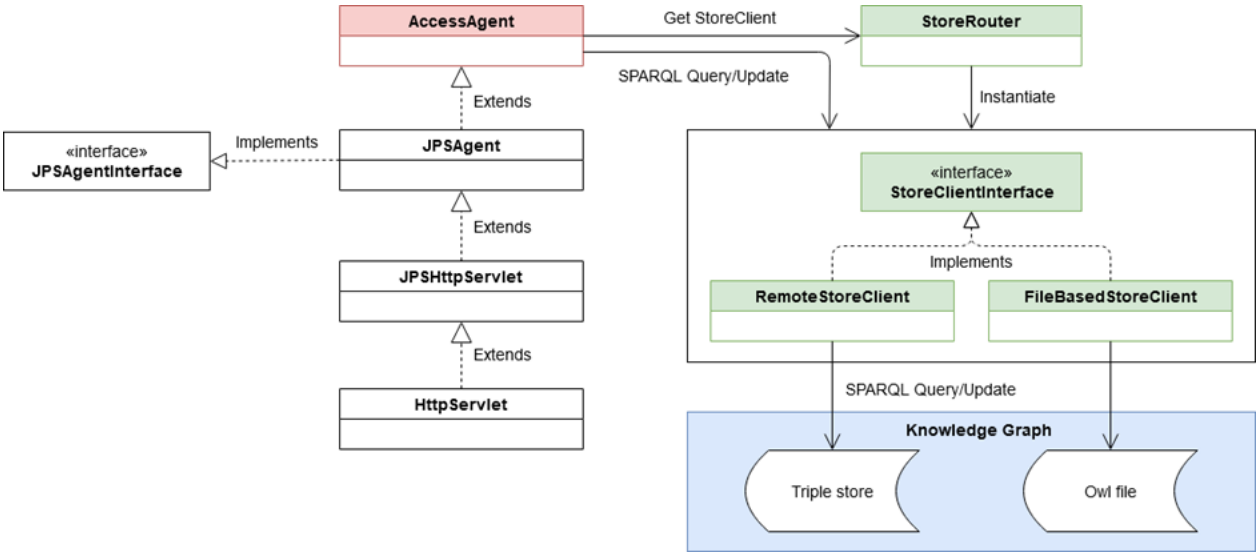


Figure 6.5: A diagram of the AccessAgent implementation within the JPSAgent framework using abstracted storage access. The AccessAgent receives a HTTP request to perform a SPARQL query or update operation on a target resource in the knowledge graph. The StoreRouter instantiates a StoreClientInterface type object connecting to the requested resource through either a RemoteStoreClient or FileBasedStoreClient. The StoreClient is used by the AccessAgent to execute the SPARQL query or update operation on the target resource.

Update on work package JPS.3

Implementation

Dr Jethro AKROYD (Senior Research Fellow, CARES), **Dr Sebastian MOSBACH (Senior Research Fellow, CARES)**, **Dr Feroz FARAZI (Research Associate, CAM)** and **Mr Tom SAVAGE (MPhil student, CAM)** have been working on the development of a dynamic knowledge graph approach for digital twins to perform "what-if" scenario analysis. The challenges posed by climate change are interdisciplinary, hence, the development of solutions requires the consideration of economic, engineering, environmental, and social factors over a range of geographic scales. These factors are strongly interconnected, and it is widely appreciated that digitalisation in the form of interoperable collaborative models that span multiple disciplines offer new ways to design and operate infrastructure and will form an important part of the response to these challenges. As data for the UK are readily and publicly available, they are utilised in the first instance to develop the "UK Digital Twin knowledge graph" as a proof of concept. This work can easily be extended and applied to other regions where data are available, in particular Singapore.

The aim of the UK Digital Twin knowledge graph is to develop a comprehensive live distributed system to support the optimal use, planning and development of infrastructure in the UK, for example to assist the decarbonisation of the energy landscape. During this reporting period, this work has focused on the electric power system, the gas grid, land use and the built environment, all of which are critical to the future of the energy landscape. Examples of data that have been instantiated in the knowledge graph include a geospatial description of the National Grid Gas Transmission system with live data feeds for the intake of gas, and a description of all regional electrical generators in the UK. During the course of this work, questions of how to use artificial intelligence (AI) to ensure alignment between the different scenarios and the goals of the society arise. To address this, the digital twins are in the process of being equipped with UN Sustainable Development Goals (SDGs) to illustrate how digital twinning and what-if scenario analysis can support decision makers to understand the effect of different design choices and policy instruments.

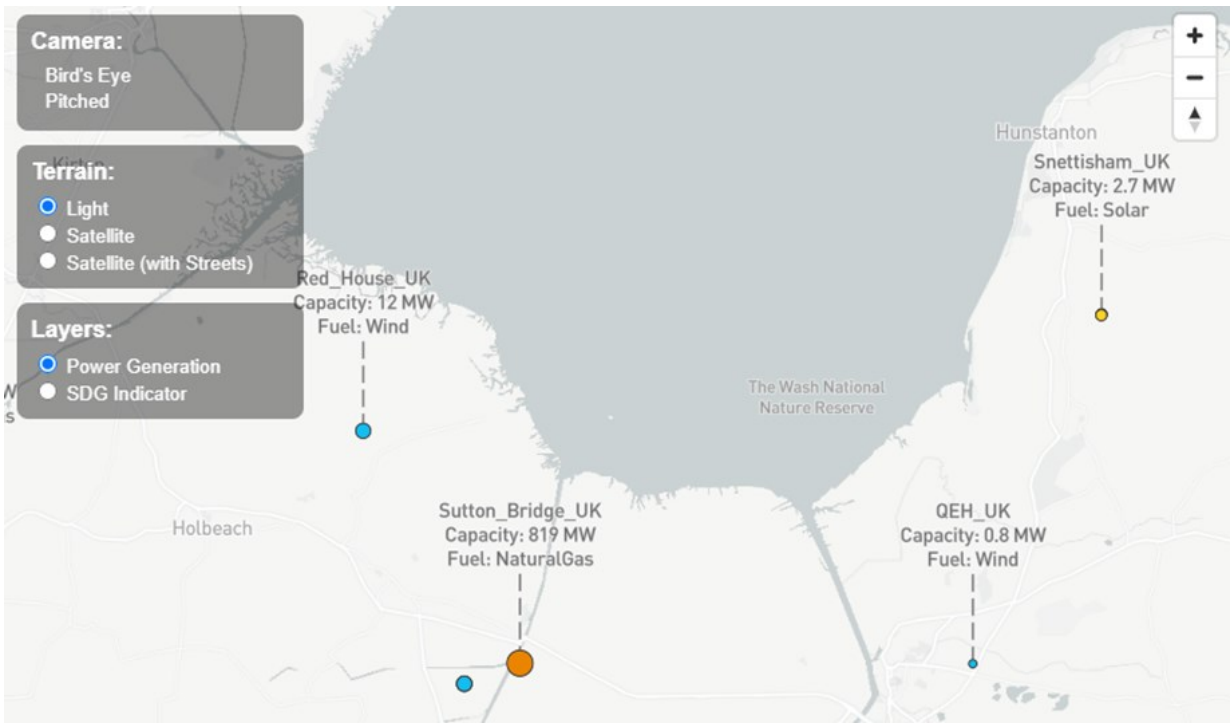


Figure 6.6: Visualisation of some electrical generators in the UK Digital Twin knowledge graph.

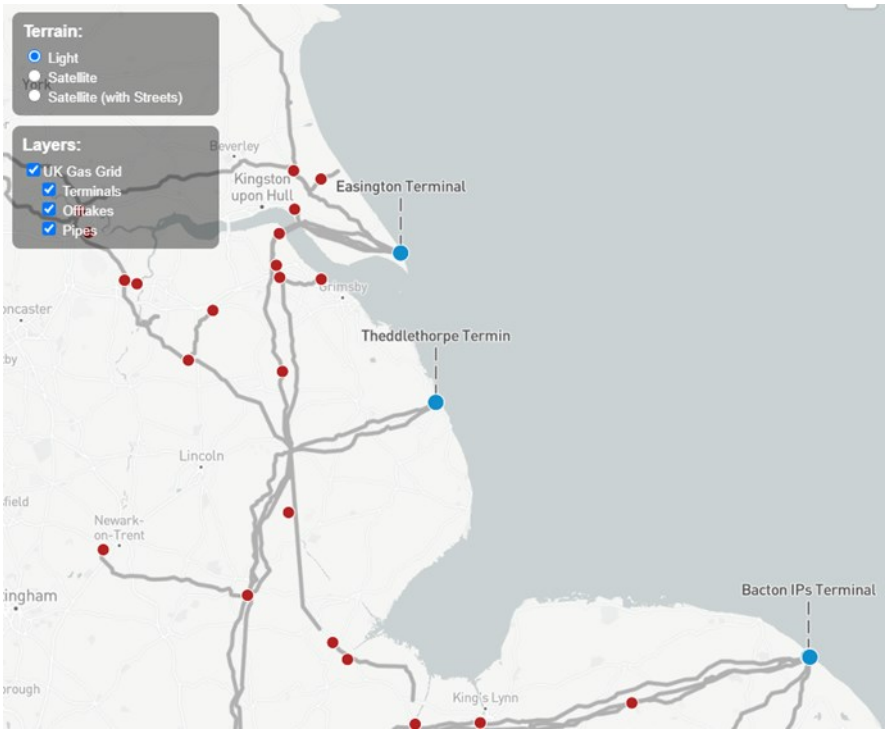


Figure 6.7: Visualisation of a portion of the natural gas transmission system in the UK Digital Twin knowledge graph, with a data feed showing the intake via the Bacton terminal.

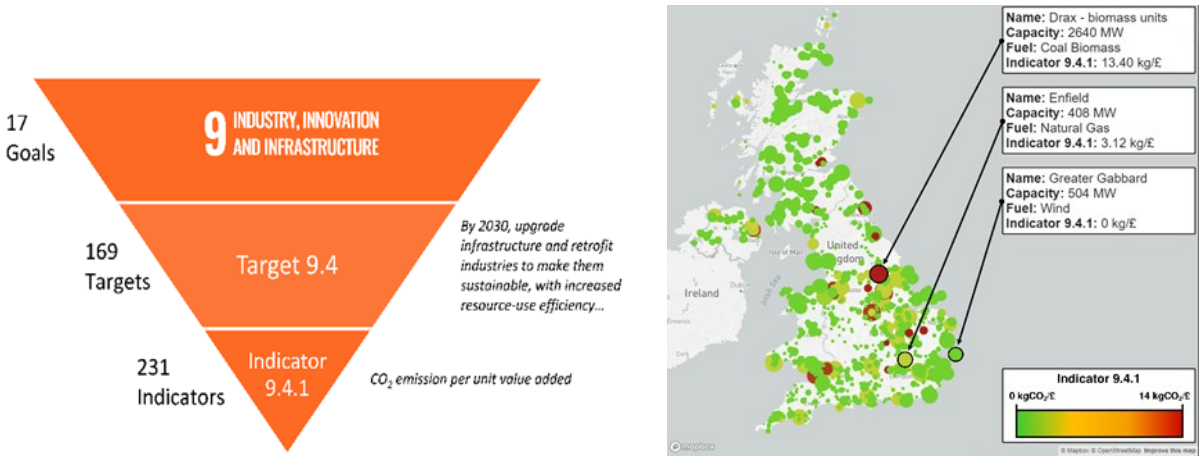


Figure 6.8: (left) UN Sustainable Development Goal (SDG) 9, Target 9.4 and Indicator 9.4.1.
(right) Visualisation of the estimated value of SDG Indicator 9.4.1 ($kgCO_2$/£) for every power generation facility in the UK Digital Twin knowledge graph. The size of the markers indicates the capacity of each facility.

Ms Wanni XIE (PhD student, CAM) has continued to work on the improvement of the automated features of the Digital Twin knowledge graph and its agent-based ecosystem. This work is motivated by the research question of how can the goal of Zero Carbon Emission be supported. In order to improve the extensibility, Ms Xie has augmented various existing agents e.g. input agents that populate the knowledge graph with information about the real-world entities and agents that modify elements at the instance-level of the knowledge graph. For instance, the input agents can now easily repopulate the portions of the knowledge graph that are describing real world entities semantically i.e., "base world" with power plant data from different data sources such as Digest of UK Energy Statistics (DUKES). **Mr John ATHERTON (PhD student, CAM)** supported this work by curating multiple models and external data sources for the UK branch model, load data and generator data. The data has been instantiated into the knowledge graph by Ms Xie. Ms Xie, in close collaboration with Mr Atherton, has also improved the design of the ontologies to allow the co-existence of electrical grid models with various levels of abstraction depicting the internal connectivity between the bus nodes and electrical lines. This is exemplified by having both the original 10-bus simplified grid model and a newly added 29-bus detailed grid model to represent the same power network in the knowledge graph. In addition, Ms Xie has integrated into the knowledge graph, clustering methods developed by Mr Atherton to automatically determine each bus's generation and demand loads based on the specified bus configurations. This allows grid studies such as Optimal Power Flow (OPF) to be performed using the data.

Furthermore, Ms Xie has created visualisation to display the wealth of data present in the UK Digital Twin knowledge graph. An example of the visualisation of the 10-bus simplified grid model and the 29-bus detailed grid model is shown in Figure 6.9.

Dr Vishvak KANNAN (Research Fellow, CARES), in close collaboration with **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, has been working on the design of linking of geospatial representations of Jurong Island described using the OntoCityGML ontology with chemical engineering representations described using the OntoCAPE ontology. This involves migrating data from OWL files to the Blazegraph triple store and instantiating Level of Detail 2 (LOD2) models of a biodiesel plant on Jurong Island with various equipment as interior building installations in the knowledge graph.

Figure 6.9: Visualisation of the 10-bus simplified grid model (left) and the 29-bus detailed grid model (right) in the UK Digital Twin knowledge graph.

Update on work package JPS.4

Model analysis and visualisation

Ms Shaocong ZHANG (Software Developer, CARES) has been working on the improvement of the quality of the current ontology matching framework, which is designed specifically to suit JPS' multi-domain and multi-level characteristics. While the previous work has been focusing on the terminology portion of the matching, Ms Zhang has been concentrating on improving instance matching during this reporting period. This involves examining a use case that aims to perform instance matching on two powerplant databases. The two new datasets (Digest of UK Energy Statistics – Global Power Plant Database and Kraftwerksliste (Germany) – Global Power Plant Database) have been chosen to establish a baseline for evaluation of the current matching framework. Ms Zhang has developed two extensional prototypes to improve the matching result metrics. One of the prototypes introduces Tversky index to factor in the effect of data quality for the source and target. The other prototype introduces background semantic knowledge, such as geographical information, into the datasets. This is to tackle the problem of a bottleneck on recall rate caused by limited information in the current data. Consequently, a prototype that includes Geonames, an external database providing semantic geographical data, was developed. As shown in Figure 6.10, compared to the baseline, the inclusion of geonames improves both the precision and recall. In particular, for the best case (threshold of 0.6), the new prototype is able to obtain a 9.6% improvement for the F-score. Ms Zhang is in the process of further improving the matching results by investigating other types of background semantic knowledge and geographical data sources.

Ms Srishti GANGULY (Project Engineer, CARES) together with **Dr Vishvak KANNAN (Research Fellow, CARES)** has been working on the extension of the knowledge graph to include varied information on chemical, pharmaceutical, semiconductor and other industries in Singapore mainland which can contribute to carbon emissions. This involves reviewing and collecting open-source geospatial data and information on business activities for such industries and companies. Ms Ganguly together with **Dr Jingya YAN (Research Fellow, CARES)** has been cleaning this data using QGIS, a geographic information system application, and developing CityGML Level of Detail 1 (LOD1) models of these buildings in Singapore using the Feature Manipulation Engine (FME) Workbench, as shown in Figure 6.11. Ms Ganguly is in the process of instantiating the models into the knowledge graph.

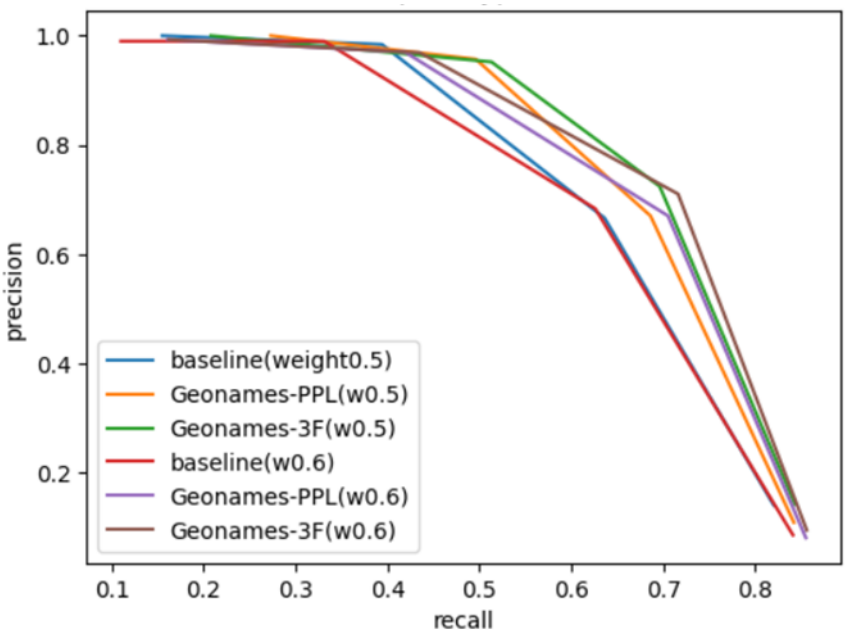


Figure 6.10: Precision-Recall curve for baseline and extended prototype that includes Geonames.

Mr Xiaochi ZHOU (PhD student, CAM) has been working on the integration of the Marie, a Question and Answering (Q&A) system, with the JPS agent system. This involves the extension of both the OntoAgent ontology and the Marie system for automated agent discovery and agent invocation. The OntoAgent ontology is extended such that any new agent described using it can be automatically included into Marie. This is achieved by adding two new properties (hasQuestionTemplate and hasQualifier) to the OntoAgent ontology. As shown in Figure 6.12, the "hasQuestionTemplate" property links "Operation" with a string that acts as a template for formulating a natural language query which the agent can answer. For example, a weather agent might have pre-defined templates such as "How is the weather in <city>?", "What is the wind speed in <city>?". The "hasQualifier" property adds qualifiers to the outputs. Qualifiers are also used to annotate attributes in Wikidata. For example, the enthalpy of a species depends on the specified temperature. However, users typically would like to know the enthalpy of a species under standard conditions when asking the question "What is the enthalpy of benzene?". In this case, the temperature is not a strict input of the function, but is an optional qualifier of the output enthalpy.

In addition, Mr Zhou has further improved the mechanism for Marie to train Natural Language Processing (NLP) models based on ontologies. This allows Marie to evolve along with the growth of the knowledge graph, in particular with the inclusion of new agents. When creating the training materials for Marie's NLP models, Marie will automatically discover all the available agents and determine their input/output types and templates. For example, in the aforementioned weather agent, its input will be annotated as "city" while its outputs such as temperature, humidity, precipitation, etc. will be annotated as "weather data". An example of an NLP template can be "What is the <weather data> in <city>?". Marie will create the training materials by first querying all the "city" in the knowledge graph to obtain their labels, e.g. "Shanghai". Similarly, Marie will query the knowledge graph to obtain all the labels for "weather data" e.g. "wind speed". Finally, Marie populates the NLP template with the labels and generates questions such as "What is the wind speed in Shanghai?". These questions are used by Marie to train its NLP models.

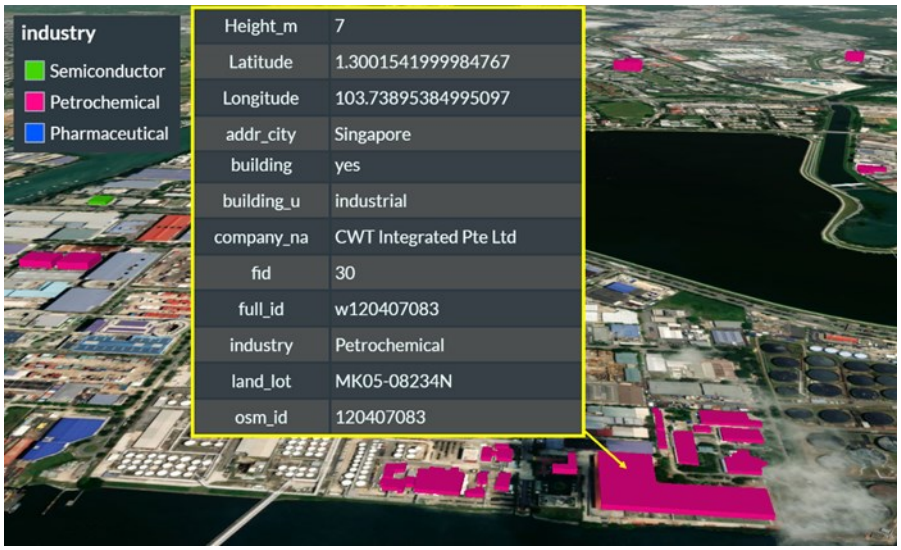


Figure 6.11: Visualisation of the CityGML LOD1 model in Singapore mainland.

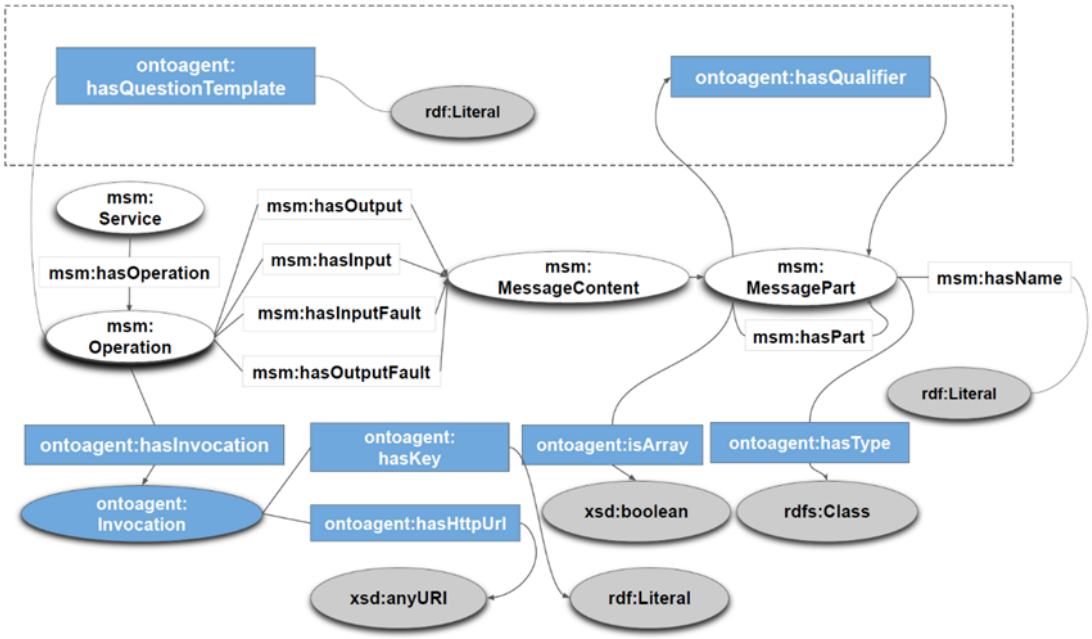


Figure 6.12: Extension (within the box) of the OntoAgent ontology for Marie.

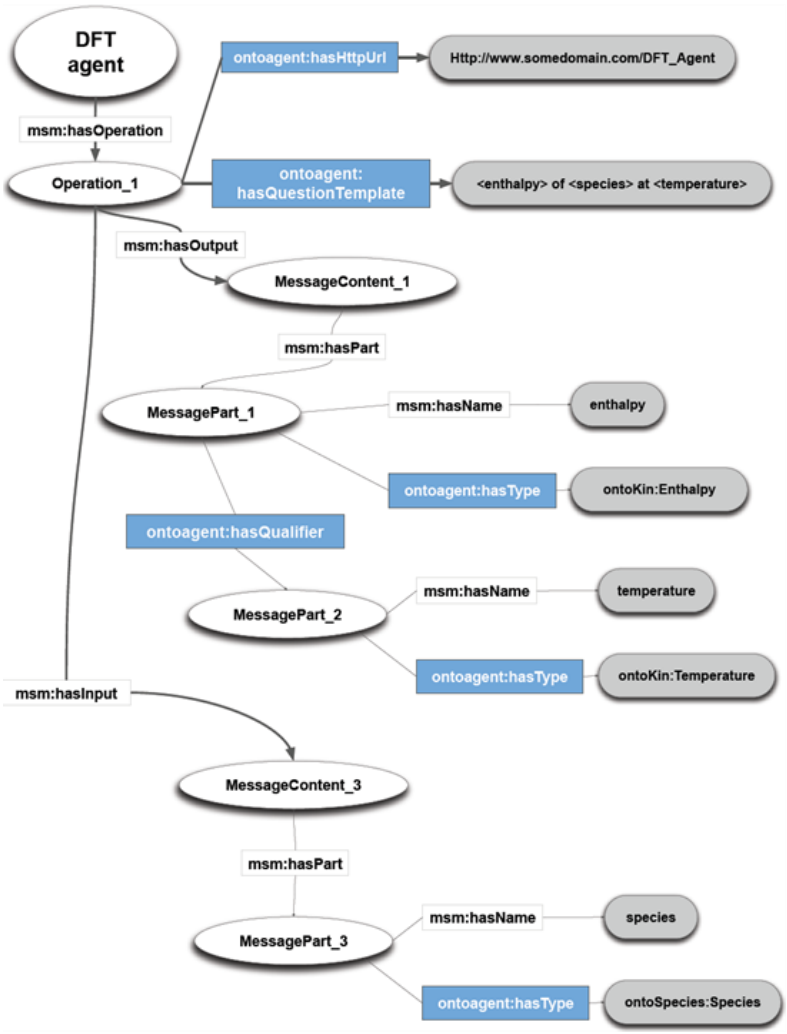


Figure 6.13: An example of an OntoAgent instance.

Scientific output

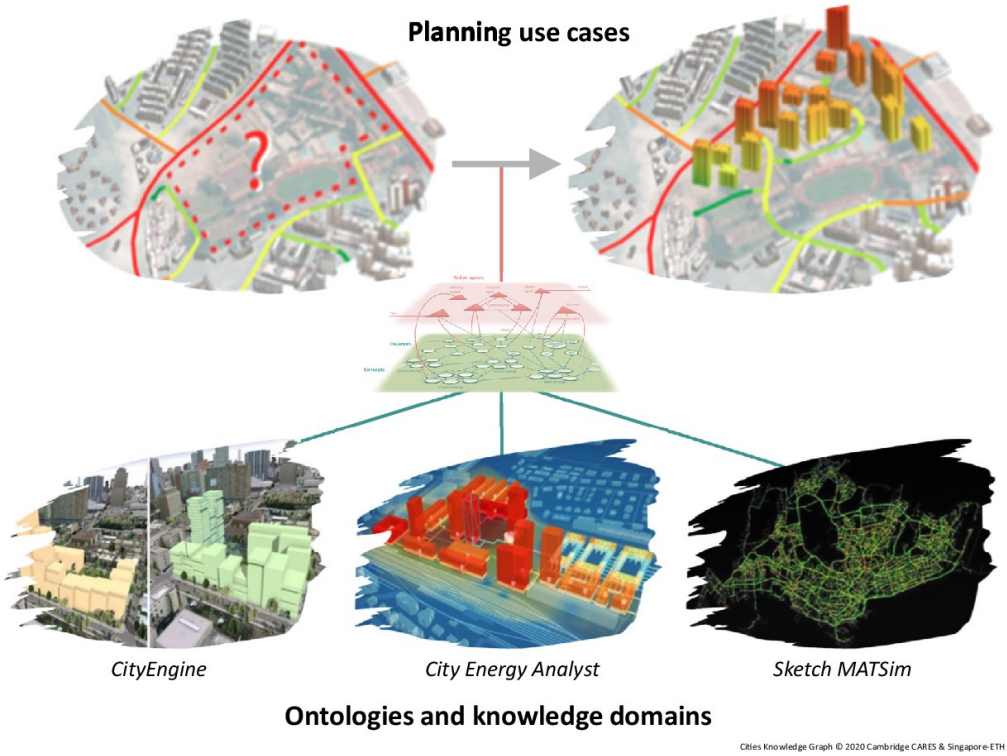
The following are the CREATE-acknowledged publications generated by IRP JPS during the reporting period, excluding those already featured in the Scientific Highlights section on page 12.

Universal Digital Twin—A dynamic knowledge graph

Jethro Akroyd, Sebastian Mosbach, Amit Bhave and Markus Kraft, *Data-Centric Engineering*

DOI: 10.1017/dce.2021.10

Abstract: This paper introduces a dynamic knowledge-graph approach for digital twins and illustrates how this approach is by design naturally suited to realizing the vision of a Universal Digital Twin. The dynamic knowledge graph is implemented using technologies from the Semantic Web. It is composed of concepts and instances that are defined using ontologies, and of computational agents that operate on both the concepts and instances to update the dynamic knowledge graph. By construction, it is distributed, supports cross-domain interoperability, and ensures that data are connected, portable, discoverable, and queryable via a uniform interface. The knowledge graph includes the notions of a "base world" that describes the real world and that is maintained by agents that incorporate real-time data, and of "parallel worlds" that support the intelligent exploration of alternative designs without affecting the base world. Use cases are presented that demonstrate the ability of the dynamic knowledge graph to host geospatial and chemical data, control chemistry experiments, perform cross-domain simulations, and perform scenario analysis. The questions of how to make intelligent suggestions for alternative scenarios and how to ensure alignment between the scenarios considered by the knowledge graph and the goals of society are considered. Work to extend the dynamic knowledge graph to develop a digital twin of the UK to support the decarbonization of the energy system is discussed. Important directions for future research are highlighted.



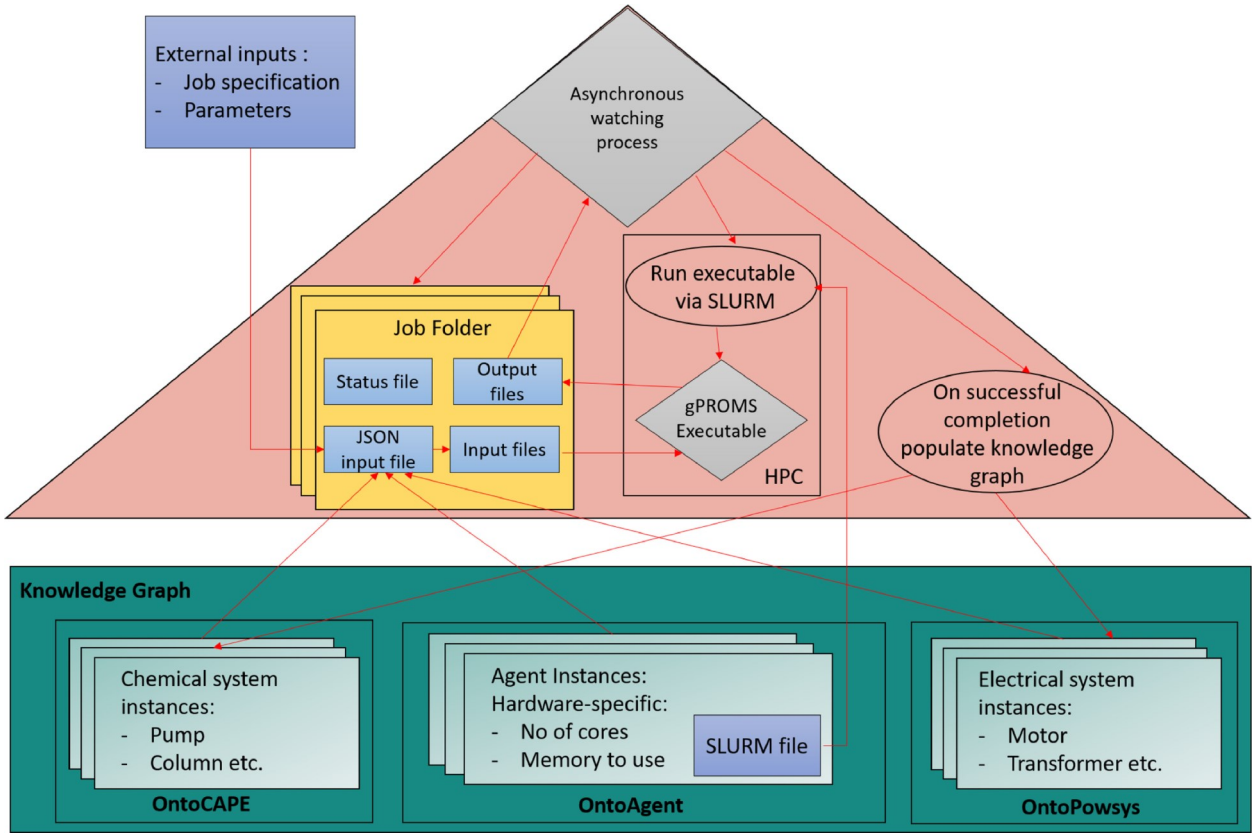
The Cities Knowledge Graph project will develop a pilot for a comprehensive knowledge management platform that provides interoperability between different types of city-relevant data to improve the precision of planning instruments and bridge the gap between planning use cases and knowledge domains.

ElChemo: A cross-domain interoperability between chemical and electrical systems in a plant

Aravind Devanand, Gourab Karmakar, Nenad Krdzavac, Feroz Farazi, Mei Qi Lim, Y.S. Foo Eddy, Iftekhar A. Karimi and Markus Kraft, *Computers & Chemical Engineering*

DOI: 10.1016/j.compchemeng.2021.107556

Abstract: The paper proposes a novel framework capable of establishing machine-to-machine (M2M) interactions between chemical and electrical systems in the industry. The framework termed as ElChemo addresses the challenges in M2M interaction of entities from different silos, such as differences in the domains' behaviour, the heterogeneities arising from different vocabularies and software. The OntoTwin ontology has been developed based on OntoPowSys and OntoEIP ontologies, which are parts of an intelligent platform called the "J-Park Simulator (JPS)". The ElChemo framework uses Description Logic (DL) and SPIN reasoning techniques to establish the interaction between the chemical and electrical systems in a plant. This paper presents a depropaniser section of a chemical plant and its corresponding electrical system as a use case scenario to demonstrate the interoperability between the two silos within the ElChemo framework. The results from the use case demonstrate, as a proof of concept, the potential of the proposed framework and can be considered as the first step towards the development of a knowledge graph based framework capable of increasing interoperability between cross-domain interactions.



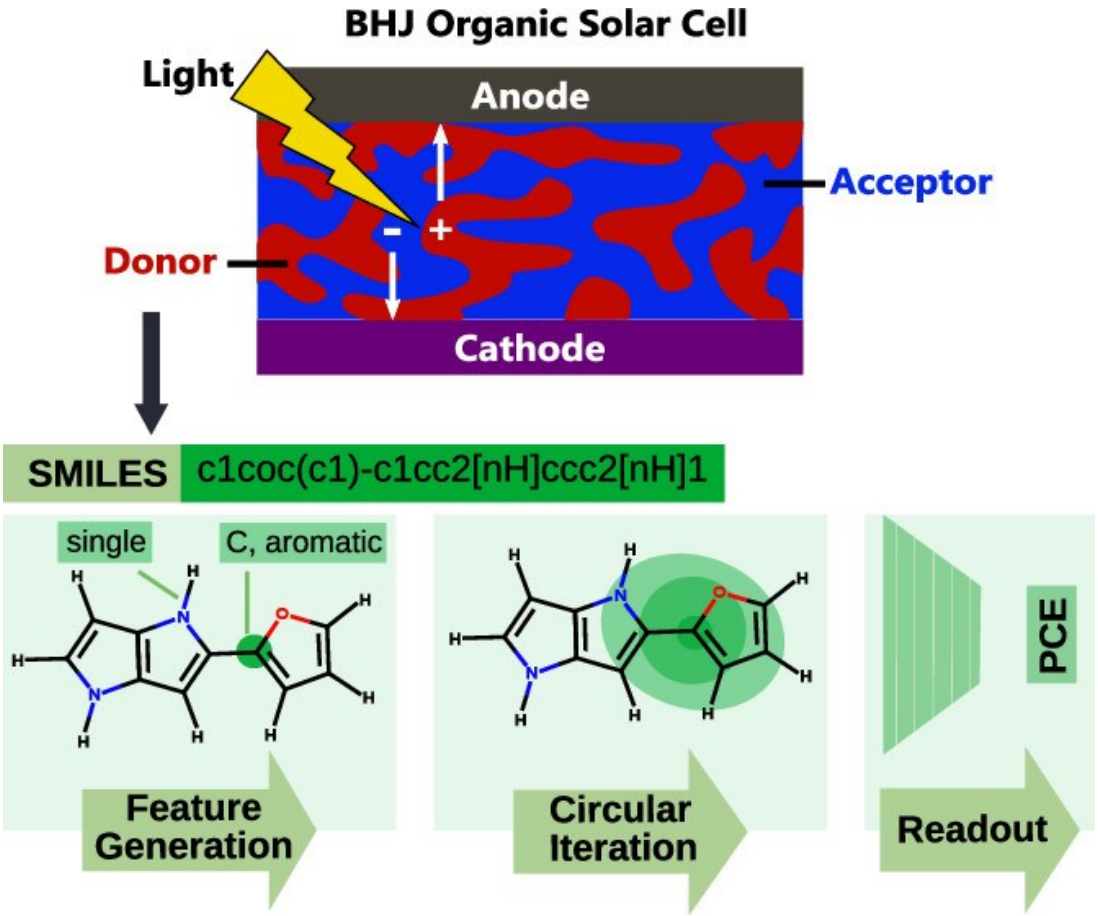
Elements of the gPROMS agent (red triangle) and how they interact with the knowledge graph (green box). An asynchronous watcher (grey diamond) manages running the gPROMS executable (grey diamond) with all associated input and output files (blue boxes).

Predicting power conversion efficiency of organic photovoltaics: models and data analysis

Andreas Eibeck, Daniel Nurkowski, Angiras Menon, Jiaru Bai, Jinkui Wu, Li Zhou, Sebastian Mosbach, Jethro Akroyd and Markus Kraft, *ACS Omega*

DOI: 10.1021/acsomega.1c02156

Abstract: In this paper, the ability of three selected machine learning neural and baseline models in predicting the power conversion efficiency (PCE) of organic photovoltaics (OPVs) using molecular structure information as an input is assessed. The bidirectional long short-term memory (gFSI/BiLSTM), attentive fingerprints (attentive FP), and simple graph neural networks (simple GNN) as well as baseline support vector regression (SVR), random forests (RF), and high-dimensional model representation (HDMR) methods are trained to both the large and computational Harvard clean energy project database (CEPDB) and the much smaller experimental Harvard organic photovoltaic 15 dataset (HOPV15). It was found that the neural-based models generally performed better on the computational dataset with the attentive FP model reaching a state-of-the-art performance with the test set mean squared error of 0.071. The experimental dataset proved much harder to fit, with all of the models exhibiting a rather poor performance. Contrary to the computational dataset, the baseline models were found to perform better than the neural models. To improve the ability of machine learning models to predict PCEs for OPVs, either better computational results that correlate well with experiments or more experimental data at well-controlled conditions are likely required.



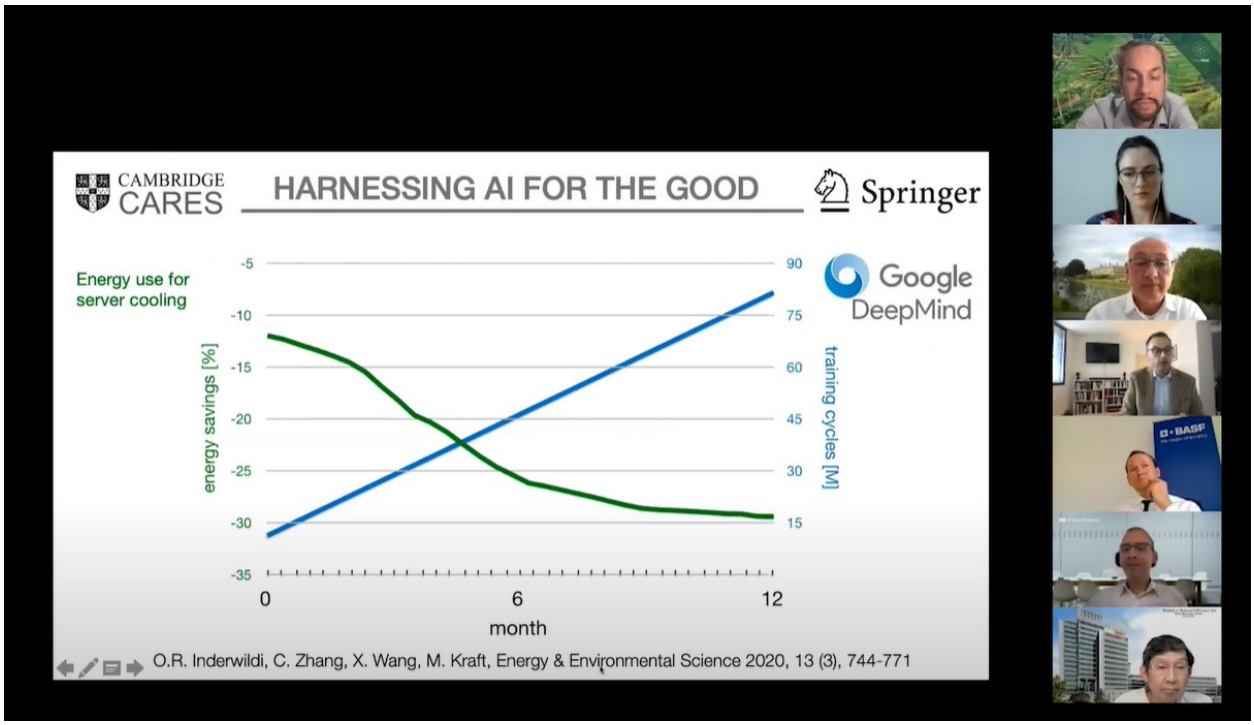
Other activities and achievements

Prof. Markus KRAFT (PI, CAM) gave a talk titled "A dynamic knowledge-graph approach to digital twin—the Universal Digital Twin" at the *2nd International Conference on Energy and AI*, 10th—12th August. The talk explained how digital technologies of Industry 4.0, such as the Internet of Things, cyber-physical systems and knowledge graphs can help to make our energy systems more efficient with reduced emissions.

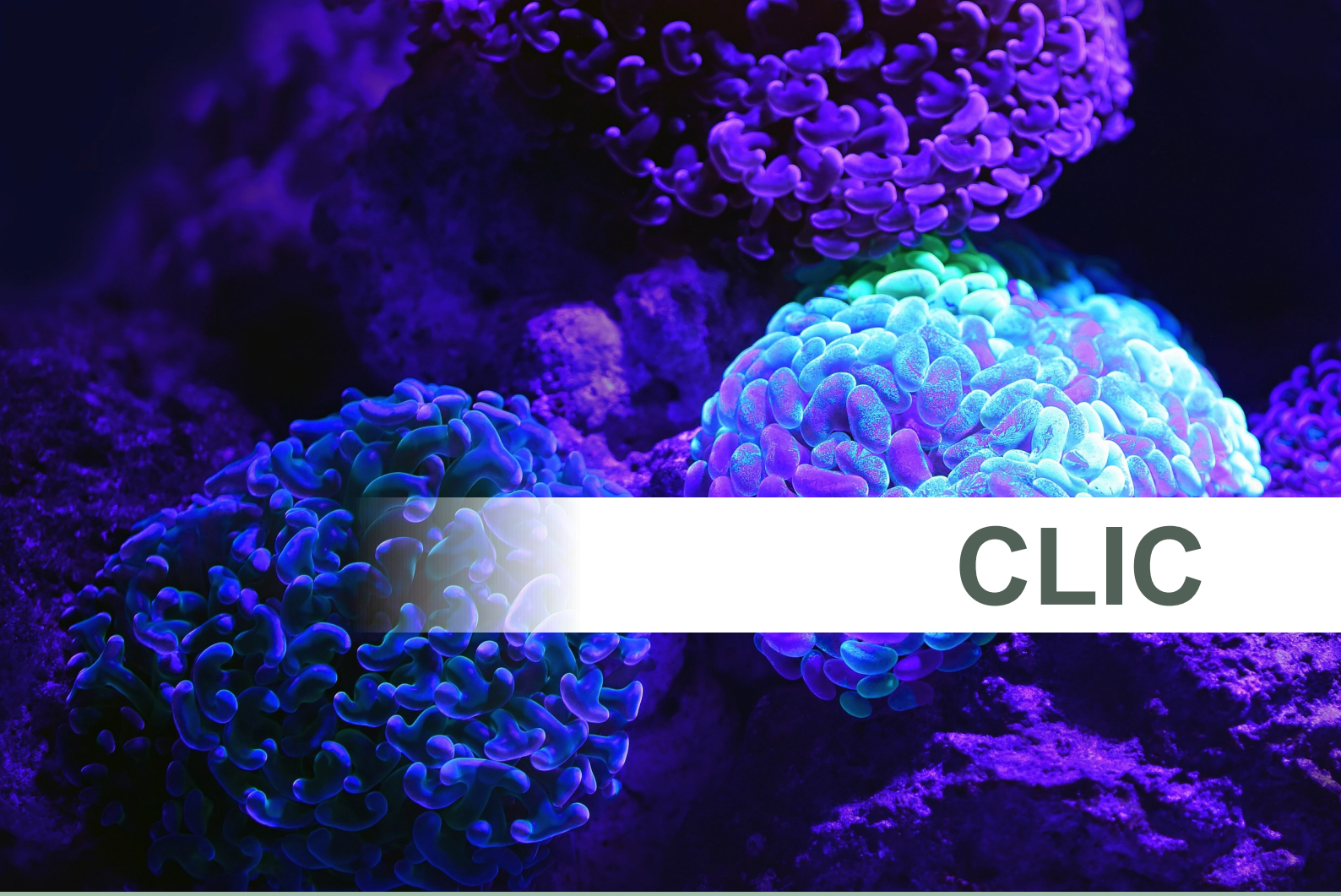
Prof. Kraft presented a talk for the monthly CREATE Webinar, titled "Intelligent Decarbonisation", on 27th August. He was joined by several panellists from academia, industry and government who each had the opportunity to talk about their work and answer questions from the audience. The event was well-attended, with nearly 200 people tuning in.

Prof. Kraft gave two talks at *Data for Policy 2021*, 14th—16th September in London: "A knowledge-graph approach to cross-domain data integration – implications for planning" and "Addressing challenges of urban policy making and city planning with a Cities Knowledge Graph". These talks were given in collaboration with other researchers from the C4T and Cities Knowledge Graph projects, including from University of Cambridge and the Singapore-ETH Centre.

Prof. Kraft gave a talk titled "Supercharging decarbonisation with a universal digital twin" as part of the *Cambridge Zero Climate Change Festival*, 15th—20th October.



A screenshot from Prof. Markus Kraft's CREATE Webinar presentation.



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 cognitive training programmes for the improvement of lifelong flexible learning, focusing initially on adolescents and young adults, but also envisaging work with infants and older adults. This is a strategic global initiative for the University of Cambridge and NTU that brings together multidisciplinary expertise from over 30 investigators in the areas of neuroscience, psychology, linguistics and education across the two universities.

CLIC Directors:

Professor Annabel CHEN Shen-Hsing
Nanyang Technological University

Professor Zoe KOURTZI
University of Cambridge

OVERVIEW

CLIC research focuses on improving cognitive flexibility across the lifespan, which means that research outcomes will address a broad age spectrum from infancy to adulthood. In particular, the age groups we are targeting are infants aged 12-24 months old, adolescents aged between 13-15 years old, young and working adults. The research we conduct will not only inform us of how cognitive flexibility interacts with learning and creativity across these various age groups but will also allow us to design and assess specific intervention programs for each age group to enhance cognitive flexibility and learning.

In addition to the learners we are targeting across the various age groups indicated above, the research outcomes are likely to inform and educate teachers and parents to pave the best way forward to embed cognitive flexibility principles into the existing curricula and lifestyle practices respectively for learners to benefit from their natural environments.

In addition, already by WP0.1, we aim to understand the relationship between cognitive flexibility and career planning. Specifically, we want to evaluate any connections between cognitive flexibility and the willingness and ability to adapt and accordingly change careers—a key factor for employability and career success. We thus believe that our results could inform the Ministry of Manpower, university career services, employers, and the students/future employees themselves.

Our research has also benefited the larger audience beyond our research participants or collaborators. The article titled "IQ tests can't measure it, but 'cognitive flexibility' is key to learning and creativity" published in The Conversation on 24th June 2021 was born out of CLIC research and had widespread public readership, highlighting the relevance of CLIC research to society.

We have planned translational outcomes given the aim of CLIC to promote and enhance lifelong learning, creativity and wellbeing by focusing on improving cognitive flexibility, a fundamental skill to learn and adapt to life's changes and challenges. Cognitive flexibility is key to learning and creativity. It supports academic and work skills such as problem solving and critical thinking, as well as learning agility to adapt and innovate solutions in the face of uncertainty. Cognitive flexibility is an essential component to living holistically and coping with uncertainty and changes that accompany the various stages of the lifespan. The research conducted at CLIC will help to inform stakeholders such as parents, educators, and employers on how they can integrate cognitive flexibility components consciously in the lives of students/employees and encourage them to embrace flexible learning instead of rote-based learning. This would involve translating research conducted at CLIC to develop procedures/strategies to embed cognitive principles into the curricula for the students and training programmes targeted towards reskilling the workforce and changing the manner of classroom delivery.

Professor Annabel Chen Shen-Hsing, Director
Nanyang Technological University

Professor Zoe Kourtzi, Director
University of Cambridge

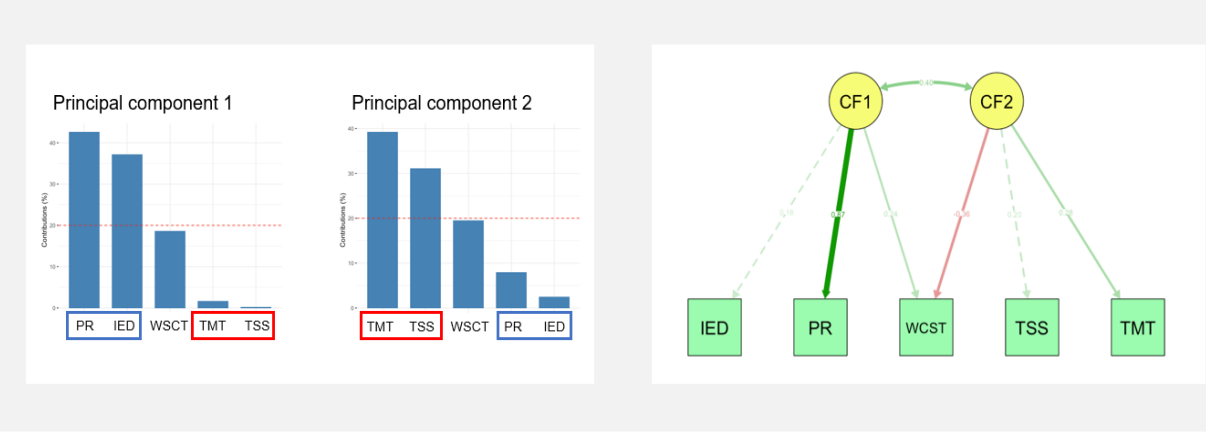
Update on Cognition Workgroup

Neurocognitive model of flexible learning

Since April 2021, the Cognition Workgroup has worked towards finalising the task battery for the WP0.1 characterisation study. **Dr Ke TONG (Research Fellow, NTU**) has modelled the pilot data that was collected from N = 85 healthy young adults on tasks measuring cognitive flexibility, structure learning, working memory, inhibition and intelligence. Initial results from the principal component analyses (PCA) suggest that the cognitive flexibility tasks may be divided into two clusters (see Figure 7.1, which could reflect different sub-components of mental flexibility. These data (and other analyses) have informed our final task selection. Further, a new collaboration with UCL Professors Jonathan ROISER and Quentin HUYS together with PhD student Ms Anahita TALWAR has been formed to apply advanced modelling to the cognitive flexibility task data. Further, **Dr Kastoori KALAIVANAN (Research Fellow, NTU)** completed a Creativity pilot study with N = 16 young adults. These data were used to establish the appropriateness of widely-used creativity tasks (e.g. Remote Associates Test (RAT), Alternate Uses Test (AUT), Torrance Tests of Creative Thinking (TTCT)) for the local Singaporean context. The Cognition workgroup has worked closely with the Social workgroup to finalise the tasks and protocols for WP0.1, and the full ethics application is now ready and pending submission.

The Cognition workgroup also organised and successfully delivered two CLIC training workshops.

CLIC Training Workshop 1: WP0.1 Task Delivery & Basic Data Checks (24th—25th May and 5th–7th July) was led by Dr Kalaivanan under the guidance of CLIC Deputy Director **Asst Prof. Victoria LEONG (NTU)**. This workshop provided a theoretical overview of WP0.1 measures, practical instruction on best practices for task administration and basic data quality checks. The workshop featured guest speakers from Cambridge including **Prof. Trevor ROBBINS (Senior Scientific Advisor, CAM)**, **Prof. Henriëtte HENDRIKS (PI and Deputy Director, CAM)** and Dr Christelle Langley, and was attended by 25 people (of which ~15 attended in person, see Figure 7.2) despite COVID-related disruptions.



Exploratory analysis-informed two-factor CF model
Left: Principal component analysis (PCA) seems to suggest two clusters of CF tasks. Probabilistic Reversal (PR) and Intra-Extra Dimensional Shift (IED) contribute mostly to the 1st extracted principal component, while Trails Making Test (TMT) and Task Set Switching (TSS) contribute mostly to the 2nd principal component. The contribution of Wisconsin Card Sorting Test (WCST) is inconclusive. **Right:** One possible structure of the proposed two-factor CF model, informed by the exploratory analysis from the pilot data.

Figure 7.1: Initial results from computational modelling analyses. *Dr Ke TONG*

CLIC Training Workshop 2: Advanced Data Analysis and Modelling (13th—15th and 22nd September) was hosted by CRADLE and led by Dr Tong under the guidance of Asst Prof. Leong. This workshop focused on advanced computational analyses of the cognitive flexibility, inhibition, and working memory tasks. Talks were given by international experts including Asst Prof. Yuval HART (Hebrew University of Jerusalem, Creative Foraging Game), Dr Vasilis KARLAFTIS (University of Cambridge, structure learning), Asst Prof Rui WANG (Chinese Academy of Sciences, structure learning under uncertainty), Ms Anahita TALWAR (University College London, attention set shifting modelling with the CANTAB IED task), Dr Leor ZMIGROD (University of Cambridge, behavioral consequences of cognitive rigidity for sociopolitical identities and beliefs) and Professor Rudolf N. CARDINAL (University of Cambridge, approaches to computational psychiatry), see Figure 7.3. This CRADLE workshop was very well-received with between 20-25 attendees on average, and modelling methods development will continue with the formation of a CLIC Computational Modelling Discussion Group.

CLIC Training Workshop 3: Introduction to EEG (27th—30th Sep) was led by **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** under the guidance of Asst Prof. Leong. This workshop aimED to provide a general introduction to EEG theory and techniques as well as hands-on training for adult and infant EEG data acquisition using the new CLIC high-density gel-based wired/wireless EEG systems. Training in EEG analytical methods will continue through the formation of a CLIC EEG Discussion Group.

Two publications have been produced by the Cognition Workgroup to date. The first article, now in press at the *Journal of Medical Internet Research* (a Tier 1 journal) reports our new Remote Guided Testing (RGT) methodology that was developed by the CLIC Cognition workgroup, led by Asst Prof. Leong. The RGT method was tested and validated against face-to-face data collection methods in a cohort of N=85 young adults, and was found to yield data of equivalent quality, including reaction time measures, for a wide range of executive function, learning and cognitive tasks. The second article appeared in *The Conversation* in June 2021 under lead authors **Prof. Barbara SAHAKIAN (Co-I, CAM)** and Dr Christelle Langley (CAM), with contribution from all Cognition workgroup members. This article, titled "IQ tests can't measure it, but 'cognitive flexibility' is key to learning and creativity", garnered substantial worldwide readership (168,707 readers), 316 tweets and 3016 shares on Facebook (as of early September 2021) and was republished by the Singapore *Straits Times* on 1st July 2021.

Figure 7.2: In-person attendees at CLIC Training Workshop 1.

Update on Social Workgroup

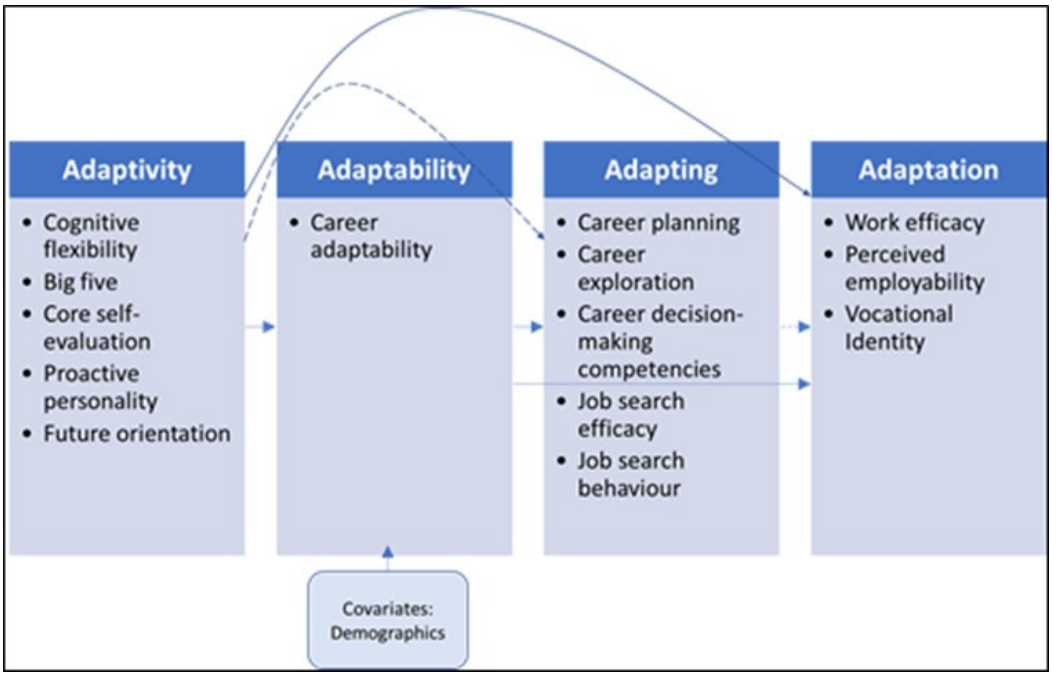
Social influences on flexible learning

Assoc. Prof. Georgios CHRISTOPOULOS is the lead PI (NTU) for the Social workgroup. He has been designing, organising, managing and preparing the WP0.1 studies and especially the measurements of social factors such as cooperation—competition and social decision making and tolerance of uncertainty. He is preparing the studies on social aspects for both the adult and adolescent samples (in collaboration with Singapore's National Institute of Education). He is managing the group of researchers mentioned below.

Ms Emma SAM Yoke Loo is a PhD student (IGP-CRADLE, NTU) under Assoc. Prof. Christopoulos's supervision. For her thesis, she will be developing a nomological network of Cognitive Flexibility (CF) to explain the role and impact of CF on career decision-making and career developmental outcomes.

Ms Sam has contributed to the general logistical and administrative planning for WP0.1 (e.g., IRB, pre-registration, developed Qualtrics questionnaire, and conducted data collection for two Pilot studies and data analyses). Specifically, she is responsible for performing the preliminary analysis of the first two pilot studies conducted by the CLIC's Social workgroup in October 2020 and January 2021 respectively. The preliminary analyses were primarily focusing on examining the quality of data and normal distribution. For instance, the construct reliability of all the scales included in the study was examined according to the factor structure suggested in the original publications. While the alpha coefficients of most of the scales were reasonable ($\alpha \geq 0.67$; Taber, 2018), few of the scales, e.g., the cultural and interpersonal dimensions of the I-ADAPT questionnaire showed unsatisfactory internal consistency (α = 0.48 and 0.40 respectively). Given the circumstance, exploratory and confirmatory factor analyses will be conducted to examine and establish more robust construct validity and reliability for all scales in the upcoming WP0.1.

Ms Sam is also assisting the participant recruitment for the WP0.1 study (determining the demographic characteristics of targeted populations). Finally, she is responsible for designing the CF and career development sub-study under WP0.1. Please refer to Figure 7.3 for the proposed theoretical framework to be tested in the sub-study of WP0.1.



The conceptual framework of the career construction model of adaptation. *Ms Emma SAM Yoke Loo*

Ms Irene MELANI (Research Associate, NTU) performed preliminary analyses on socio-cognitive variables of interest of the CLIC's Social Workgroup based on the pilot data collected by CLIC's Schools Workgroup from the adolescents sample. These analyses were aimed at examining the quality of the obtained data (e.g., whether the data distribution and properties met statistical assumptions and deemed to be acceptable) and suitability of the tasks/measures for adolescents sample and in Singapore's context. The results of these analyses were used to inform and decide the tasks/measures to be included in WP0.1, making sure that there is a significant overlap in the tasks/measures administered across the Social and Schools Workgroups to address relevant research questions of interest (e.g., socio-cognitive moderators of cognitive flexibility in young adults versus adolescents). In addition, to probe the relationships between socio-cognitive variables of interest and the hypothesised moderation by socio-cognitive variables with creative outcomes, a series of correlation and linear regression analyses were performed. One noteworthy result suggested the potential negative relationships between intolerance of uncertainty and creativity, as expected. Specifically, a higher score on the Need for Closure measure (Roets & Van Hiel, 2011) was negatively associated with performance on a creative drawing task (Urban, 2005; see Figure 7.4). For an overview, the correlation matrix showing the relationships of the variables of interest is presented below (see Figure 7.5).

Ms YAP Hui Shan (Research Assistant, NTU) contributed to the general logistical and administrative planning for WP0.1, e.g. preparations of IRB and pre-registration, setup the survey forms—including designing ways to allow for some questionnaires to be administered online—that will be used for data collection for both adults and adolescents study and drafted a portion of the SOP. In addition, she conducted data collection for one of the pilot studies and examined descriptives for data collected in the pilot study (for example, the time taken for each session) which allows for better planning for the subsequent WP0.1 study.

Ms TAN Yan Fen (Research Assistant, NTU) is the Variable Naming and Data Codebook Lead of the Social Workgroup and is in charge of setting up the pilot and WP0.1 data codebook, renaming raw pilot data and developing the data management plan. In addition, she is the Recruitment Team Lead and is in charge of WP0.1 participant recruitment (e.g., working on the screening questionnaire and developing the recruitment plan). She has also contributed to the general logistical

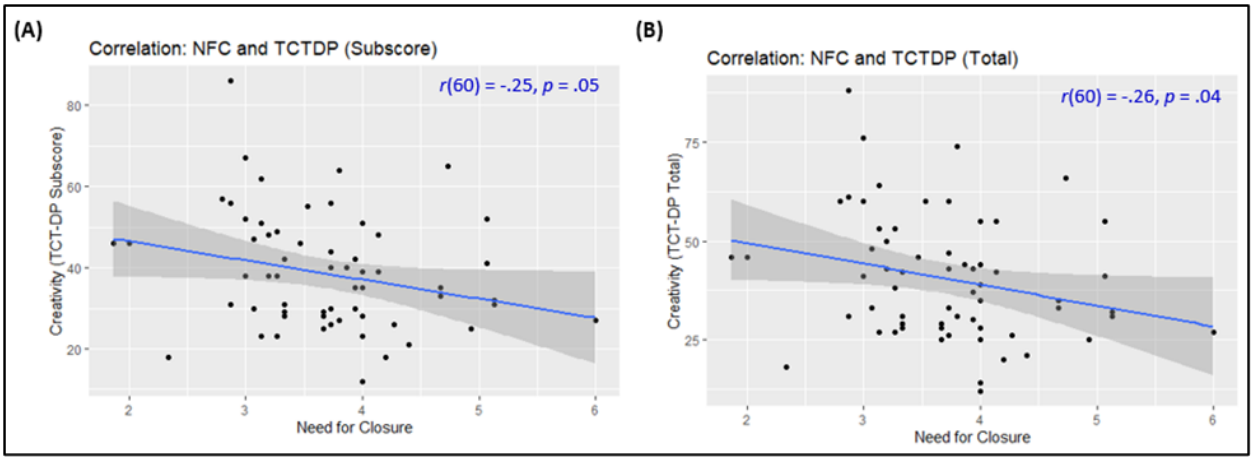


Figure 7.4: Correlation between measures of intolerance of uncertainty (Need for Closure; Roets & Van Hiel, 2011) and creative drawing task (TCTDP; Test for Creative Thinking - Drawing Production; Urban, 2005) score before (A; Subscore) and after (B; Total) bonus points for completion time were added. The higher one's need for cognitive closure (indicative of lower tolerance to uncertainty), the lower one's creative performance.

Ms Irene MELANI

and administrative planning for WP0.1 (e.g., preparing for the pre-registration of a study).

Ms LEE Li Ling (Research Assistant, NTU) contributed to the general logistical and administrative planning for WP0.1 (e.g., preparations of IRB and setup of questionnaire). In addition, she is part of the recruitment team for WP0.1 where she contributed to the logistical and administrative planning for participant recruitment (e.g., preparations of recruitment plan).

Ms CHAN Yuan Ni (Research Assistant, NTU) assisted in contributing to the general logistical and administrative planning for WP0.1 (e.g., IRB and pre-registration preparations). Ms Chan is also responsible for updating a manual consisting of detailed descriptions of the questionnaire used in the study for the social workgroup. She is also currently involved in setting up the Qualtrics survey form that will be used for data collection.

Ms PEI Jia Ying (Research Assistant, NTU)'s main research interest lies in the relationships between social and cognitive factors of adolescents and adults. Ms Pei is the data management lead of the Social Workgroup and ensures data compliance within the workgroup by adhering with the data management guidelines. She is also involved in setting up the Google Workspace structure for the Social team to allow ease of sharing of files and information. She worked with her team members with setting up the pilot and WP0.1 data codebook.

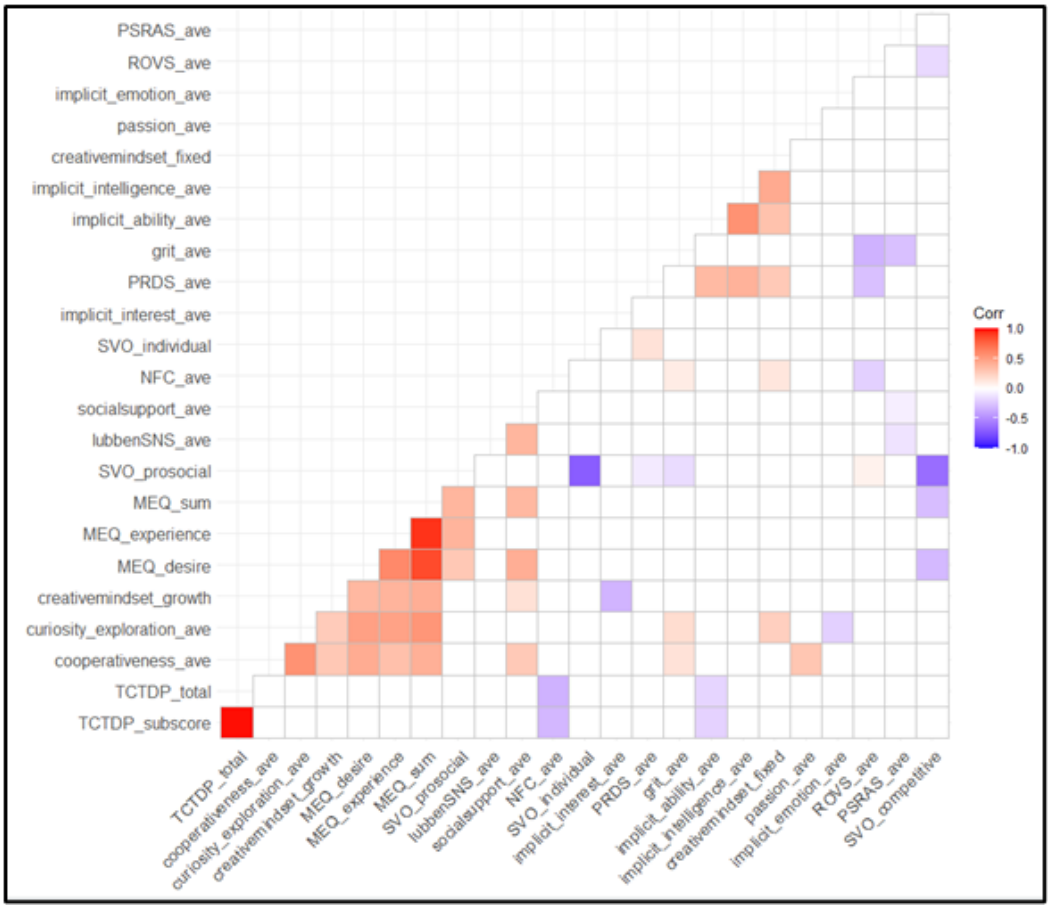


Figure 7.5: Correlation matrix of variables of interest obtained by the Schools Workgroup from the adolescents sample in a pilot data collection. Coloured boxes represent correlations that are statistically significant or tend towards statistical significance. Red indicates positive correlations; purple indicates negative correlations. The intensity of the colour represents the magnitude of the correlations, with darker shades representing greater and lighter shades representing smaller magnitudes of correlation.

Ms Irene MELANI

Update on Schools Workgroup

Real-world translation to education

Under the guidance of **Prof. David HUNG (PI, NTU/NIE)** and **Dr TEO Chew Lee (Co-I, NTU)**, **Dr Nastassja LOPES FISCHER (Research Fellow, NTU)** has been assigned to coordinate the Schools Workgroup team regarding their day-to-day tasks in order to successfully accomplish the project's milestones. Together with the Schools team, she has been involved in planning and delivering two workshops that communicate the relevance of research related to the CLIC project to educational practice. In the first workshop she delivered a component on Digital Technology in Education to Humanities Master Teachers from Singapore's Ministry of Education. In another workshop, she introduced teachers from Singapore, Hong Kong and China to the neuroscientific basis of executive functions studied by CLIC, highlighting their relevance to Knowledge Building pedagogical practices. Moreover, she organised a training workshop for CLIC's project members about the best practices for electroencephalography data collection and analysis. Dr Fischer has also been involved in the data collection preparation of the secondary students' cognitive performance in a classroom setting, including liaising with schools and coordinating the technical and logistics needs to ensure a smooth data collection process. In addition, under the guidance of **Asst Prof. Victoria LEONG (PI, NTU),** Dr Fischer has been involved in establishing a modelling approach for a statistical learning task integrating behavioural and electrophysiological measures.

Ms Phillis FU Wei Li (Research Associate, NTU) has been working under the supervision and guidance of Prof Hung and Dr Teo. She has contributed to preliminary data analysis from pilot study conducted earlier and collaborated with members of other workgroup on data analysis. Ms Fu is involved with project dissemination with schools which participated in the pilot study to work on their further involvement in the project. Under the guidance of **Prof. Henriëtte HENDRIKS (PI and Deputy Director, CAM)**, she is also a member of the social media team of CLIC project. Currently, she is working on the data collection plan for the actual study in the face of COVID-19 restrictions.

Mr Timothy LEE (Research Associate, NTU) has been involved in planning and delivering two workshops that communicate the relevance of CLIC-related research to educational practice. He delivered a component on Digital Technology in Education in a workshop to Humanities Master Teachers from Singapore's Ministry of Education. In another workshop, he introduced teachers from Singapore, Hong Kong and China to the executive functions studied by CLIC, highlighting their relevance to Knowledge Building pedagogical practices. Mr Lee has also been involved in data preparation for analysis, including setting up a team data dictionary and writing scripts to process data collected in earlier CLIC pilot studies. In addition, under the guidance of Asst Prof. Leong, Timothy has been involved in establishing CLIC's data handling guidelines and ensuring that they are compliant with university policies and other requirements.

Dr Ryutaro UCHIYAMA (Research Fellow, NTU) has been conducting data analysis of pilot data collected earlier across three schools, and has found preliminary patterns among the cognitive and social variables. He has given a tutorial on data analysis in the statistical programming language R to the CLIC research staff in an internal workshop, and has also co-hosted a seminar on "Digital Media and the Student's Mind" that the Schools Workgroup offered to the MOE Master Teachers Humanities Cluster.

Update on Neuroimaging Workgroup

Neuroimaging

The Neuroimaging Workgroup in CLIC has set up and piloted the WP0.2 MRI protocol used to measure changes in brain activity before and after the structure learning intervention. This comprises pulse sequences such as resting-state functional magnetic resonance imaging (fMRI), multiparameter mapping (MPM) and magnetic resonance spectroscopy (MRS). Pilot data has been pre-processed and checked for data quality through consultations with experts at the University of Cambridge. Planning of the analyses pipelines is in the works. Close collaboration with the team at the Cognitive Neuroimaging Centre (CoNiC) NTU has been initiated to coordinate a tight schedule planned for the MRI data collection. Bi-weekly meetings with CoNiC have been scheduled to discuss the complex logistics involved to ensure smooth MRI data collection.

In addition, the Neuroimaging Workgroup is in the midst of preparation for a pilot of the WP0.2 structure learning intervention programme. Pre- and post-cognitive flexibility measures will be collected during the pilot kickstarted in mid-October. This pilot will play a pivotal role in allowing the team to better stage the intervention programme and evaluate its potential efficacy at training cognitive flexibility. Training manuals and logistics protocols have been developed to familiarise part-time NTU undergraduate student Research Assistants hired to support the administration of the cognitive behavioural task battery and the month-long cognitive flexibility intervention.

Apart from developing research protocols, preparing for and implementing the studies for WP0.2, the team is also the main lead in the procurement and setup of CLIC's data and IT infrastructure. This involves the following: (1) network-attached storage (NAS) system that will mainly be used to store personal identifiable and neuroimaging data (e.g., MRI and EEG), as well as back-ups of all data generated by CLIC; (2) physical analyses servers to support computationally intensive research work needed by CLIC's research staff; (3) REDCap system to establish a data dictionary for CLIC. This infrastructure will play a particularly critical role in the support of current ongoing work programmes (i.e., WP0.1 and WP0.2) as well as future work programmes within CLIC.

Other activities and achievements

Prof. Annabel CHEN Shen-Hsing (Director, NTU) has received the following grant awards since the last report:

- NIE Education Research Funding Programme (external Co-I)—Growth in Bilingual & Biliteracy Proficiency: Environmental, Individual & Experiential Factors (GIBBER)—Project 4 (2021-2025)
- Workforce Development Applied Research Fund (Institute for Adult Learning) Grant (Co-I) Dialogical Inquiry: Developing Quantitative Instruments for Profiling Future Skills (2021-2024)
- WDARF (IAL) Grant (collaborator) Measuring employability and life-long learning mindsets needed for careers in the 21st century (2021-2023)

Asst Prof. Victoria LEONG (Deputy Director, NTU) has received the following grant awards since the last report:

- Wellcome Trust LEAP Award
- Singapore Social Sciences and Humanities Research Fellowship—The digital future of human learning: Social optimisation of digital media for early learning
- Singapore Ministry of Education Tier 2 Grant (SGD$628,040, 2021-2024)—How do depressed and anxious maternal moods shape infant affective cognition?

Dr Kastoori KALAIVANAN (Research Fellow, NTU) gave a presentation at The Centre for Research and Development in Learning (CRADLE) booth showcasing CLIC as one of the Science of Learning projects at the *Singaporean Researchers Global Summit 2021*.

Ms Phillis FU Wei Li (Research Associate, NTU) gave a virtual presentation titled "Perfectionism, anxiety and depressive symptoms in adolescents: The mediating role of temporal focus" at the *32nd International Congress of Psychology 2020*+ on 21st July 2021.

The Schools Workgroup has been involved in several engagements with Singapore school teachers to connect CLIC's research in psychology and neuroscience with the educational experience of teachers.

Thus far, the team has planned to deliver three workshops. Two of these, "Digital Media and the Student's Mind" and "The Psychology and Neuroscience of Knowledge Building" have been delivered, while "The Neuroscience and Psychology of Learning Workshop" was planned for 25th-26th October 2021.

eCO$_2$EP

CARBON CAPTURE AND UTILISATION USING A TABLE-TOP CHEMICAL FACTORY

This was CARES' first large Intra-CREATE project and was aimed at developing a "table-top chemical factory" that uses electrochemical processes to convert CO_2 into ethylene or to 1-propanol – two molecular products widely used in the chemical industry. Earlier research carried out at CREATE had demonstrated that CO_2 molecules could be transformed into hydrocarbons through the application of electro-catalysis. eCO$_2$EP's research studied the viability of scaling CO_2 reduction processes, including techno-economic evaluation of the use of off-peak renewable electricity in areas with excess capacity, with the goal of developing new energy-chemistry solutions for a more sustainable future. The project completed in June 2021.

eCO$_2$EP Principal Investigators:

Professor Alexei LAPKIN
University of Cambridge

Professor Joel AGER
University of California, Berkeley

OVERVIEW

eCO$_2$EP: A Chemical Energy Storage Technology was established in 2018 as an Intra-CREATE collaboration between the University of Cambridge, University of California, Berkeley, the National University of Singapore and Nanyang Technological University. The objective of the project was to develop ways of transforming carbon dioxide (CO_2) emitted as part of the industrial process into compounds that are useful in the chemical industry supply chain. To this end, researchers aimed to produce a "table top chemical factory" which uses electrochemical processes to convert CO_2 into ethylene or to 1-propanol—two molecular products widely used in the chemical industry.

The eCO$_2$EP project completed in June 2021, following a six-month no cost extension to the original term. This final update presents a summary of the project's achievements, along with some recent updates from researchers who have since transferred to other CARES research projects.

Professor Alexei Lapkin, PI
University of Cambridge

Professor Joel Ager, PI
University of California, Berkeley

Update on work package 1

New catalyst discovery and characterisation

The project developed cathode materials with leading performance characteristics and, keeping in mind the scale-up goals of the project, scalable deposition methods for them. In order to greatly reduce the cycle time for catalyst design-synthesize-test, the project has pioneered the use of proton ionisation mass spectroscopy for reaction products monitoring. This method provides real-time (50 ms) and sensitive (ppb) detection of target products of our reactors. Importantly, the method's extreme sensitivity revealed previously unseen reaction intermediates and by-products. We learned that that elementary steps of the chemical network in the high-rate, high pH conditions used in our production reactor are quite different than those in investigated in prior studies at lower current density in smaller reactors. We also found new reaction mechanistic pathways and generation of polymer by-products that affect the catalyst stability.

By performing rapid vetting of catalyst formulations at small scale (1 cm^2) and evaluating promising candidates and addressing issues of overall reactor design at intermediate scale (2-4 cm^2), we were able to select a gas diffusion electrode approach suitable for use in our 100 cm^2 table top reactor. In doing so, we identified a number of critical issues, such as the importance of metal precursor and impact of dopants. Notably, our GDE cell performance in terms of rate/current density and selectivity to the C2 projects which are the goal of the eCO_2EP study are at or beyond published reports from similar GDE-based reactors, Table 1.

Table 8.1: Performance parameters of eCO_2EP gas diffusion meet or exceed those of published reports.

	Partial current density of C2+ products	**vs. RHE**	**Electrolyte**
eCO_2EP	1.3 A/cm^2	-0.60 V	3.5 M KOH
Science, 2018	0.6 A/cm^2	-0.67 V	3.5 M KOH + 5 M KI
Science, 2020	1.3 A/cm^2	-0.91 V	7 M KOH

Update on work package 2

Modelling and data informatics

While some initial kinetic and process models have been published for electroreduction of CO_2 into ethylene, none have so far attempted to capture the complexity of the physics involved to enable inverse design. The project has developed a detailed microkinetic model, linking with the observed experimentally intermediates and dynamic data, and a detailed GDE model that allows to link the nature of a catalyst with the structure of GDE and final experimental observations.

Mr Simon RIHM (PhD student, CAM) continued his work on kinetic modelling of the CO_2 Reduction Reaction (CO_2RR) by utilising data from first-principle calculations as well as analysing possible reaction pathways towards products observed in the table-top reactor.

He proposed reaction paths towards all observed products by comparing experimental data collected within the project to reaction steps and data reported in the literature. For this, he focused on C2+ products as well as different functional groups such as carboxylic acid. Different hypotheses regarding the formation (electrochemical as well as subsequent reactions in aqueous solution) were formulated and further experiments proposed to assess them.

Based on these assessments he identified coupling reactions and different types of reduction and hydrogenation reactions as the key selective mechanisms and drew up a complex reaction mechanism accordingly. He developed a collection of different software tools for micro-kinetic modelling of electro-catalytic processes: From pre-processing the data to achieve thermodynamic consistency to simulation kinetics of different operating modes and post-processing the data as Flux Diagrams and Faradaic Efficiency graphs.

Mr Rihm is currently finalising the calibration of the model parametrisation by comparison with measurement data. He intends to publish the results as first-ever micro-kinetic study of an elementary-step-based CO_2RR mechanism to a wide variety of C1 and C2 products where coverages, efficiencies and fluxes can be assessed individually.

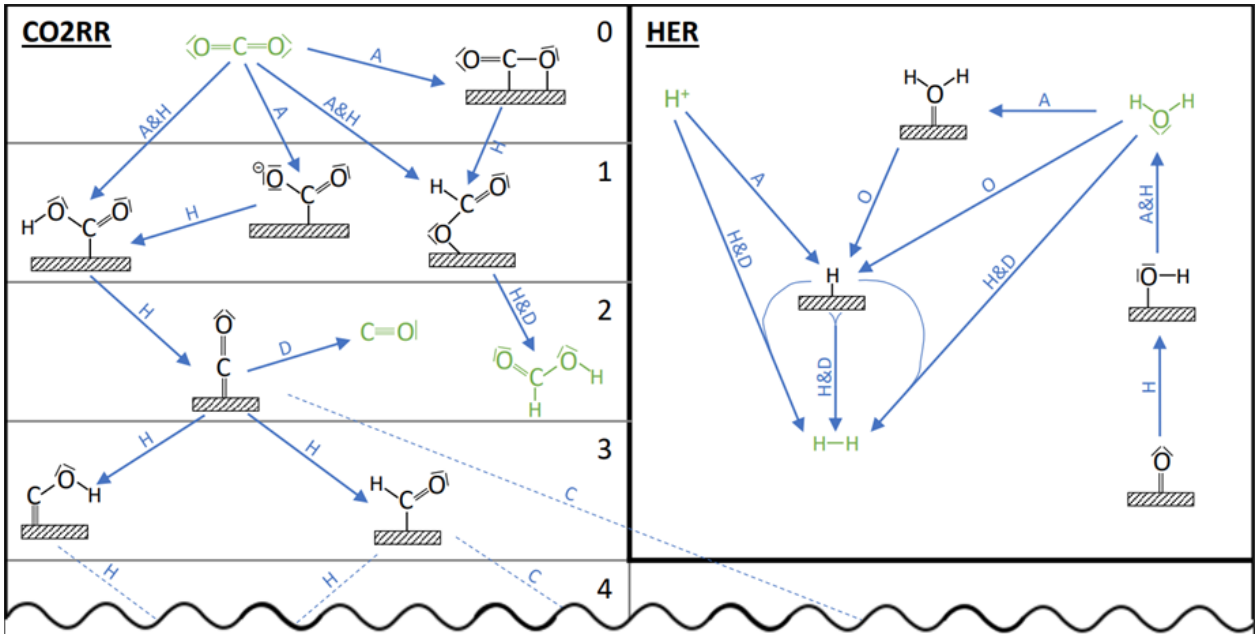


Figure 8.1: Initial section of the CO2RR mechanism used for the microkinetic modelling, showing adsorption (A) and desorption (D) reactions as well as hydrogenation (H) and coupling (C) elementary steps.

Update on work package 3

Chemical factory on a table

Separations: The topic of product separation at the end of the electrocatalytic reaction of CO_2 into ethylene was not addressed in prior literature in depth. In the project this problem was explored systematically, looking at gas-phase separation, liquid-phase separation and an alternative process via ethanol as the main product. The project outputs include:

- Design and experimental validation of liquid products separation; these were integrated into the test bed reactor.
- Development of new adsorbents, process characterisation and technoeconomic analysis of gas products separation.

Gas Diffusion Electrode (GDE) and electrolysis cell development: The aim of GDE development was to achieve a 100x100 mm scale at high current, high ethylene selectivity and good stability. All these aims were achieved through systematic design of the electrode and the cell. Areas of significant cooperative work between all the work packages were as follows:

- Cathode materials: conductors, catalysts, gas diffusion membrane.
- Cell design: gas and liquid flows and controls.
- Anode materials and environment, including stability.

Integrated chemical plant: The key aim of the project was to demonstrate the feasibility of scaled reaction and separation as an integrated process. This was achieved by combining the scaled 100x100 mm GDE cell with liquid products separation based on a membrane process developed in the project (Figure 8.2). Additionally, extensive data on gas products separation was collected and the integrated plant performance will be demonstrated in publications through simulations. The eCO$_2$EP table top chemical factory has multi-hour stability at commercially viable current densities and also the ability to work with intermittent electrical power. These data are unique so far in the literature and will lead to a much more detailed technoeconomic analysis of this technology.

Figure 8.2: Table top chemical reactor constructed in eCO$_2$EP for the conversion of CO_2 to value-added chemicals.

Dr Magda BARECKA's (Research Fellow, CARES) main research interest lies in the development of CO2-based manufacturing concepts that can be scalable and viable on the current market. Within eCO2EP project, Magda worked towards the design of the entire table-top factory for manufacturing of ethylene from CO_2. She has also integrated the techniques that she developed for liquid products separation with the electrochemical reactor. Till May, she continued to supervise an internship (under the NTU Professional Internship programme) that supports testing a wide variety of membranes and perform long-term separation runs. Till the end of June, she has been primarily focusing on supporting team efforts towards reaching the ultimate goal of eCO2EP project: demonstration of the entire plant, that was successfully achieved. She has also published two papers (with *Cell Press*, see Figure 8.3 for a graphical abstract).

Dr Mikhail KOVALEV's (Senior Research Fellow, CARES) research interests focus on the area of gas diffusion electrode preparation (GDE) and analytical studies of its performance. The complicated GDE structure comprises many layers that were optimised for large size – over 100 cm^2 – which is an increase from the previously reported size of 16 cm^2. Large electrodes tested in a flow cell with working size of 10x10 cm^2 shown similar efficiency as in a small cells 1x1 cm^2 and 2x2 cm^2. As a summary, developed GDEs during the eCO_2EP project met project goals of increasing CO_2 reduction process to an industrial scale where GDEs can perform 8+ h at the current density J = 0.5 A/cm^2 and 2+ h at J = 1.5 A/cm^2. A SEM picture of a GDE cross-section is shown in Figure 8.4.

Another of Dr Kovalev's activities is to set up analytical methods for reaction products analysis. Insights of the surface analysis and the use of Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer (PTR-TOF-MS) revealed possible routs of copper-based GDEs failure. The used GDEs were subjected to heating up to 300 °C where outgassed products were sampled and analysed with PTR-TOF-MS. The analysis of used GDE thermolysis products shown the formation of acrolein which is preciously have been detected and existed only in theoretical studies.

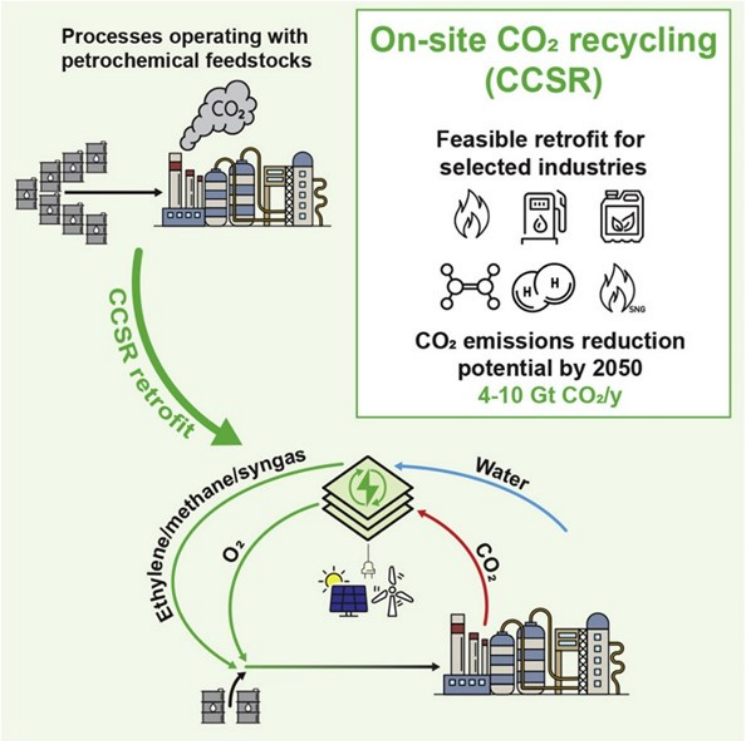


Figure 8.3: Graphical abstract from the article "Carbon neutral manufacturing via on-site CO_2 recycling", published recently in iScience. This manuscript showcases the global potential of the new carbon utilisation approach (Carbon-Capture On-Site Recycling) proposed to drastically reduce CO_2 footprint of chemical manufactures with a minimum interruption to their operation. Credit: iScience, Cell Press.

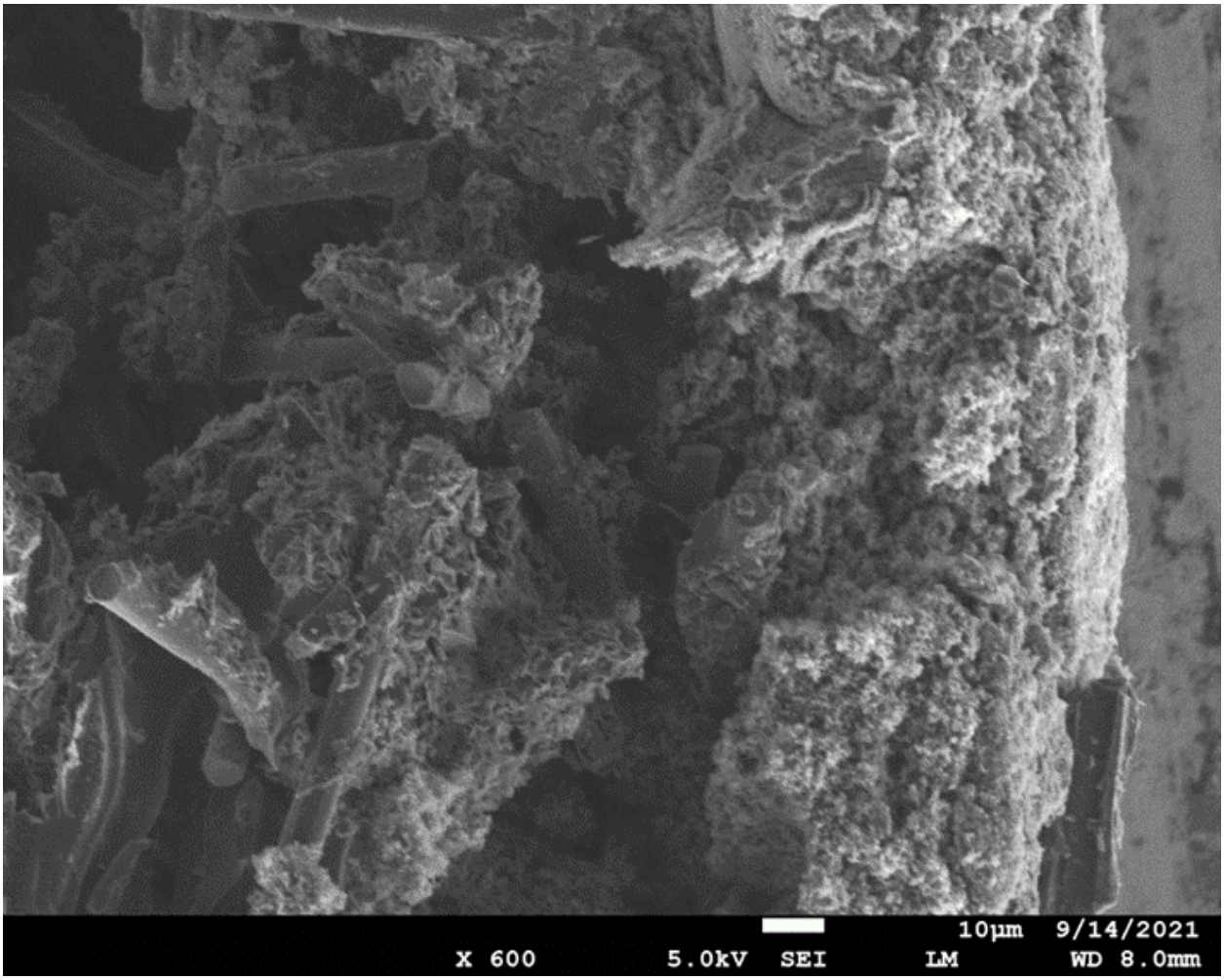


Figure 8.4: Cross-section SEM image of copper-based GDE.

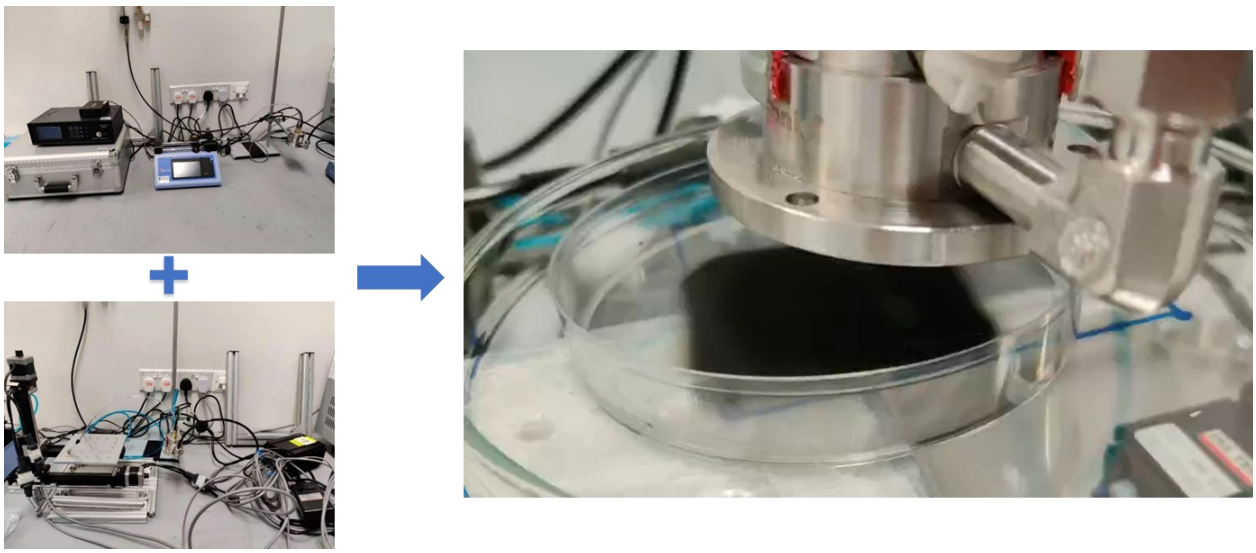
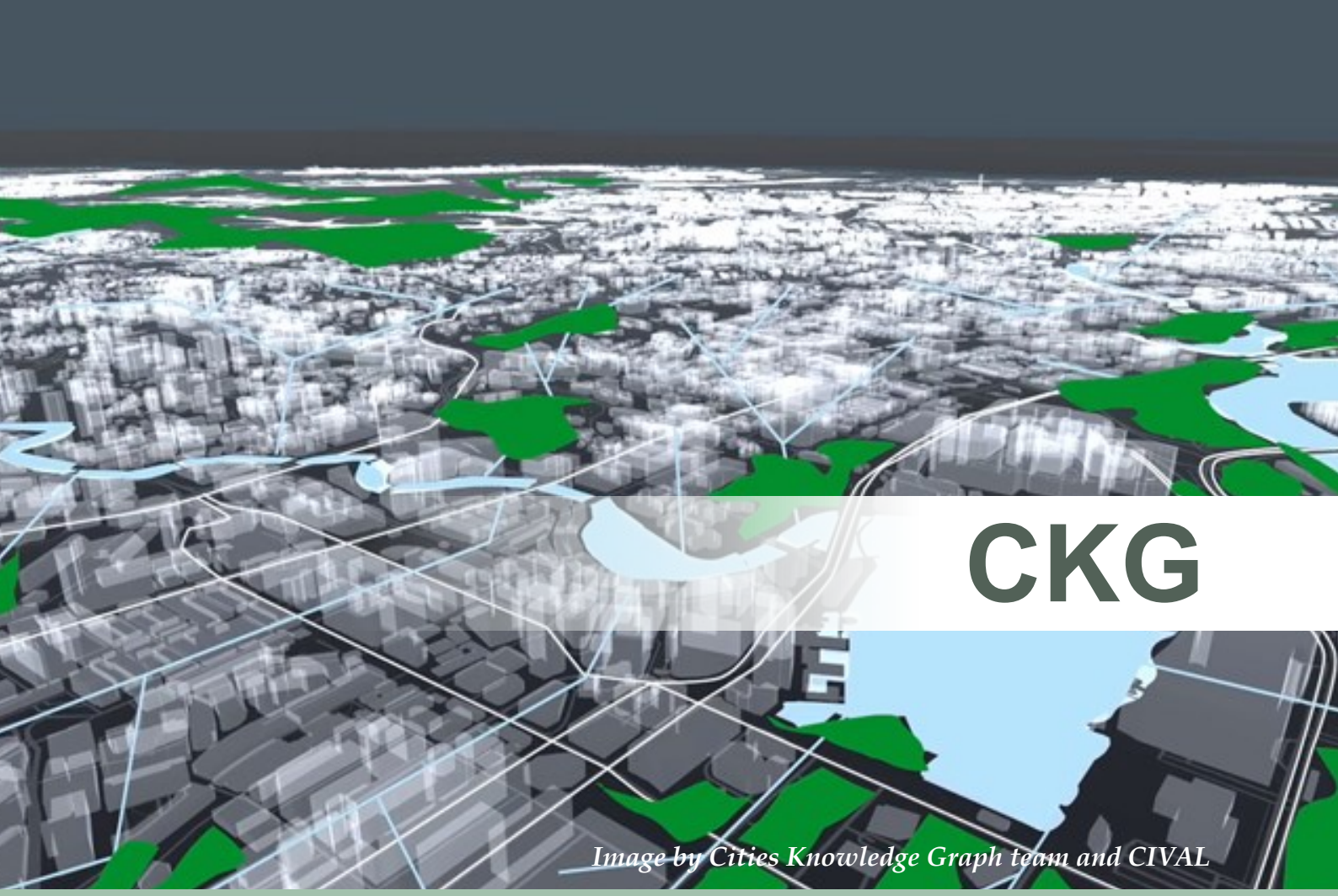


Figure 8.5: Scalable fabrication of CO_2R cathode; spray coating of Cu nanoparticles on carbon paper.

Other activities and achievements

Dr Magda BARECKA (Research Fellow, CARES) gave an invited talk titled "Economically viable pathways for solar fuels production by means of CO_2 electrolysis" at the *AIChE 3rd Solar Energy Systems Conference*, 4-6 August 2021.

Mr Simon RIHM (PhD student, CARES) was admitted for PhD studies at the University of Cambridge where he will continue to work on the development and integration of novel computational models under the supervision of Prof. Markus KRAFT. Mr Rihm's studies will be supported by the CARES studentship programme as well as the Cambridge Trust International Scholarship and the Fitzwilliam College Lee Kuan Yew NUS PhD Studentship.



CKG

Image by Cities Knowledge Graph team and CIVAL

CITIES KNOWLEDGE GRAPH

Cities Knowledge Graph (CKG) aims to transform master-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 policy makers and planners by mapping interesting planning directions. It further ties together existing 3D geo-databases, such as URA Space, as well as novel analysis, simulation and visualisation tools developed by CARES and SEC, creating an unprecedented knowledge graph for master-planning.

CKG Principal Investigators:

Professor Markus KRAFT
University of Cambridge

Professor Stephen Cairns
ETH Zürich

OVERVIEW

Cities Knowledge Graph (CKG) is an Intra-CREATE collaborative project in the urban systems 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).

Over the past six months, we have progressed on several fronts with regard to developing new capabilities for the CKG. For instance, we have developed a mixed-use zoning ontology to link geospatial plot data with highly granular programme types that are allowed on the plot, based on its zoning type. Knowledge of the programme types that are allowed on each plot can help planners select a site for a specific function, or analyse the impact of zoning decisions on outcomes such as mobility or energy use and supply. In addition to the mixed-use zoning ontology, ontologies are being extended to describe all the thirty-two zoning types in the Singapore Master Plan. We have also linked available planning datasets from different governmental entities in Singapore, such as the Urban Redevelopment Authority (URA) and Singapore Land Authority (SLA) using the OntoCityGML ontology. By linking and instantiating these heterogeneous datasets in the dynamic knowledge graph, we could execute useful planning queries and derive various planning metrics, such as Site Coverage, Zoning Fragmentation, Zoning Density and Unbuilt Gross Plot Ratio (GPR) Potential.

Furthermore, we have been working on the addition of elements of a cognitive architecture that allows the automation of data processing tasks as well as sample analytical capabilities. This includes: 1) a CityImportAgent that automates the data validation and instantiation of CityGML 2.0 city models in the knowledge graph upon detecting the specified file type in the given directory; 2) a CityExportAgent which automates the export of the city model data needed for visualisation – the data could be exported for the whole model, or for different areas found via geospatial search, or for individual city object members, stored in the knowledge graph and 3) a Distance Agent which autonomously calculates the physical distance between two data instances in the knowledge graph by tracking external interactions with the representation via a web map client.

Moreover, we have evaluated the definitions of additional OntoCityGML concepts used in generating Level of Detail 4 (LOD4) models against the CityGML specifications and extended the 3D City Database Importer/Exporter tool developed at the Technische Universität München (TUM) to import LOD4 building data into the knowledge graph.

Professor Markus Kraft, PI
University of Cambridge

Professor Stephen Cairns, PI
ETH Zürich

Update on work package 1

Developing master-planning ontologies

Ms Heidi SILVENNOINEN (Researcher, SEC), supported by **Dr Pieter HERTHOGS (Senior Researcher, SEC)**, **Dr Zhongming SHI (Postdoctoral Researcher, SEC)**, and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES),** has been developing the mixed-use zoning ontology using Protégé, an ontology editor. This ontology can be used to link geospatial plot data (in CityGML format) with highly granular programme types that are allowed on the plot, based on its zoning type. These programme types include medical services, restaurants and apparel stores. Knowledge of the programme types that are allowed on each plot can help planners select a site for a specific function, or analyse the impact of zoning decisions on outcomes such as mobility or energy use and supply.

Analysing the impacts of zoning is particularly enabled by the mixed-use zoning archetypes developed by Dr Shi with the help of Ms Silvennoinen. In this work, Google Place data were used to formulate programme archetypes of all plots in Singapore, given their zoning type and gross plot ratio (GPR). These archetypes can be used to inform new development. Using an archetype for a plot with a similar GPR and zoning type, planners can simulate the energy and mobility performance of a plot that is currently being planned or developed.

In addition to the mixed-use zoning types, Ms Silvennoinen, with the help of Mr Chadzynski, is leading the expansion of the ontology work to all the thirty-two zoning types in the Singapore Master Plan. Currently, the team is finalising a manuscript on the mixed-use zoning ontology work. Ms Silvennoinen has also commenced work on a manuscript on the general zoning ontology work.

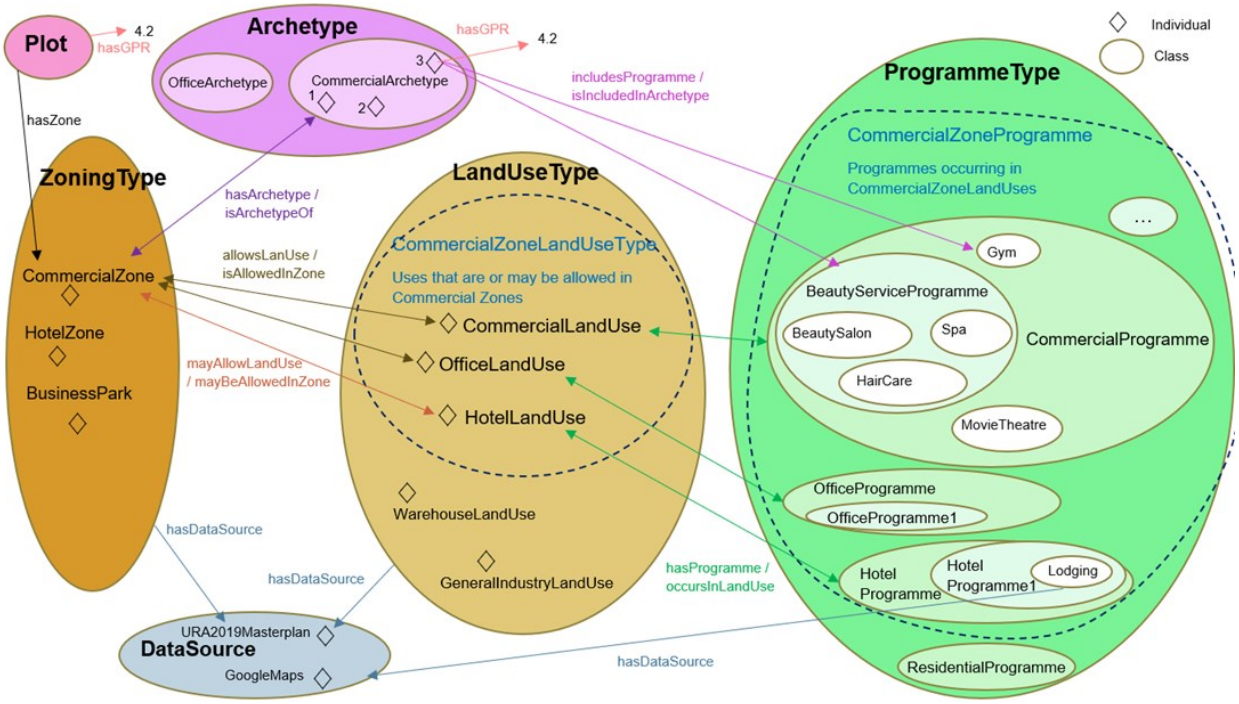


Figure 9.1: Diagram illustrating the ontoMixedUsezoning ontology for Singapore.

Ms Ayda GRIŠIŪTĖ (Researcher, SEC) and **Dr Aurel von RICHTHOFEN (Senior Researcher, SEC**) have linked available planning datasets from different governmental entities in Singapore, such as the Urban Redevelopment Authority (URA) and Singapore Land Authority (SLA) using the OntoCityGML ontology. These heterogeneous datasets include land use, ownership, building and transportation related data. By linking and instantiating these data in the dynamic knowledge graph, Ms Grišiūtė could execute useful planning queries and derive various planning metrics, such as Site Coverage, Zoning Fragmentation, Zoning Density and Unbuilt GPR Potential. For example, unbuilt GPR potential metric estimates unused plot's GPR capacity by comparing planned GPR with built GPR. These data can be further linked with more open datasets such as information of building programme types or with building energy simulation software for the assessment of urban building energy performance. This work demonstrates how the knowledge graphs enable the creation of planning indicators, that otherwise would not be possible to retrieve from individual datasets, by building on various openly available datasets in Singapore.

In order to import CityGML Level of Detail 4 (LOD4) model data into the knowledge graph, **Dr Jingya YAN (Research Fellow, CARES)** has evaluated the definitions of additional OntoCityGML concepts used in generating LOD4 models against the CityGML specifications. A total of ten concepts have been evaluated and Dr Yan concluded that the current definitions can adequately describe a LOD4 model example. Dr Yan has also modified six classes of the 3D City Database Importer/Exporter tool developed at the Technische Universität München (TUM) to use SPARQL based on the OntoCityGML ontology.

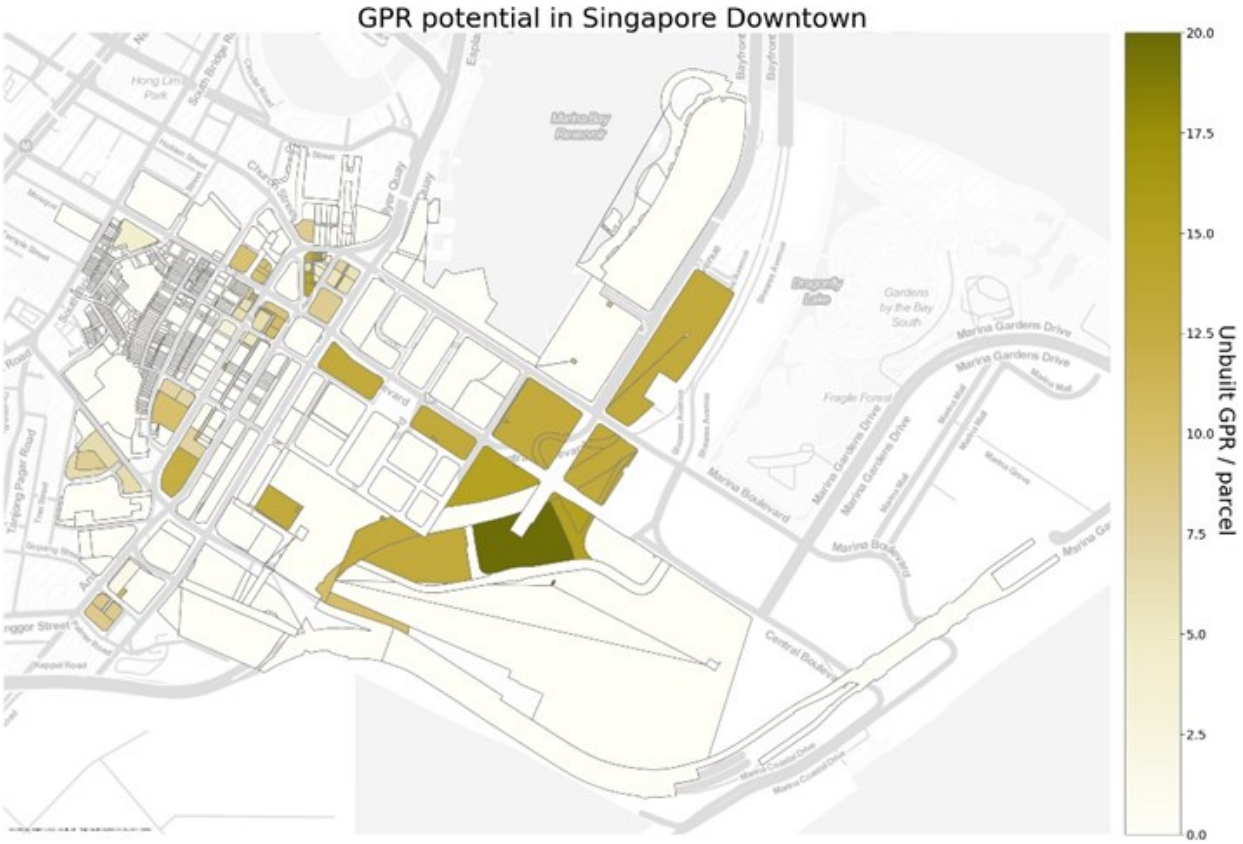


Figure 9.2: An example of a map of unbuilt GPR potential in Singapore downtown.

Update on work package 2

Developing the knowledge graph's architecture

Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES) has continued working on an architecture which is required for importing and exporting large datasets into the knowledge graph. Creating and updating City Information Models (CIM) via existing data curating techniques can be error-prone and time-consuming as this is usually done manually. Furthermore, legacy geographic information systems (GIS) also lack dynamics; existing data formats and modelling techniques make it difficult to keep the models up-to-date as they were designed to work with data distributed over multitude of different flat files. Such static models remove the historical aspect and do not allow insights on evolution, stagnation or deterioration of cities. Changes in CIM are also not visible without a complex process of importing/exporting multiple types of files for the entire city. Examples of such CIMs include extensible markup language (XML) file-based models describing various urban elements in CityGML standard, provided by the Open Geospatial Consortium (OGC). These are commonly used as a data exchange standard for city landscape management and planning systems, or even as a file-based data source for applications that visualise 3D city landscapes on the Web.

3D City Database that was developed at the Technische Universität München (TUM) aims to add flexibility and scalability to the CityGML based models by transforming XML into Relational Database Management System (RDBMS). Better data interoperability is also supported by the implementation of domain specific extensions. Despite this, utilising its Importer/Exporter tool application for data transformation processes to create and visualise CIM are still highly manual, making it error-prone, especially when larger models are taken into consideration. Consequently, Semantic 3D City Database, which is based on a semantic triple store backend instead of RDBMS, is introduced to enable dynamic geospatial knowledge graph capabilities. Most importantly, it removes the data interoperability limits of the original 3D City Database imposed by its default Closed World Assumption (CWA) in relational databases. This also opens a possibility of turning it into a semantic knowledge base instead, by enabling reasoning and truth maintenance capabilities via inferencing engines, together with OntoCityGML as its schema. In addition, the added geospatial search features allow for efficient retrieval of CIM data from specific regions bounded by a set of coordinates. However, in the last reporting period, data import as well as export still relied on the appropriately augmented Importer/Exporter tool and remained manual. While this approach successfully produces a semantic twin of Charlottenburg-Wilmersdorf CityGML 2.0 Level of Detail 2 (LOD2) model, the lack of automation became more prominent for the instantiation and linking of the remaining eleven districts of Berlin in the knowledge graph.

Hence, Mr Chadzynski, in close collaboration with **Ms Shiying LI (Software Engineer, SEC)**, **Ms Ayda GRIŠIŪTĖ (Researcher, SEC)** and **Dr Pieter HERTHOGS (Senior Researcher, SEC)**, has been working on the addition of elements of a cognitive architecture that allowed the automation of data processing tasks as well as sample analytical capabilities. This was used to produce a semantic representation of all the remaining Berlin districts in the knowledge graph, as well as

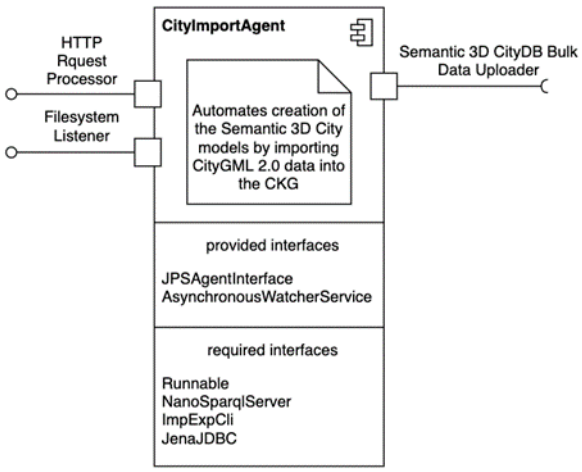


Figure 9.3: A component diagram of the CityImport Agent that automates the instantiation of city models in the knowledge graph.

visualise it using a web map client, along with obtaining some insights about distances of interest automatically by tracking external interactions with the representation.

In addition, Mr Chadzynski has been working on the CityImportAgent (as shown in Figure 9.4) that automates the instantiation of CityGML 2.0 city models in the knowledge graph by listening on two Internationalized Resource Identifiers (IRIs). Upon receiving a request on the Listen IRI, the CityImportAgent calls the JPS Asynchronous Watcher Service to watch for the appearance of new Geography Markup Language (GML) files in a directory specified by the request, in a separate thread. Upon receiving a request on the Action IRI, the CityImportAgent splits the file into smaller and more manageable sizes before importing each using four tasks running in separate threads. BlazegraphServerTask creates local instances of the NanoSparqlServer and puts them on a BlockingQueue that are to be picked up by the ImporterTask. The ImporterTask imports a CityGML portion into the local instance of the triple store using an augmented code. This process makes it possible to detect any import errors isolated to the particular portion. NquadsExporterTask uses the ExportKB Blazegraph code to create N-Quads files containing data transformed by the importer into a semantic form. At this point, local IRIs are replaced with The World Avatar (TWA) IRIs. NquadsUploaderTask reads the updated N-Quads file and uploads it to the BulkDataLoad endpoint of TWA.

Ms Huay Yi TAI (Software Developer, CARES), in close collaboration with Mr Chadzynski, is in the process of implementing a feature in the 3D City Database Importer/Exporter tool to support the import of coordinate reference system information into the knowledge graph. This involves reviewing methods which use Structured Query Language (SQL) queries in the original tool, and implementing their equivalents in SPARQL. The feature will allow for the storage of multiple datasets with different geospatial representations in the knowledge graph according to their coordinate reference systems and for efficient geospatial searches using the existing capabilities.

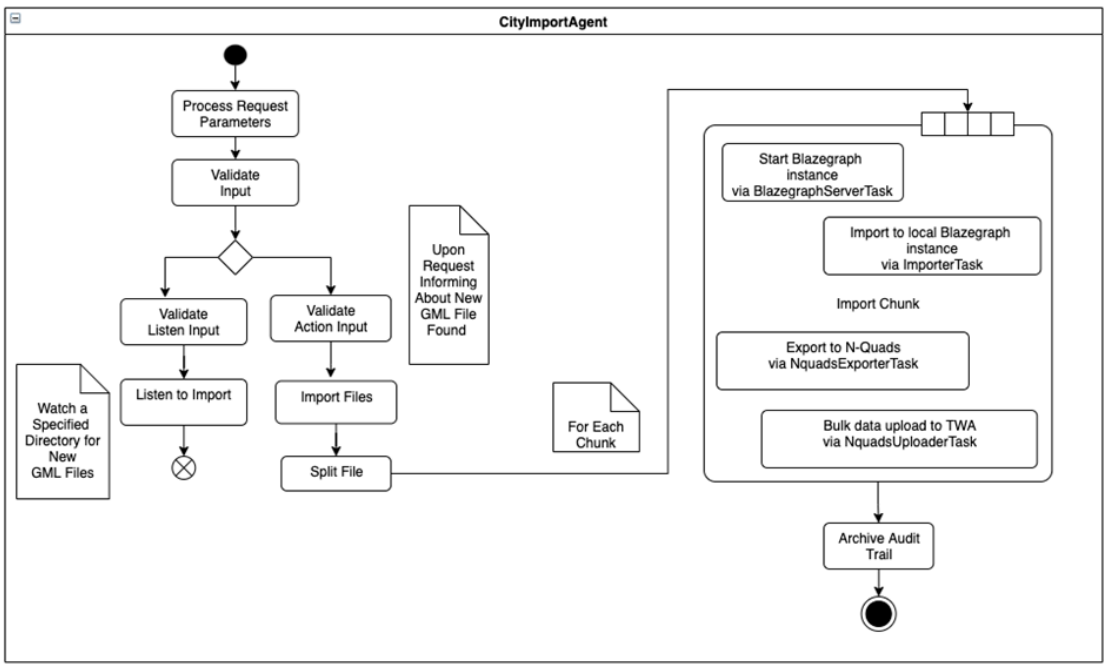


Figure 9.4: An activity diagram of the CityImportAgent that automates the instantiation of CityGML 2.0 city models in the knowledge graph by listening on two IRIs. Upon receiving a request on the Listen IRI, it calls the JPS Asynchronous Watcher Service to watch for the appearance of new GML files in a directory specified by the request, in a separate thread. Upon receiving a request on the Action IRI, it splits the file into smaller and more manageable sizes before importing each using four tasks running in separate threads: BlazegraphServerTask, ImporterTask, NquadsExporterTask and NquadsUploaderTask.

Ms Li has successfully extended the 3D City Database Importer/Exporter tool for extracting the geometry information of 3D city models from the Blazegraph triple store. In order to maximise the reusability of the legacy code and preserve the existing functionalities with relational databases like PostGIS and Oracle, two main components are implemented for the export operation (KMLexporter) with semantic databases: SQL2SPARQL Transformer and GeoSpatial Processor. The SQL2SPARQL Transformer translates the SQL statements to equivalent SPARQL statements according to the OntoCityGML schema. However, some SQL statements in the original tool make use of the built-in geospatial functions provided by PostGIS database, which are not present in the current Blazegraph version. Examples of such functions are: ST_TRANSFORM, ST_Area and ST_IsValid. These functions are used for filtering the query results. Therefore, the GeoSpatial Processor is implemented to provide geospatial functionalities to post-process and filter the query results to produce exactly same results as the built-in functions of PostGIS and Oracle geospatial databases. The query results are used for generating Keyhole Markup Language (KML) files. The exported KML files can be used to illustrate the city model in Level of Detail 1 (LOD1) with extruded display form. Figure 9.5 illustrates an example of the exported KML model in a close-up view.

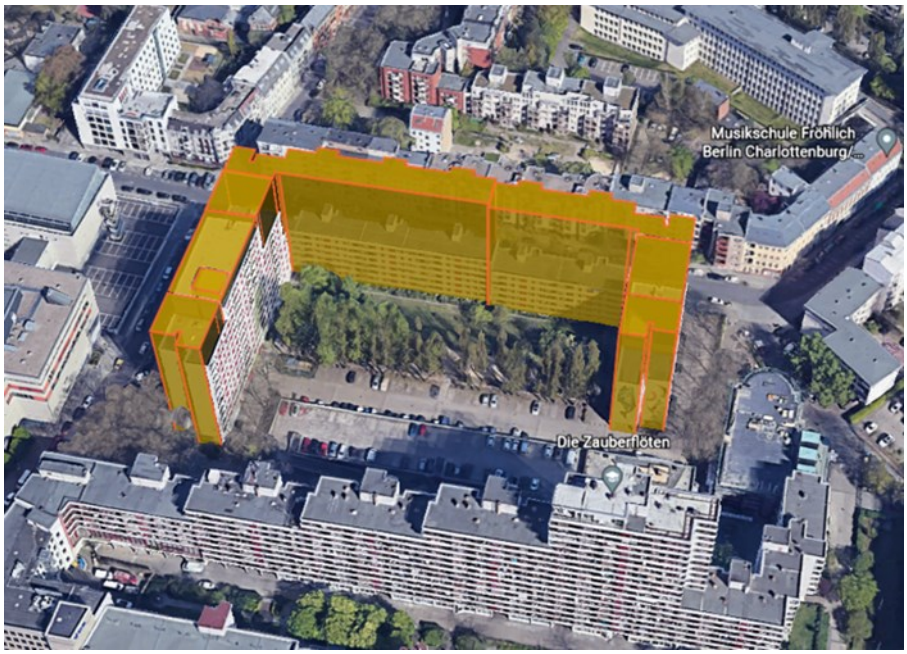


Figure 9.5: Visualisation of the exported KML model with extruded display form.

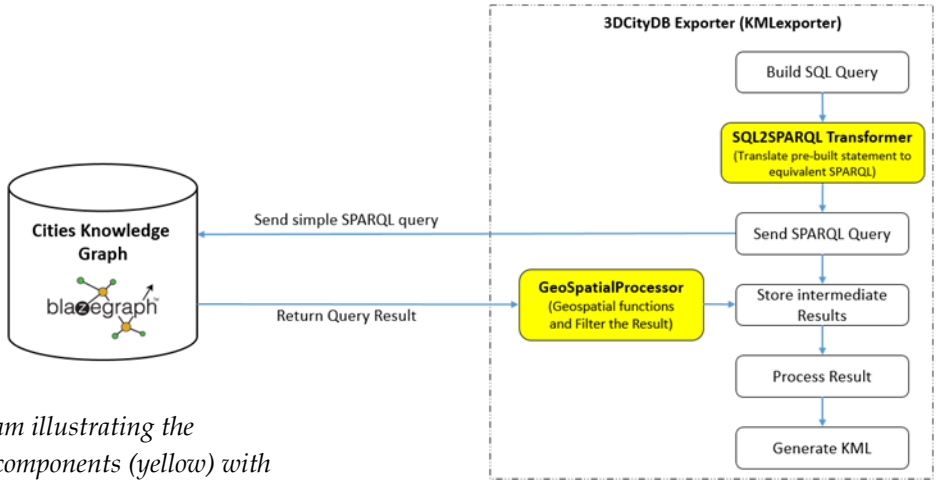


Figure 9.6: Workflow diagram illustrating the integration of the extended components (yellow) with KMLexporter.

Update on work package 3

Developing agents to operate software and integrate data

Dr Emily LLOYD (Research Fellow, CARES), in close collaboration with **Dr Zhongming SHI (Postdoctoral Researcher, SEC)** and **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, is in the process of packaging the City Energy Analyst (CEA) software as an agent that can apply the Semantic Web stack to read and understand information (e.g. Singapore building data) from the knowledge graph and modify its data values. In the first instance, the agent will store key CEA outputs such as buildings' energy demands and their photovoltaic energy potential in the knowledge graph. As the concepts required to store the output data are not currently available in the knowledge graph, Dr Lloyd has conducted research on the various existing energy ontologies including Semantic Web for Earth and Environmental Terminology (SWEET), Smart Appliances Reference (SAREF) ontology and Ontology for Energy Management Applications (OEMA), and concluded that the Domain Analysis-Based Global Energy Ontology (DABGEO) is most suitable to represent the CEA outputs in the knowledge graph.

Ms Ayda GRIŠIŪTĖ (Researcher, SEC), in close collaboration with Mr Chadzynski, has developed the Distance Agent which measures the physical distance between two data instances in the knowledge graph (Blazegraph), with the places represented as 2D polygons, 3D objects or points. This agent also updates the dynamic knowledge graph with distance information using a Units of Measure (OM) ontology. By considering the Z coordinate, the agent provides more accurate results and expands its application scope. The Distance Agent can be used to query the knowledge graph for answering questions such as "how many MRT Stations are within a walkable distance from a land plot?" or "which plot is the furthest away from a school?" Ms Grišiūtė is in the process of developing use cases to demonstrate the capability of the Distance Agent in answering more complicated planning queries using the knowledge graph, as illustrated in Figure 9.8.

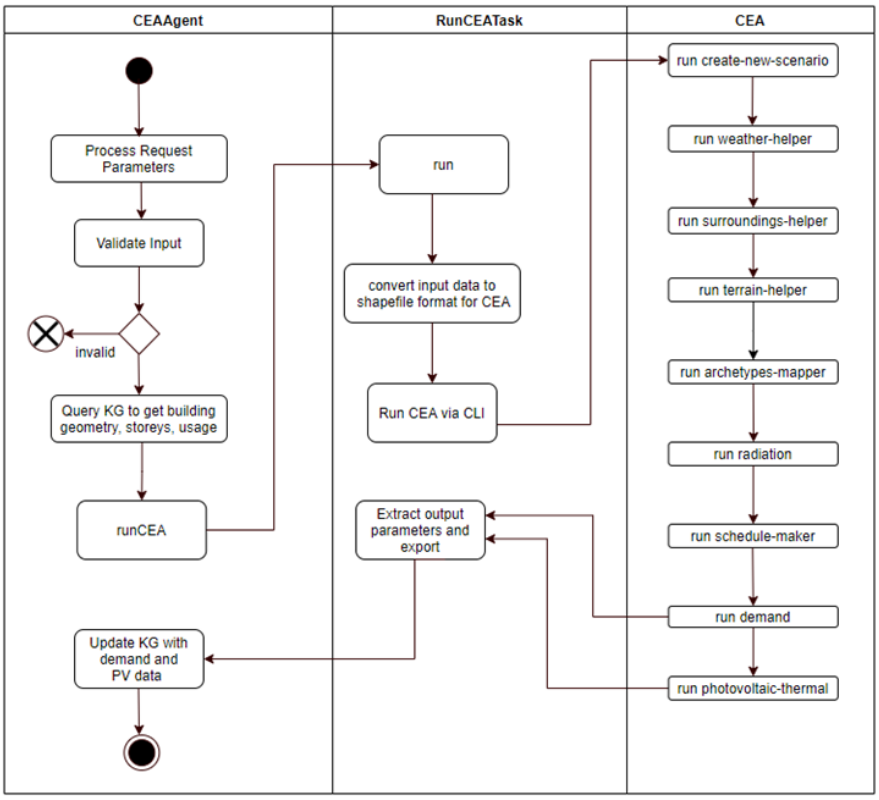


Figure 9.7: UML activity diagram of the initial design of the CEA agent.

Furthermore, Ms Grišiūtė has integrated the Distance Agent with the web-based front-end 3DCityDB-Web-Map-Client, as illustrated in Figure 9.9. The Distance Agent is used for intelligent analytical functionalities by autonomously calculating distances of city objects while the front-end visualisation displays the acquired information upon selecting the city objects and displays distance information between them.

Dr Vishvak KANNAN (Research Fellow, CARES), in close collaboration with Ms Grišiūtė, **Ms Huay Yi TAI (Software Developer, CARES)** and Mr Chadzynski, has been working on the instantiation of various data into the knowledge graph. For instance, Dr Kannan has extended the 3D City Database Importer/Exporter tool to import Level of Detail 2 (LOD2) model of the CREATE Enterprise wing and LOD1 models of all the Housing Development Board (HDB) buildings in Singapore.

```
PREFIX om:<http://www.ontology-of-units-of-measure.org/resource/om-2/>
SELECT DISTINCT ?distance ?NumericValue ?unit
WHERE {
 GRAPH <http://localhost/blazegraph/namespace/SLA/distance/> {
  ?distance   om:hasPhenomenon <http:cityobjectxample/cityobject1> ;
              om:hasPhenomenon <http:cityobjectxample/cityobject2>;
              om:hasValue ?value .
  ?value      om:hasNumericValue ?NumericValue ;
              om:hasUnit ?unitURI .
   BIND(SUBSTR(STR(?unitURI), 59) AS ?unit ) }
`
```

distance	NumericValue	unit
<http:distexample/distance1>	10.0	metre

Figure 9.8: An example of using the Distance Agent to retrieve the distance between two objects.

Figure 9.9: 3DCityDB-Web-Map-Client front-end demo visualisation of the Distance Agent autonomously calculating distance for selected objects.

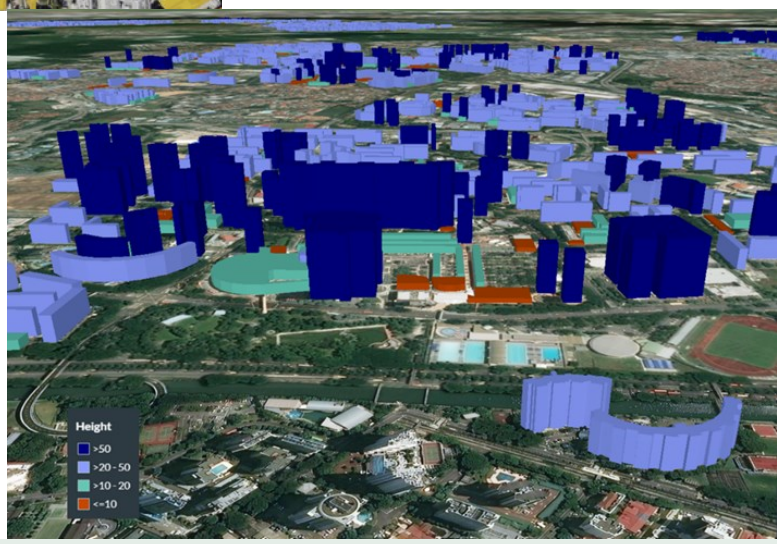


Figure 9.10: Visualisation of the LOD1 HDB building models in the knowledge graph classified by their heights.

Update on work package 4

Developing interfaces and planning libraries for the CKG

Ms Shiying LI (Software Engineer, SEC), in close collaboration with **Mr Arkadiusz CHADZYNSKI (Senior Research Fellow, CARES)**, has developed the CityExportAgent which automates the export of the city model data needed for visualisation. The data could be exported for the whole model, or for different areas found via geospatial search, or for individual city object members, stored in the knowledge graph. Figure 9.11 illustrates the exported Keyhole Markup Language (KML) models of Charlottenburg-Wilmersdorf datasets that consist of 22,771 buildings, and are visualised on the web-based platform, Cesium ion. The 3D City Database Importer/Exporter tool offers a Command Line Interface (CLI) which allows the embedment of this tool in a third-party application such as CityExportAgent. When an export operation is required, a HTTP POST request with the request parameters in a JavaScript Object Notation (JSON) format is sent to the CityExportAgent. After the successful validation by the agent, the parameters are inserted into the configuration file of the 3D City Database Importer/Exporter tool, and the export process is triggered automatically in the background to update the model.

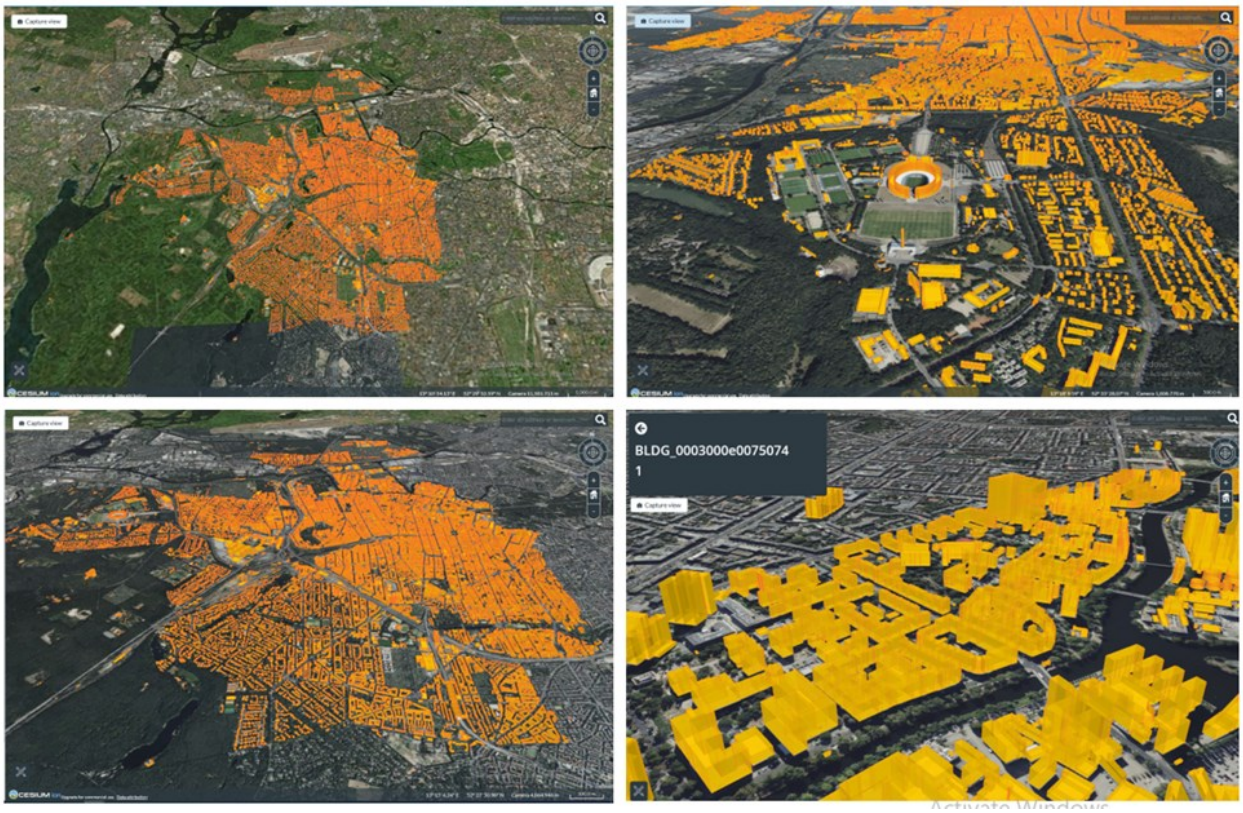


Figure 9.11: Visualisation of the exported KML models of Charlottenburg-Wilmersdorf LOD2 building data from different view angles.

Update on work package 5

Developing design informatics functions

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

Ms Ayda GRIŠIŪTĖ (Researcher, SEC) has been working on a use case of SWOT analysis for assessing the potential of on-site solar energy use in a case study of Singapore downtown area. This experimental use case is developed to explore how SWOT analysis can be used to inform the urban planners of how a variety of urban planning metrics may impact a certain planning target, which is improving the on-site solar energy use in the experimental use case. This effort has been translated into the format of a poster and was submitted to the "International Conference on Evolving Cities 2021 (ICEC 2021)" that was held on September 22-25 by University of Southampton.

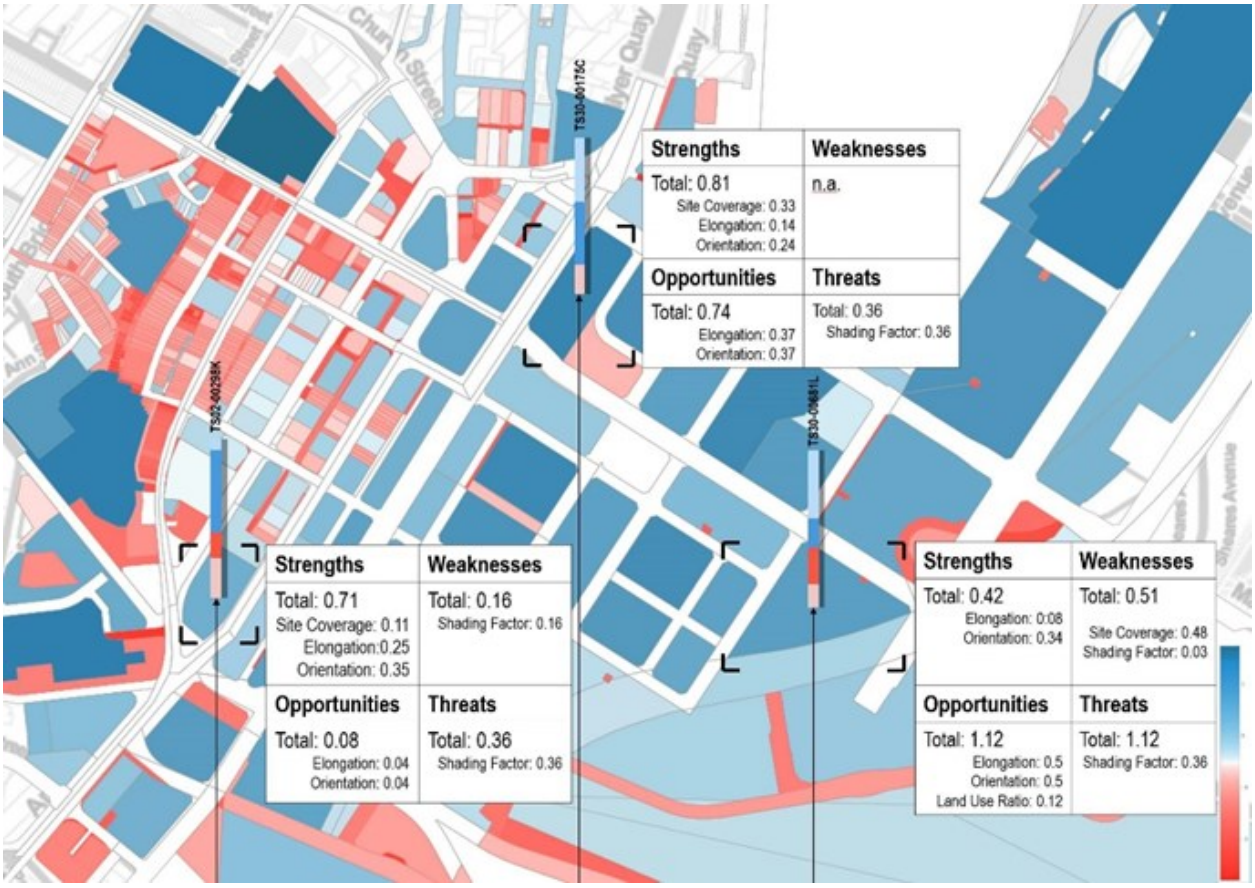


Figure 9.12: The use case of SWOT analysis for assessing the potential of on-site solar energy use in a case study of Singapore downtown area. This work has been submitted to ICEC 2021 as a poster presentation.

Update on work package 6

Demonstrators: horizontal and vertical use cases

Dr Zhongming SHI (Postdoctoral Researcher, SEC) has applied the above-mentioned mixed-use zoning archetypes in a use case of urban building energy performance assessment and estimation for greenfield projects. The use of mixed-use zoning archetypes aims to improve the simulation results of urban building energy modelling's accuracy. Compared to the conventional methods, the data-informed mixed-use zoning archetypes offer more in-detail programme profiles for energy demand simulation. In a case study for a commercial plot above the future Cantonment MRT Station in Singapore, the simulated hourly electricity demand can be up to approximately 84% different when compared to using the conventional method that relies on experts' rules-of-thumb. Dr Shi is in the process of preparing a journal publication pre-print to describe this work.

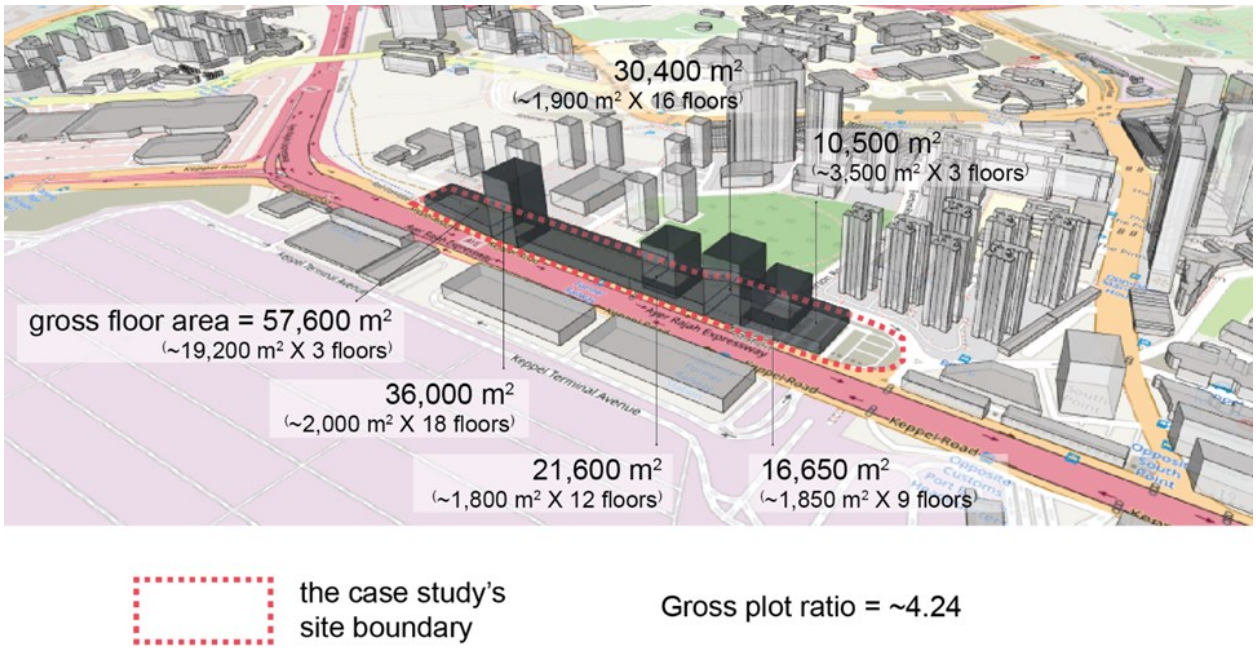


Figure 9.13: The use case of assessing urban energy performance using mixed-use zoning archetypes.

Scientific output

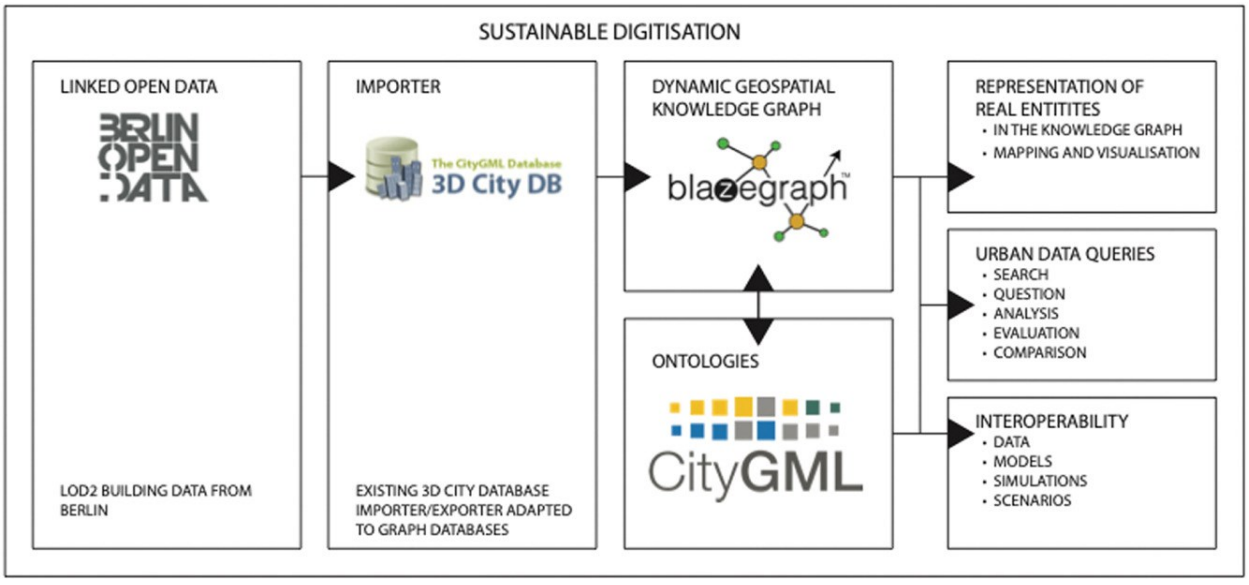
The following are the CREATE-acknowledged publications generated by CKG during the reporting period.

Semantic 3D City Database — An enabler for a dynamic geospatial knowledge graph

Arkadiusz Chadzynski, Nenad Krdzavac, Feroz Farazi, Mei Qi Lim, Shiying Li, Ayda Grišiūtė, Pieter Herthogs, Aurel von Richthofen, Stephen Cairns and Markus Kraft, *Energy & AI*

DOI: 10.1016/j.egyai.2021.100106

Abstract: This paper presents a dynamic geospatial knowledge graph as part of The World Avatar project, with an underlying ontology based on CityGML 2.0 for three-dimensional geometrical city objects. We comprehensively evaluated, repaired and refined an existing CityGML ontology to produce an improved version that could pass the necessary tests and complete unit test development. A corresponding data transformation tool, originally designed to work alongside CityGML, was extended. This allowed for the transformation of original data into a form of semantic triples. We compared various scalable technologies for this semantic data storage and chose Blazegraph™ as it provided the required geospatial search functionality. We also evaluated scalable hardware data solutions and file systems using the publicly available CityGML 2.0 data of Charlottenburg in Berlin, Germany as a working example. The structural isomorphism of the CityGML schemas and the OntoCityGML Tbox allowed the data to be transformed without loss of information. Efficient geospatial search algorithms allowed us to retrieve building data from any point in a city using coordinates. The use of named graphs and namespaces for data partitioning ensured the system performance stayed well below its capacity limits. This was achieved by evaluating scalable and dedicated data storage hardware capable of hosting expansible file systems, which strengthened the architectural foundations of the target system.



Other activities and achievements

As part of the stakeholder engagement strategy, the team has conducted a wide range of outreach activities towards academia, industries of urban project consultants and developers, and government agencies, such as the Urban Redevelopment Authority (URA) in Singapore. Researchers have met URA's Design & Planning Lab on 18th August 2021, shared research results, and discussed potential CKG functionalities, use cases and demonstrators that might be of interest to URA in particular, and the urban development domain in Singapore in general.

Dr Pieter HERTHOGS (Senior Researcher, SEC) has presented the CKG project virtually during the inaugural meeting of the Urban Tech Stack Alliance (April 2021), a newly established international network of computational city planning experts from industry, academia, and government domains.

Dr Zhongming SHI (Postdoctoral Researcher, SEC) has presented the CKG project virtually at an international conference of *DigitalFUTURES: 2021 InclusiveFUTURES*. DigitalFUTURES, an educational initiative launched in 2011, is an annual series of activities consisting of workshops, lectures, conferences, and exhibitions hosted by Tongji University over the summer months in Shanghai, China.

Ms Ekaterina VITITNEVA (Bauhaus University Weimar, main supervisor Prof Dr Reinhard KOENIG), a Master student co-supervised by SEC researchers, has presented her master thesis work in two conferences: *CISBAT 2021* in Lausanne, Switzerland and *ISUF 2021* in Glasgow, United Kingdom.

Dr Aurel von RICHTHOFEN (Senior Researcher, SEC), Dr Herthogs and **Prof Markus KRAFT (PI, CAM)** have recorded and virtually presented the panel talk "Addressing Challenges of Urban Policy Making and City Planning with a Cities Knowledge Graph" at *Data for Policy 2021* held in September 2021 by University College London, as part of the special session "Towards smart city planning – digital twins and parallel world scenarios to support better public policies?" organised by **Dr Franziska SIELKER (Co-I, CAM).**

An industry collaboration between Takenaka Corporation (Japan) and SEC has officially started in August 2021. The CKG team welcomed **Mr Genki UNNO**, a Takenaka architect and engineer who will join the project for a research visit of up to two years.

SMALL PROJECTS

OTHER CARES-FUNDED PROJECTS

In addition to C4T and CLIC, CARES hosts a number of other projects. These give our researchers an opportunity to explore new areas, develop technologies for commercialisation or build relationships with new industry partners or public sector collaborators. The smaller projects are also often a good opportunity for interns (such as Mr Aman SINGHAL, pictured above during his time working on the RINGs project in 2019) to have a novel experience of research and technology development not easily available during their undergraduate degrees.

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

This section also includes updates on the ten projects under the C4T Emerging Opportunities Fund, which was created to support exciting new ideas that have arisen since the start of C4T Phase 2.

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

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

In 2018, the liberalisation of Singapore's electricity market gave consumers more choice and flexibility in selecting suitable electricity retailers and plans to meet their needs while enjoying the same supply and convenience. In lieu of this, CEUS aims to develop a knowledge-enabled, data-driven common platform on Singapore's real-time consumer energy usage using the Common Information Model (CIM) to standardise data formats. This adds value to stakeholders by supporting the individual consumers and local government with evidence to make more informed decisions. With the CEUS platform, consumers would be able to analyse their real-time energy consumption levels and make more informed decisions to manage their energy usage and costs. This allows for more active participation in the energy market.

CEUS acts as a testbed for greater interoperability between diverse technological systems to share data with more stakeholders while respecting consumer privacy. The project is linked up with the existing platform developed by CARES—the J-Park Simulator (JPS) Project—to enable seamless and unambiguous data exchange with third party services. Furthermore, CEUS tests how this data can be made interoperable and allow seamless integration between Geographic Information System (GIS) and Building Information Modelling (BIM) software. Over the course of the project, the researchers identified that the data siloes in public administration is one significant hurdle to interoperability, and has put increasing attention to understanding this issue and proposing suita-

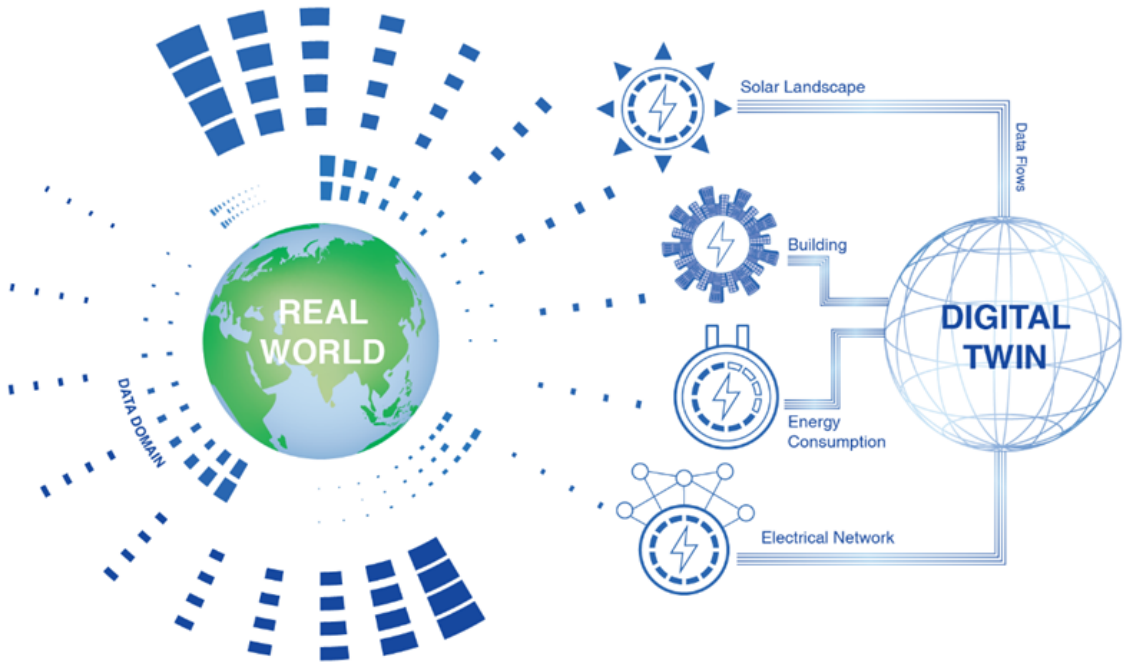


Figure 10.1: An image showing the interface between the digital and real world in the CEUS model.

ble solutions. By laying a foundation for the integration of real-time energy consumption data into city information modelling, the information provided by the CEUS platform paves the way towards a consumer digital-twin.

To empower consumers, foster innovation for a consumer-oriented energy grid, and provide more decarbonised, resilient and affordable electricity, the CEUS project has three overarching aims:

- *A common language*—New forms of consumer semantics will be incorporated to expand the smart city planning of the future. A Singapore-specific Common Information Model will allow consumers to make better decisions around their energy consumption.
- *More effective data sharing*—An autonomous agent framework will be developed in the CARES JPS Project that enables a seamless and unambiguous consumer energy data exchange with third party services.
- *Smart city energy policies*—Identify and suggest implementation solutions to overcome the existing data siloes that hinders data sharing through digital twins in a smart city environment.

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

Led by SEC and developed in close cooperation with other entities, WP1 aimed to develop a standardised CIM grammar in Singapore's energy consumer domain to empower consumers and encourages active consumer participation in the electricity market. CIM is a well-established open standard for information modelling in the power systems domain through the provision of standard unambiguous definitions and representations of various energy related concepts. With a robust framework for accurate data sharing, merging and transformation into reusable information, CIM has been considered an enabler of smart grids. The developed CIM grammar for Singapore's consumer energy domain builds on the Enterprise Architect tool and IEC TC57 specifications. Parameters defined in the energy usage information and grid parameters are used as inputs. Figure 10.2 depicts the CIM development process.

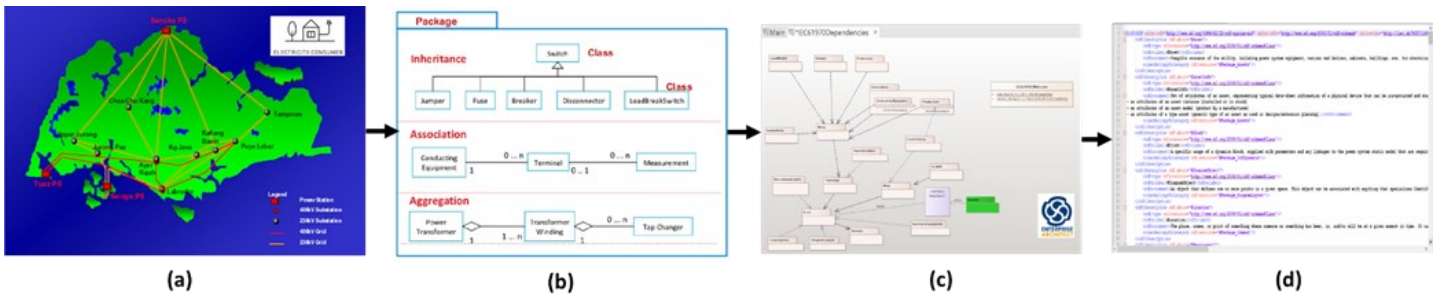


Figure 10.2: (a) Horizon scan of electricity consumer space for knowledge gathering. (b) Describing relationships between different electricity parameters. (c) Developing UML diagrams and establishing upstream link with CIM. (d) Schema XML file generation.

Work package 2: Knowledge graph ontology development

From the literature review, it is observed that CIM grammar only provides formal definitions, and does not encode the necessary contextual information to carry out complex tasks such as automation and reasoning. Led by CARES and working actively with **Dr VSK Murthy BALIJEPALLI (PI, SEC)**, this work package aims to enhance the expressivity of the CIM grammar, developed in WP1, through the development of a knowledge base and ontology schema for Singapore's consumer energy domain. This establishes the relationships between the CIM concepts and is then integrated within the CARES JPS framework for the use case further elaborated in WP3. Through an ontology-based model-driven knowledge approach, the JPS agent architecture utilises the energy consumption data to automatically execute specific tasks within the electricity domain.

For this work, **Dr Vishvak KANNAN (Research Fellow, CARES)** assisted in the development of a Level of Detail 4 (LOD4) model for the housing unit. Dr Kannan retrieved images of the apartment block's escape plans, floor plans, and building facades to support the models' development (See Figure 10.3). By generating a LOD4 model, users can visualise and identify the sensors' positions and the corresponding power consumption of different appliances within the household. This approach is beneficial as knowledge of the sensors and appliances' geo-spatial information could expand the understanding of current power consumption patterns for different households and different appliances at a more granular level. This understanding would then empower consumers with recommendations to optimise their interior layout inclusive of the appliances and furniture to reduce energy consumption.

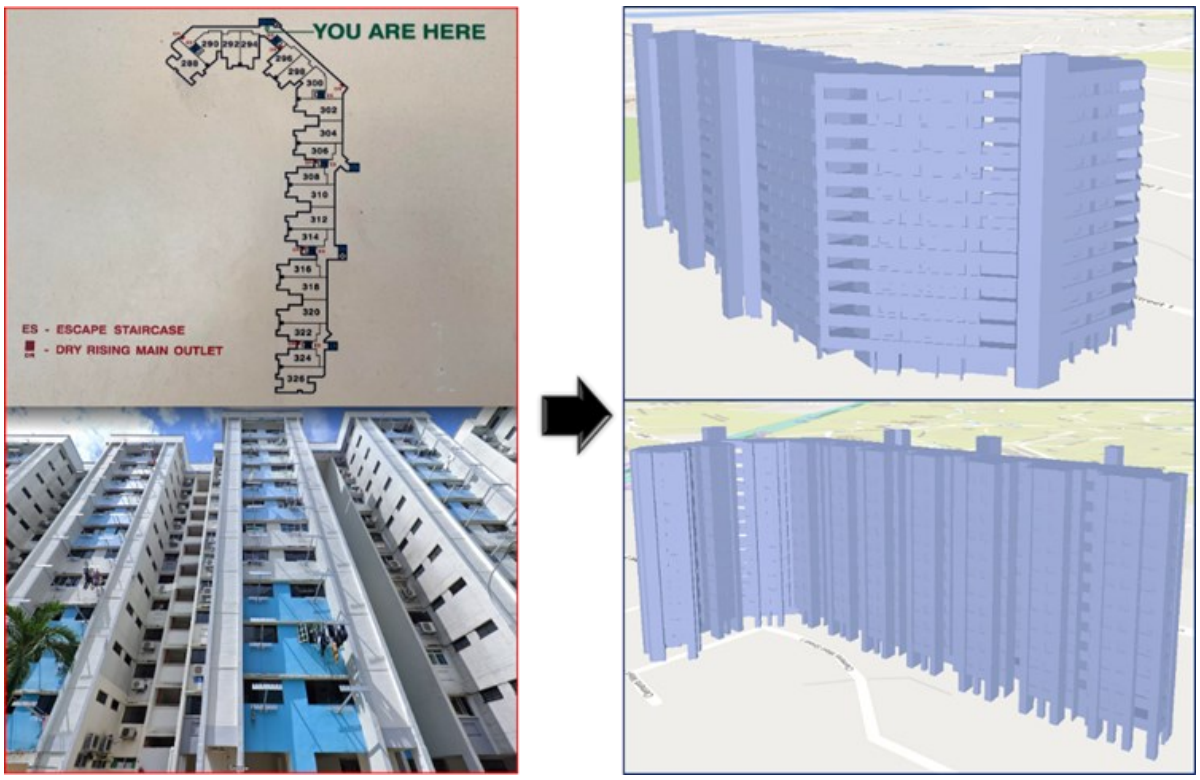


Figure 10.3: The Level of Detail 4 (LOD4) model of the selected HDB block in JPS.

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

Led by SEC, this work package handles the development and implementation of the use case as a real-time consumer energy usage data exchange interface. Real-time consumer energy data will be integrated using the consumer energy ontology developed in WP2 to become a part of the JPS knowledge graph to run consumer applications (See Figure 10.4). The knowledge from the use case can be used to make an informed decision on infrastructure provision or energy policies at the consumer level. For example, the knowledge of real-time energy consumption patterns provides input to policies targeted at reducing urban heating and increasing consumer uptake of smart city solutions.

In this period, the researchers have successfully established the Internet of Things (IoT) hardware setup using micro-components to capture the energy usage data of different consumer appliances in real-time. This data is then aggregated to a live dashboard interface and is made available in the public domain at http://ceus.live. In the future, there are plans to execute extensive model calibration alongside contextual schema profiles to incorporate these aggregated datasets as inputs in the testing of various contextual consumer applications.

Work package 4: Planning and energy consumption information for policy-making

Adding an urban planning and policy perspective to the technological developments in CEUS, this work package aims to provide a thorough analysis of Singapore's governance model in energy and city planning to understand the value of CIM in city planning and energy systems, how CIM could enable interoperability with the diverse urban information systems available and how it can be implemented in practice.

Joining the project in June 2021, **Mr QUEK Hou Yee (Research Associate, CARES)** is working with **Dr Franziska SIELKER (PI, CAM and CARES)** on preparations for the upcoming stakeholder dialogue. One key outcome is the institutional mapping that highlights the structure of Singapore's energy market and governance. This aids the identification and formulation of suitable interview themes such as to inquire into the existing data silos. Mr Quek is also exploring how BIM could be integrated into The World Avatar knowledge graph.

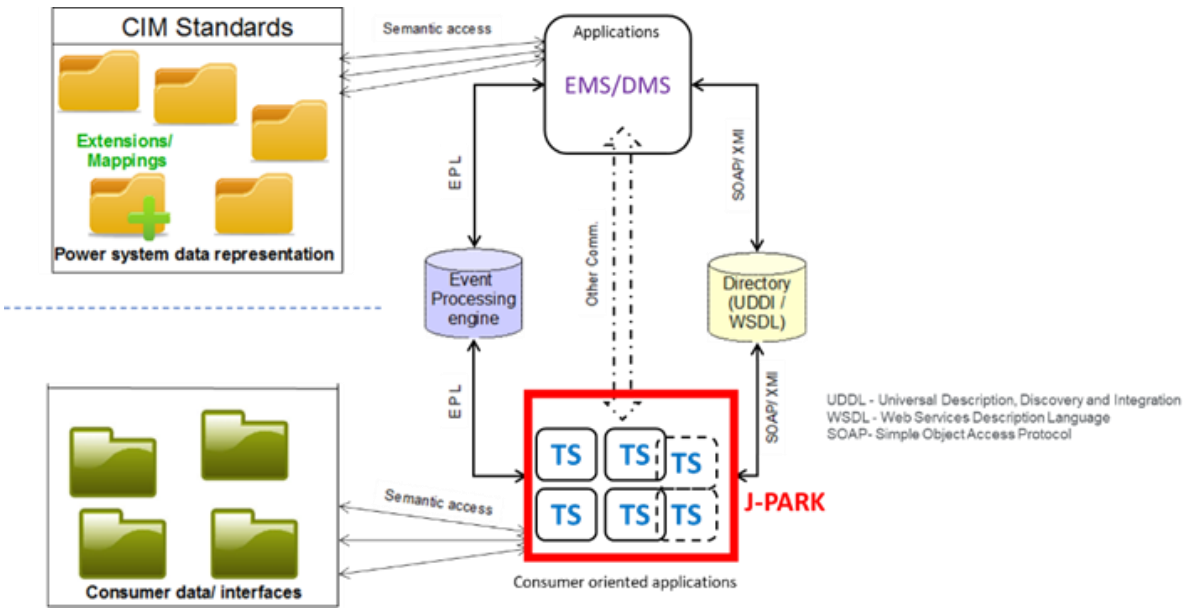


Figure 10.4: Positioning of standardised real-time data and consumer applications with J-Park Simulator and electricity distribution operator (EMS/DMS).

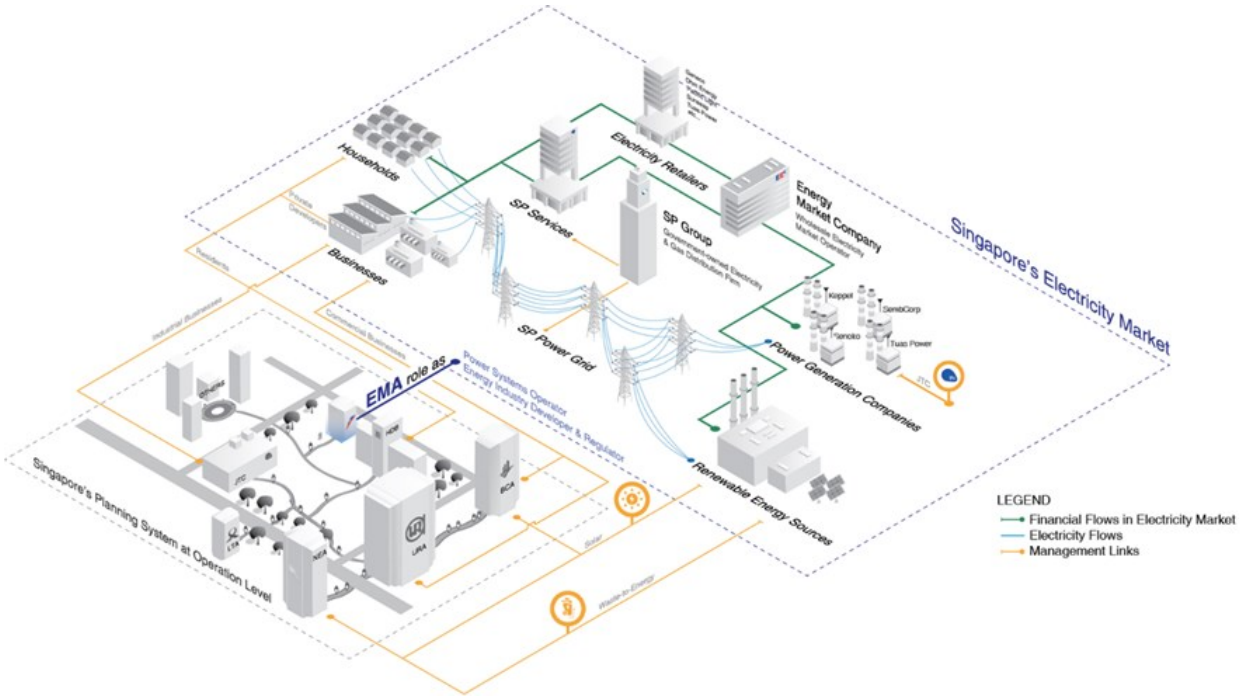


Figure 10.5: Interactions between Singapore's Energy and City Governance Model.

The key outreach and publication activities in this period are as follows:

- **Stakeholder Dialogue:** A brochure introducing the knowledge graph and its digital twin applications.
- **IEEE PES ISGT Europe 2021 Conference:** The paper "Evolution of Power System CIM to Digital Twins - A Comprehensive Review and Analysis" led by SEC has been accepted.
- **International Conference on Evolving Cities 2021:** The poster presentation "Can different urban information systems speak to one another? Using the World Avatar Knowledge Graph for Singapore's energy planning" led by CARES has concluded.
- **Data for Policy 2021 Conference:** In collaboration with CMCL Innovations Cambridge, University of Cambridge, Future Resilient Systems and SEC, the four-member panel presentation "Towards smart city planning—digital twins and parallel world scenarios to support better public policies?" has concluded.

The corresponding conference paper "Digital Twins for Smart Cities: A Knowledge Graph Approach" is currently under revision before submission to the *Data & Policy* journal. Another paper titled "Knowledge Graphs for Urban Planning: A Literature Review" is currently being written. This paper summarises the current research on the application of semantic web technology in urban planning and key research challenges and sets a future research direction for efficient knowledge and data management in the architecture, engineering and construction (AEC) domains.

Development of Multi-Step Processes in Pharma

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

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

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

Despite the success of existing active learning ML methods when applied to individual chemical reactions, results in the optimisation of larger multi-step chemical system have proven demonstrably poorer. Dr Sung and Dr Jeraal have therefore developed a new optimisation algorithm for the multi-step optimisation of chemical processes for multiple simultaneous objectives. The holistic end-to-end machine pipeline collectively utilises a range of supervised and unsupervised learning methods for a synergised approach to the representation and optimisation of chemical systems.

The new algorithm has been seamlessly integrated into the robotic flow platform that Dr Sung and Dr Jeraal designed and created. The multi-step optimisation for an antiviral drug analogue has been successfully performed to produce a trade-off curve between maximal yield and minimal materials costs. Multi-step reaction yields were higher than those observed in pre-optimisation testing via batch experimentation. Following a training set size of 50 experiments, 60% of optimisation experiments resulted in yields over 10%. Factorial studies of the same optimisation space indicate only 2% of the space capable of producing yields in this range which indicates good selectivity for ideal conditions. Future work aims to further increase the optimisation space with larger chemical systems to determine the capabilities of the newly developed machine learning toolset.

Dr Magda BARECKA (Research Fellow, CARES) joined this project in July 2021, working towards development of first principle models that will be used together with machine learning automatic process optimisation. The overarching goal is to propose accelerated methods for process design, suited for the needs of the pharmaceutical industry.

Data2Knowledge in the Digital Manufacture of Pharmaceuticals

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

Data2Knowledge in the Digital Manufacture of Pharmaceuticals is a project funded under the Pharma Innovation Programme Singapore (PIPS) programme and led by **Professors Alexei LAPKIN** and **Markus KRAFT (PIs, CAM)**. This is a 15-month project and commenced in December 2020.

The digitalisation of chemical manufacturing is one of the critical technology paths towards a more sustainable society, as it promises to deliver a significant level of decarbonisation of industry. It focuses on creating a digital twin of the physical entities that bridges the gap between the cyber - and the real-world, shortening the time span from design to the delivery of the target product to the end-users. Data2Knowledge is a project that aims to develop a fully automated data exchange and knowledge management within a closed-loop self-optimisation experiment.

The first stage of this project (December 2020—March 2021) focused on a literature review of the existing data schema and exchange protocols. This report concludes the progress made in the second stage of the project (April 2021 – September 2021). The findings of **Mr Jiaru BAI (PhD student, CAM)** and **Dr Liwei CAO (Research Associate, CAM)** have been prepared into a paper and submitted for publication. Their findings were also presented as a talk at the *4th Machine Learning and AI in Bio(Chemical) Engineering Conference* in Cambridge. Subsequently, Mr Bai and Dr Cao focused on proposing a complete dynamic knowledge-graph-based framework of an existing automated closed-loop optimisation setup, which was originally demonstrated in a platform-based approach.

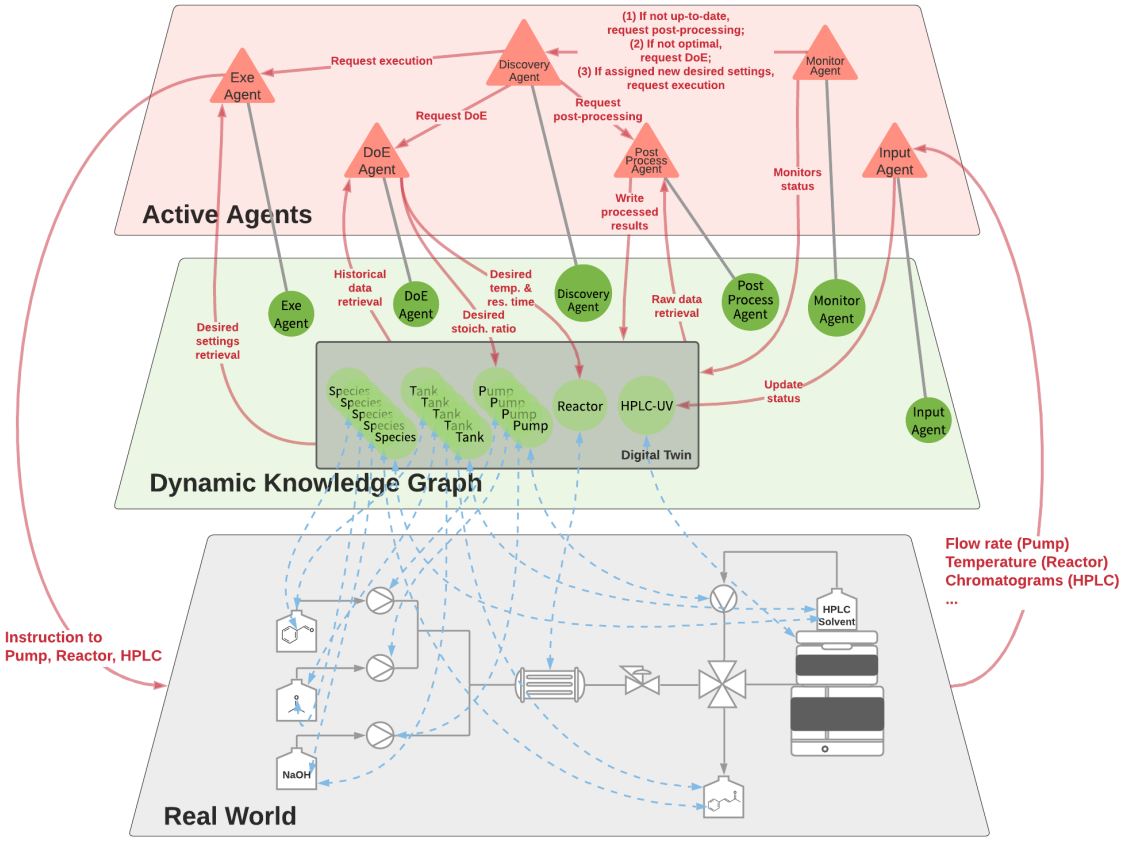


Figure 10.6: Dynamic knowledge-graph-based approach towards automated closed-loop optimisation. The real-world layer represents the existing physical entities, adapting from the experimentation setup of CARES lab.

As a first step of turning the current platform-based approach into a knowledge-graph-based approach, understanding the workflow of the monolithic automation code and the experimental setup it controls is crucial to the success of the project. The existing codes have been reviewed to identify the core variables, the dependency between these variables and the concepts they represent in the chemistry domain. Based on the identified concepts and relationships, a short literature review was conducted on the existing reaction ontologies and schemas to propose the suitable ontology to instantiate the experimental setup in this project. From a preliminary assessment, two ontologies were identified to cover different perspectives of the framework, including reaction experiment and digital twin of the equipment.

A flowchart was also made to break down the logic encoded in the existing code. The code was modularised and will be turned into autonomous agents, in line with The World Avatar coding practice. This includes wrapping agent as an HTTP servlet, expressing agent capabilities using OntoAgent ontology and deploying it in the Docker environment.

Figure 10.6 illustrates the proposed framework. It consists of three layers, namely the real-world, knowledge graph, and active agents. The knowledge graph represents the "digital twin" of the physical world and hosts additional intelligent agents responsible for data management and utilisation. Once activated, these agents act autonomously over the knowledge graph and keep the cyber- and the real-world synchronised. The update of "digital twin" based on the readings from the equipment is managed by the input agent. As the monitor agent is responsible for monitoring the state of the "digital twin", it assesses if the current reaction has reached the optimal and invokes the DoE agent for a suggestion of a new experiment if further optimisation is required. Once the suggestion is ready, the DoE agent requests a new configuration of the physical equipment to the execution agent, who is responsible for updating the real-world to reflect the changes made in the knowledge graph. This loop of self-optimisation continues until the monitor agent decides the optimal condition is reached.

Work is now in progress for creating the proposed ontology and refactoring the existing code into the proposed agent framework.

Digital Workflow and Continuous Processing in Pharmaceuticals Manufacturing

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

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

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

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

The objectives of this project are:

- To develop a technical solution for exploration of a maximally diverse range of operating conditions using a minimal set of reactor components.
- To explore a multi-modal analytics approach for rapid generation of data from experimental systems.
- To demonstrate the application of rational design of a continuous flow process to industrially relevant case studies.

A new Research Fellow, **Dr CHEN Guoying (CARES)**, started on the project in March. Dr Chen has been working on assembling flow chemistry devices and evaluating the batch process. A new batch process was successfully developed in the lab and could be transferred to flow process once the assembly of the flow equipment is finished.

Cambridge Alternative Finance Collaboration Network

University of Cambridge Judge Business School

Since January 2021, the CAFCN has been active in the Asia-Pacific region through the establishment of a research collaboration with Cambridge CARES alongside a bi-lateral programmatic relationship between the Asian Development Bank Institute and the Cambridge Centre for Alternative Finance (CCAF), with the aim of accelerating tech-enabled financial innovation and knowledge sharing across the region.

CCAF is an interdisciplinary academic research institute at the University of Cambridge Judge Business School, dedicated to the study of alternative finance, which includes technology-enabled financial instruments, channels and systems that emerge outside of the traditional financial system. The CCAF is leading the establishment of a global knowledge network that accelerates the creation and transfer of knowledge relating to FinTech: the Cambridge Alternative Finance Collaboration Network (CAFCN). Earlier this year, the CAFCN launched operations in Sub-Saharan Africa and in the Middle East, North Africa and the Mediterranean. As a cross-sectoral and cross-regional network, the CAFCN can facilitate FinTech market development and effect evidence-based regulatory changes in economies seeking to promote the sustainable growth of FinTech industries. This programme has established the CAFCN in Singapore for coverage across the Asia Pacific region (APAC), starting in January 2021.

Recent highlights include: Asia Pacific data insights from the second Global Benchmarking study' digital tools demonstrations (Atlas and Benchmarking tools) to funders and selected FinTech associations in the region; Cambridge FinTech and Regulatory Innovation course embedded with Asia Pacific focused "live" sessions and plans to deepen regional imprint, with support of the UK Foreign, Commonwealth & Development Office; planning grant for Indonesia awarded by a major philanthropic organisation; successful closed-door regional (AP) roundtable organised and executed with World Economic Forum with senior participants from alternative finance markets, regulatory and government ecosystem and global roundtable planned to coincide with Singapore FinTech Festival on 11th November; regular collaboration network deepening and broadening across Asia Pacific.

Cooling Singapore 2.0

In collaboration with the Singapore-ETH Centre

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

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

Dr Vishvak KANNAN (Research Fellow, CARES) has identified the major heat emitters of the industrial sector of Singapore as Chemicals and Petroleum Refining, of which the top three emitters are ExxonMobil (605,000 bbl/day), Shell (500,000 bbl/day) and Singapore Refining Corporation (290,000 bbl/day). Furthermore, to facilitate a preliminary study to examine the effect of industries on Jurong Island, heat emissions (as heat fluxes) were provided to the Weather Research and Forecasting (WRF) model to estimate the ambient temperatures. The WRF model estimates the ambient temperatures based on the heat fluxes assigned in specific geo-spatial locations coupled with different climatic conditions, traffic, and power plant models. Heat fluxes on Jurong Island were estimated through a top-down approach from the total heat emissions from industry which is reported as 11906 kToe (138 TWh) in a report entitled "Anthropogenic heat sources in Singapore". In order to study the effects of the industry, three scenarios based on different assumed operating conditions and distributions of the plants were formulated.

Dr Kannan has also collected information pertaining to the geo-spatial representation of the heat emissions from Jurong Island e.g. locations, addresses, land lot numbers, areas of the land parcels and to the industries on Jurong Island e.g. design capacities, types of reactants and products and production technology. With the collected information, Dr Kannan together with **Dr Jingya YAN (Research Fellow, CARES)** and **Ms Huay Yi TAI (Software Developer, CARES)** have developed Level of Detail 1 (LOD1) models for the selected major heat emitters on Jurong Island. These models have been instantiated in the knowledge graph to enable automated coupling of the heat emissions estimations with the individual emitters i.e. heat emissions can be automatically assigned to their geo-spatial locations. Dr Kannan has also developed an agent to perform cross-domain query for the geo-spatial and chemical engineering information simultaneously from the knowledge graph.

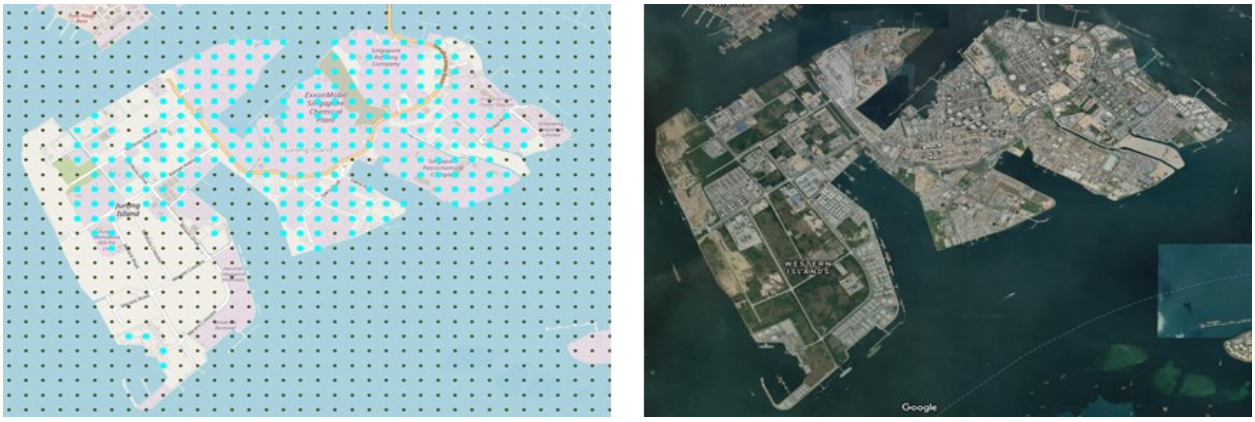


Figure 10.7: Selected grid points for heat emissions distribution and a corresponding satellite image for clarity. The unselected points correspond to empty spaces or storage tanks.

C4T Emerging Opportunities Fund

1) Brown carbon laser characterisation and light-absorbing property

Prof. Markus KRAFT and Dr Yichen ZONG

The purpose of this project is to investigate the brown carbon (BrC, a light-absorbing organic carbonaceous species) from combustion emissions. BrC is a major air pollution source in Southeast Asia and a possible cause of climate change. The research has continued in the last six months, despite the fact that the Covid-19 situation in Singapore continues to slow down progress. The project's experimental work is carried out in partnership with CARES researchers and researchers from the Department of Environmental Engineering, NUS. Our recent paper "Effects of Polyoxymethylene Dimethyl Ether (PODE) on Diesel Engine Emission" was presented at the *American Association for Aerosol Research Annual Conference* (AAAR 2021), which finds BrC absorption across all PODE blends with the highest contribution to the total aerosol absorption under low loading conditions. The BrC contributing factors in this study are similar to those from on-road engine emissions, according to the Positive Matrix Factorisation (PMF) result.

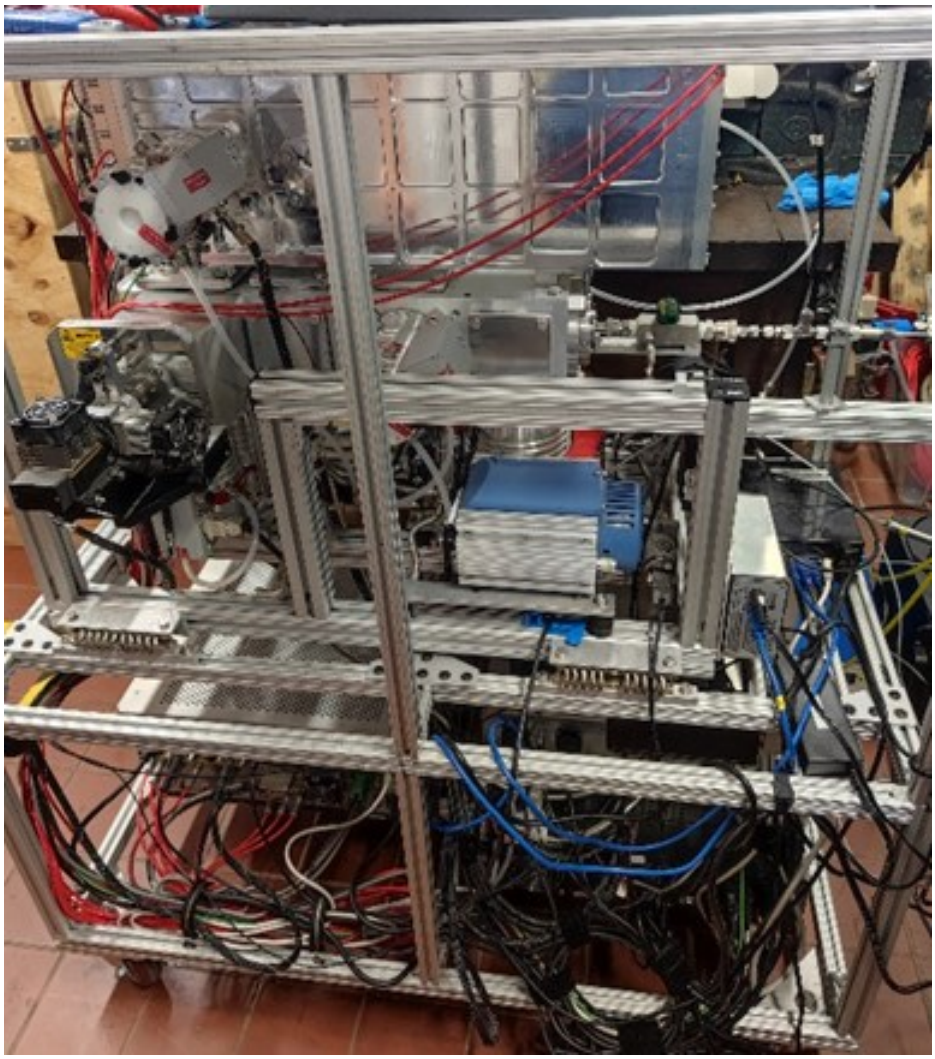


Figure 10.8: SP-AMS (Soot Particle-Aerosol Mass Spectrometer) used in this study to detect organics from engine emissions.

2) Chemical farming

Assoc. Prof. YAN Ning, Prof. Alexei LAPKIN, Dr DING Shipeng and Dr PHAM Thuy Trang

The main research topic in this project is the synthesis of primary amines, which are key intermediates in the production of amino acids. Ru-based catalysts were proven to be active for the alcohol amination to form amines. However, the selectivity toward primary amines is always unsatisfactory and the understanding of the key factors in affecting its catalytic performance is still lacking, especially for the determinative induction in selectivity. It was reported that the product selectivity could be effectively optimised by modulation of the structure of catalysts in heterogeneous catalysis.

To illustrate the structure-performance relationship in direct amination of alcohols to produce primary amines, in the past a couple of months, **Dr DING Shipeng (Research Fellow, NUS)** and the team dispersed Ru nanoparticles on a CeO_2 matrix with various crystal facts (nanocubes and nanorods). The cube-shape and rod-shape of CeO_2 supports were clearly identified by TEM images. After depositing Ru species, the morphology of the CeO_2 matrix was well reserved. Besides, the presence of Ru element is definitely confirmed by the liner EDX results. The catalytic performance of Ru species dispersed on CeO_2 nanocubes and nanorods was evaluated in the directed amination of iso-propanol with NH_3. As shown in the figure, the two catalysts showed similar iso-propanol conversion, while the selectivity for the desired product iso-propylamine was significantly different. The Ru/CeO_2 nanocube exhibited a high selectivity of 83% for iso-propylamine at 200 °C. On the other hand, the iso-propylamine selectivity of Ru/CeO_2 rod was only 33%. Preliminary results indicated that the oxygen vacancies in supports played a key role in determining the selectivity towards the target product. The effect of oxygen vacancies will be further investigated in the future.

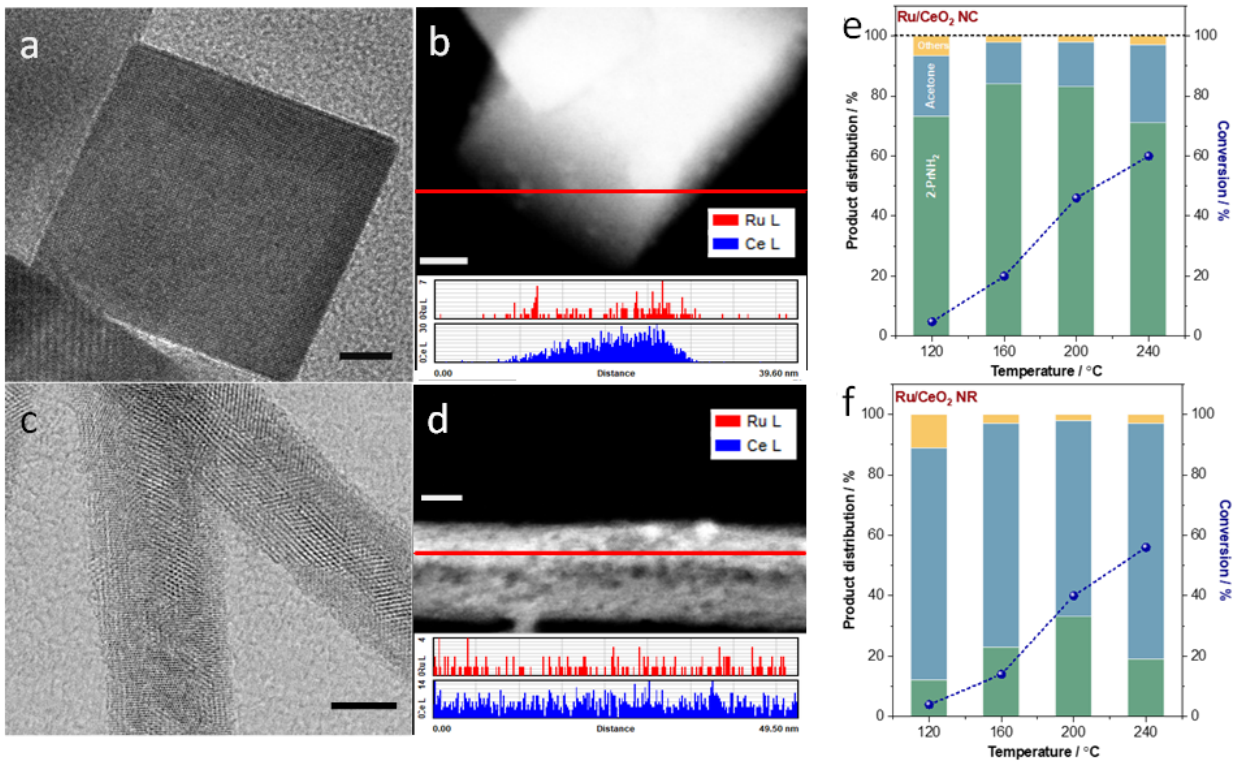


Figure 10.9: HRTEM images of Ru/CeO_2 catalysts after H_2 pre-treatment at 200 ˚C: (a) Ru/CeO_2 nanocubes and (b) Ru/CeO_2 nanorods. HRTEM images of spent catalysts after reductive amination of isopropanol at 200 ˚C (c) Ru/CeO_2 nanocubes and (d) Ru/CeO_2 nanorods. Scale bar: 5 nm. Conversion and production distribution at various temperature over catalysts of (e) Ru/CeO_2 nanocubes and (f) Ru/CeO_2 nanorods in propanol amination.

Dr PHAM Thuy Trang's (Research Fellow, CARES) primary research lies in the synthesis of platform chemicals from biomass-derived substrates. Pyrrole-2-carboxylic acid (PCA) is a versatile platform chemical and building block for a number of high-value products, including bioactive marine natural products as well as synthetic bioactive compounds. Recently, she has been focusing on the synthesis of pyrrole-2-carboxylic acid and its derivatives from chitin-derived D-glucosamine and bio-derived α-keto acids, with some results achieved during past six months. First, she has conducted the optimisation of the synthesis of pyrrole-2-carboxylic acid from D-glucosamine and pyruvic acid with the yield of up to 40%, compared to 20% in the original research. With the optimised conditions, different bio-derived a-keto acids have been used to react with D-glucosamine to give various 3-substituted pyrrole-2-carboxylic acid derivatives. At this stage, four derivatives have been successfully prepared. Furthermore, she has studied the reaction mechanism by using ^{13}C NMR to analyse the plausible intermediates formed during the reaction. Finally, further transforming PCA into valuable *N*-containing building blocks has also been carried out, with several pyrrole-2-carboxamide/carboxylate derivatives and several valuable nitrogen-containing heterocycles being synthesised recently (Figure 10.10).

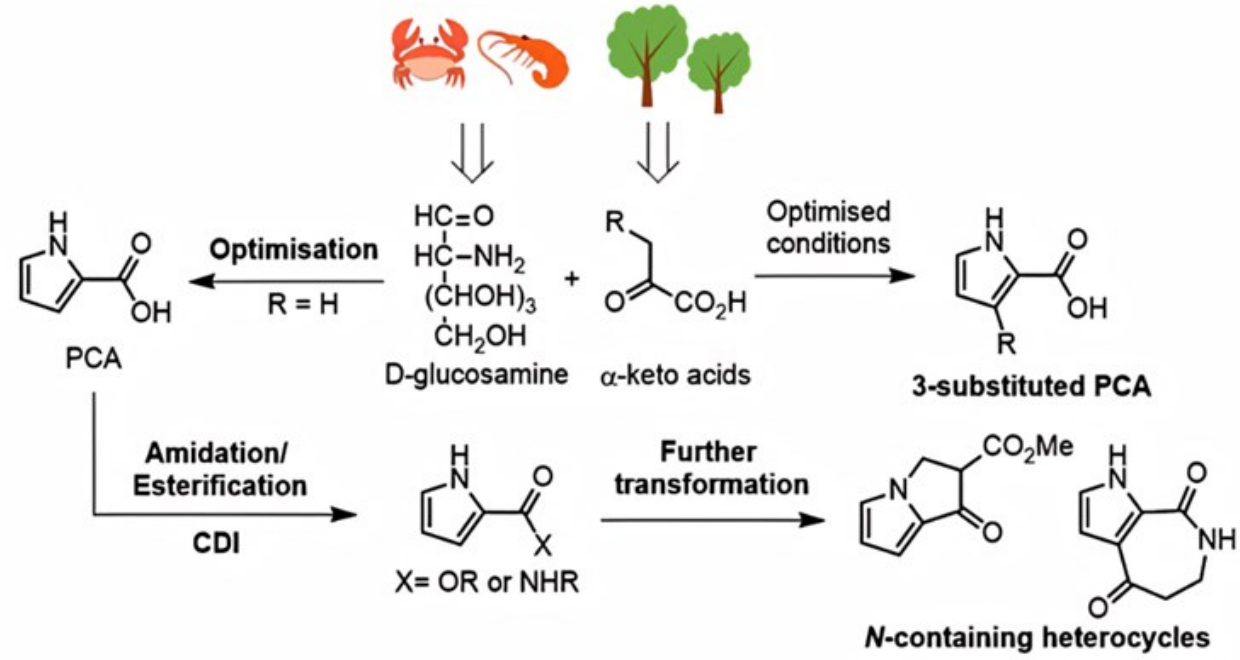


Figure 10.10: Synthesis of pyrrole-2-carboxylic acid (PCA) and its derivatives from biomass-derived substrates.

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

Prof. Markus KRAFT, Ms Mei Qi LIM and Mr Jiaru BAI

The initial motivation of this work is to evaluate the impact of emissions from shipping activities on air quality in Singapore and to demonstrate the knowledge graph technology in handling a cross-domain application. The data required to simulate the dispersion of pollutants are highly heterogenous as they are collected from different sources. Using knowledge graphs, data from different domains are stored semantically and this eliminates data silos. Over the past six months, the researchers have continued to improve the knowledge graph infrastructure especially for the handling of time series data and the dependency among different instances in the knowledge graph through a derivation framework.

In order to describe and store the time series measurement data of virtual sensors and AQ-Mesh (a small-sensor air quality monitoring system that offers real-time localised outdoor weather and air quality information) in the knowledge graph, a framework was developed to allow data to be stored and queried in a consistent manner across the knowledge graph with a relational database. A relational database is typically accessed via the knowledge graph with a URL along with a set of credentials (username and password) and queried/updated using a standardised query language, SQL. The main advantages of using a relational database over a local storage system such as CSV files are that it is highly portable, scalable, and efficient especially for large datasets.

Another key development during this reporting period is the derivation framework that allows instances in the knowledge graph to be linked in a consistent manner. The main feature provided by this framework is the ability to update quantities calculated by agents acting on the knowledge graph when the inputs to the calculations are found to be out-of-date. This is especially useful for this work that involves multiple cascading dependencies between different time-varying instances e.g. weather and marine traffic data.

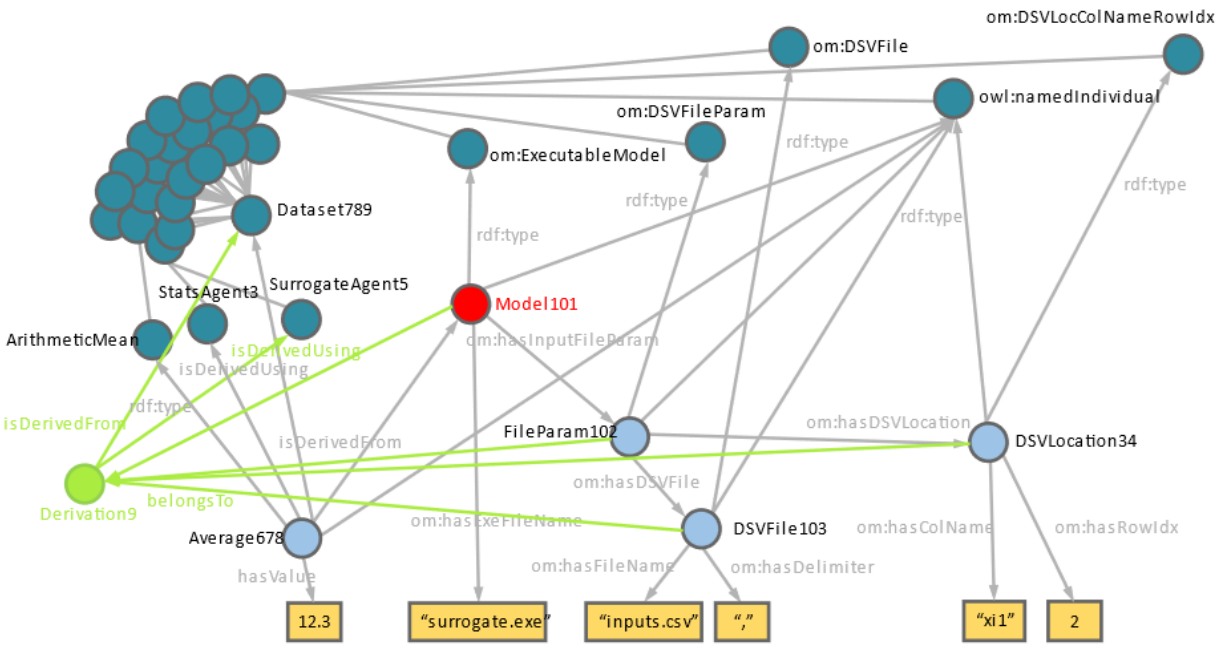


Figure 10.11: An illustration of the derivation framework implementation for a simple surrogate agent example.

4) Ignition systems and methane slip in marine natural gas engines

Prof. Epaminondas MASTORAKOS

The project involves modelling of methane slip and ignition systems (pilot, jet) with Large-Eddy Simulation and finite-rate kinetic sub-grid combustion models. Work on the theoretical and code development front has started at Cambridge and the project is ready to launch upon the permission of the new Singapore-based researcher to enter the country.

5) Future marine economy

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

This project identifies 22 potential marine fuels to be used as bunkering fuel in Singapore towards zero carbon in shipping. The production pathway of these fuels is shown in Figure 10.12. Life cycle assessment for these fuels was carried out using results from Aspen simulation and data from literature. Comparisons were carried out and outcomes put together in a ranking system. This ranking system has included 14 assessment criteria, and each of the marine fuels is assigned under green, yellow and red categories based on the outcome from life cycle assessment. One of the most important assessment criteria is the well-to-wake energy consumption (see Figure 10.13 for the summary of this assessment). As shown in the chart, installation of carbon capture and storage (CCS) downstream of a heavy fuel oil (HFO) combustion engine results in 22% more energy consumption, and production of hydrogen using natural gas as the feedstock results in 12-38% more energy consumption depending on type of energy converters. On the other hand, production of ammonia and methanol result in 45-77% and 122% more energy consumption respectively. In term of energy consumption, hydrogen, biofuels and electrification are competitive to HFO, but not for ammonia and methanol which involve energy intensive production steps.

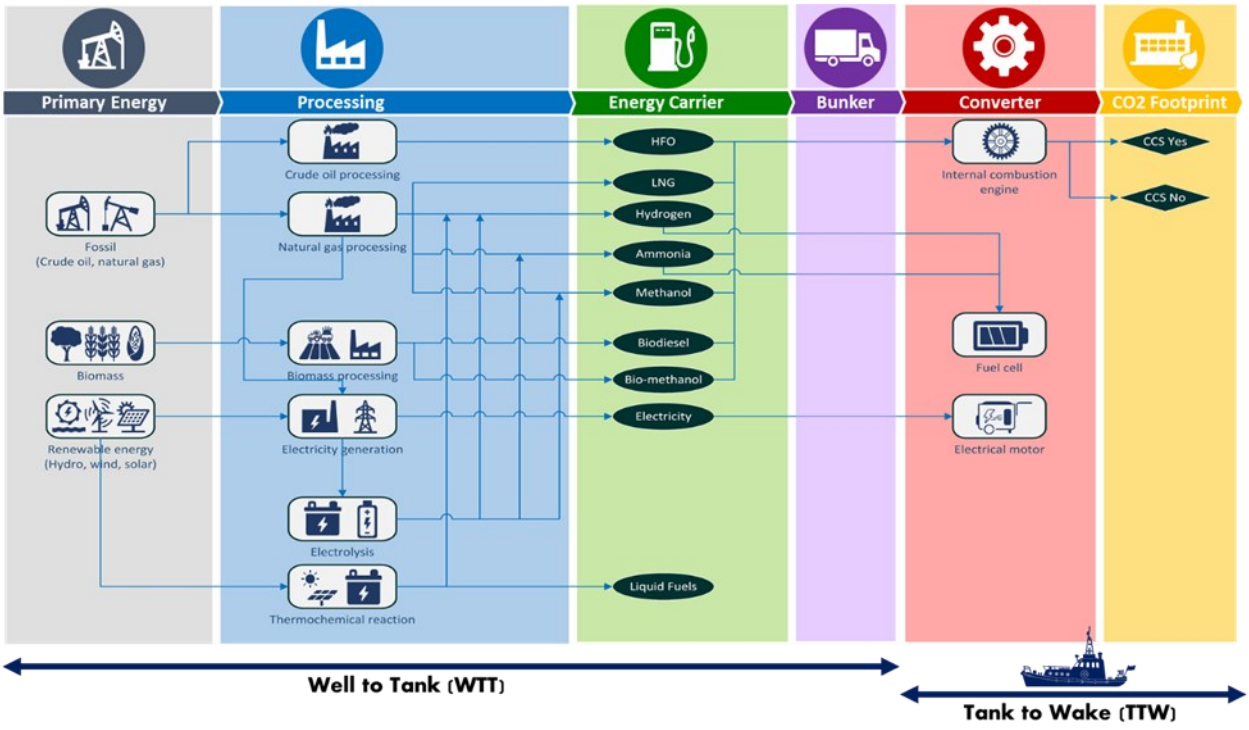


Figure 10.12: Potential marine fuels and their production pathways.

Figure 10.14 (next page) shows the ranking table which has included all 14 assessment criteria. This table has quantified the potential of each alternative fuels. The marine fuel with highest score has the most potential as an alternative fuel for shipping, and vice versa. As shown, fossil fuels with carbon capture technology achieve the highest score and are identified as the best decarbonisation pathways, followed by biofuels, hydrogen, electrification, methanol and lastly ammonia produced from various production pathways. This table can be used as a guideline for fuel selection. For example, comparing LNG with CCS installation and natural gas-based hydrogen, LNG is better which requires smaller storage volume and results in lower well-to-wake CO_2 emission due to lower energy consumption in the production phase (well-to-tank). In term of safety, LNG with its smaller flammability range is safer, and the readily available IGF code (International Code of Safety for Ship Using Gases or Other Low-flashpoint Fuels) for LNG application gives it more potential than hydrogen which requires amendment of IGF code for onboard application. This table summarises the overall project outcome at the current stage. More detail is to be included in the future publication.

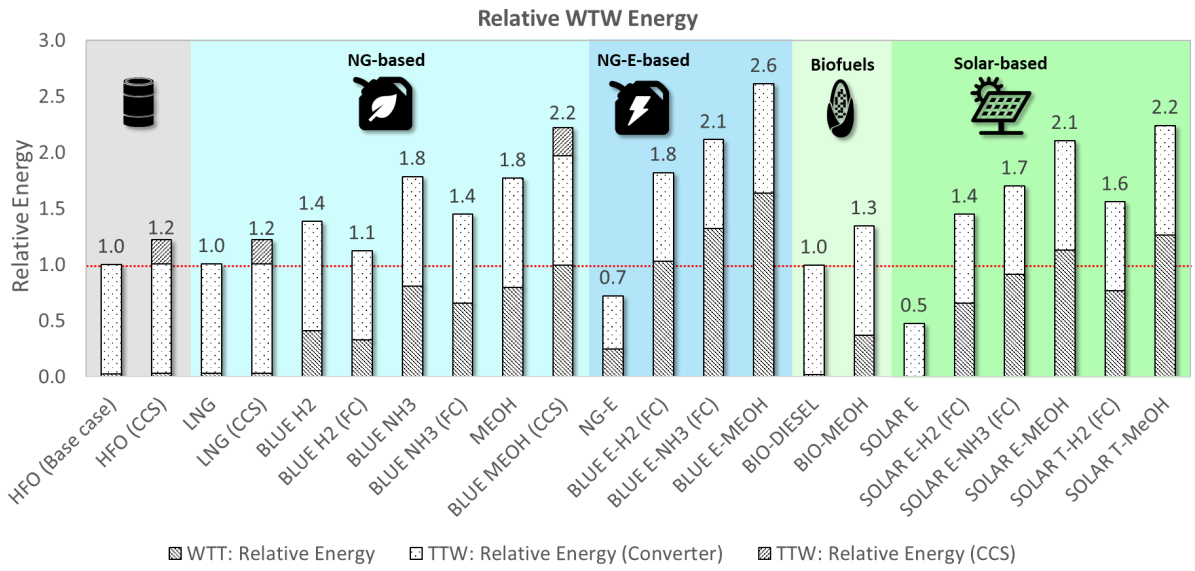


Figure 10.13: Well-to-wake (WTW) relative energy consumption for various marine fuels.

Based on latest research direction)

Marine Fuel	Onboard fuel mass = Light = Medium = Heavy	Onboard fuel volume = Small = Medium = Large	Relative WTW Energy = Low = Medium = High	Relative WTW Cost = Low = Medium = high	Relative WTW CO_2 Emissions = Low = Medium = High	Relative Non-GHG Emissions = Low = Medium = High	WTT Scalability = Scalable = Challenging = Unlikely	Fuel safety = Safe = Intermediate = Dangerous	Regulations & guidelines = Available = Amendment = N.A.	Technology readiness = Commercial = Small scale = R&D	Total Scores
HFO (base case)	G	G	G	G	Y	R	G	G	G	G	83.4
HFO (ICE,CCS)	G	G	Y	G	G	R	G	G	G	Y	86.3
NG-LNG (ICE)	G	G	G	G	Y	G	G	G	G	G	87.1
NG-LNG (ICE,CCS)	G	G	Y	G	G	G	G	G	G	Y	89.2
NG-H2 (ICE)	G	Y	Y	G	G	G	G	R	Y	Y	71.6
NG-H2 (FC)	G	Y	G	Y	G	G	G	R	Y	Y	71.3
NG-NH3 (ICE)	G	Y	Y	Y	Y	G	G	R	R	Y	59.4
NG-NH3 (FC)	G	G	Y	Y	Y	G	G	R	R	Y	61.1
NG-MeOH (ICE)	G	G	Y	G	R	G	G	Y	Y	Y	60.7
NG-MeOH (ICE,CCS)	G	G	R	G	R	G	G	Y	Y	Y	59.5
NG-E (EM)	R	R	G	R	G	G	G	G	G	G	65.7
BLUE-E-H2 (FC)	G	Y	Y	R	G	G	Y	R	Y	Y	63.2
BLUE-E-NH3 (FC)	G	G	R	R	Y	G	Y	R	R	Y	53.7
BLUE E-MeOH (ICE)	G	G	R	Y	R	G	Y	Y	Y	Y	51.8
BIODIESEL (ICE)	G	G	G	G	G	Y	Y	Y	G	Y	85.7
BIO-MeOH (ICE)	G	G	Y	Y	G	Y	Y	Y	Y	Y	69.4
SOLAR E (EM)	R	R	G	R	G	G	R	G	G	G	65.5
SOLAR-E-H2 (FC)	G	Y	Y	R	G	G	R	R	Y	Y	63.4
SOLAR-E-NH3 (FC)	G	G	Y	R	G	G	R	R	R	Y	58.7
SOLAR E-MEOH (ICE)	G	G	R	Y	G	G	R	Y	Y	Y	63.6
SOLAR-T-H2 (FC)	G	Y	Y	R	G	G	R	R	Y	Y	62.7
SOLAR-T-MeOH (ICE)	G	G	R	R	G	G	R	Y	Y	Y	58.1

Figure 10.14: Marine fuel ranking system.

6) Carbon reduction strategies of top chemical companies

Prof. S. VISWANATHAN, Dr Abhiruchi GADGIL, K. R. Preethi

To understand the decarbonisation strategies of big emitting chemical industries and oil and gas, the research recently (in August 2021) procured the Trucost datasets. These datasets have exhaustive information on companies' complete environmental profiles. Using these datasets, they have started analysing the oil and gas sector for their comparative emissions (Scope 1, Scope 2, Scope 3 upstream and downstream, based on environmentally extended input-output model). They are also comparing their overall sustainability ESG (Environmental, Social and Governance) scores, their emission reduction targets and Paris Agreement alignment levels, and based on their current decarbonisation actions and future carbon pricing hike, their overall earnings at risk. As integrated oil and gas industry have a lot of variation in their portfolio, the team are also trying to understand the effect of their different business activities on their decarbonisation strategies.

For the project on analysis of internal carbon pricing, a manuscript is being written for the work on understanding a multi-unit firm strategy for designing the internal tax based on a game-theory model.

7) Carbon capture, storage and utilisation roadmap 2050

Asst Prof. Paul LIU, Prof. Markus KRAFT

Dr Erika Lorenz-Calderon's (Research Fellow, NTU) main research consists of reducing carbon emissions by developing a 2050 roadmap towards achieving, at least partially, a carbon-circular economy in Singapore. In this field of study, Dr Lorenz-Calderon aims to develop solutions that could decarbonise Singapore, in particular, its chemical sector on Jurong Island, as well as other sectors such as transport, buildings, households, etc. In order to understand the Singapore carbon dioxide emission landscape, Dr Lorenz-Calderon and her team will use a knowledge-graph based approach developed by the same team at CARES.

Dr Lorenz-Calderon has recently found that in the road transport sector the light and heavy goods vehicles seem to emit the highest CO_2 (2,265.6 Gg CO_2e/year in total) in comparison with private cars, which are shown to emit 1,877.2 Gg CO_2e/year. In comparison to the literature, she has found that her values seem to be in agreement presenting a 0.94% error.

Figure 10.15: Singapore's Jurong Island.

8) Designing the structure and composition of active site motifs in CO_2 hydrogenation catalysts with atomic-level specificity

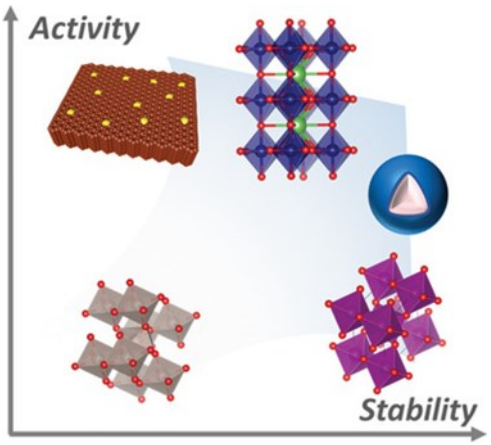
Asst Prof. Paul LIU, Prof. Alexei LAPKIN, Asst Prof. Tej CHOKSI

Asst Prof. Tej CHOKSI's (Co-I, NTU) research group employs density functional theory, molecular thermodynamics, and microkinetic modelling to understand how catalysts work at the atomic scale and improve their performance. In collaboration with **Asst Prof. Paul LIU (PI, NTU)**, a Strong Metal Support Interaction (SMSI) for metal nanoparticle supported on two-dimensional borides was reported. First principles calculations indicate that the SMSI phenomena arises from a combination of electrostatic and covalent interactions between the metal boride (TiB_2) and the metal nanoparticle. Asst Profs Choksi and Liu are now taking this study forward to understand how these low-dimensional boride overlayers improve the rate of formic acid dehydrogenation.

9) Electrified chemical production: AI strategies for accelerated intelligent design of disruptive technologies and electrochemical processes

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

Proton exchange membrane (PEM) water electrolysis is one of the most promising hydrogen production techniques. The oxygen evolution reaction (OER) occurring at the anode dominates the overall efficiency. Developing active and robust electrocatalysts for OER in acid is a longstanding challenge for PEM water electrolysers. Most catalysts show unsatisfied stability under strong acidic and oxidative conditions. Such a stability challenge also leads to difficulties for a better understanding of mechanisms. Work on this project aims to provide the current progress on understanding of OER mechanisms in acid, analyse the promising strategies to enhance both activity and stability, and summarise the state-of-the-art catalysts for OER in acid. First, the prevailing OER mechanisms are reviewed to establish the physicochemical structure–activity relationships for guiding the design of highly efficient OER electrocatalysts in acid with stable performance. The reported approaches to improve the activity, from macroview to microview, are then discussed. To analyse the problem of instability, the key factors affecting catalyst stability are summarised and the surface reconstruction is discussed. Various noble-metal-based OER catalysts and the current progress of non-noble-metal -based catalysts are reviewed. Finally, the challenges and perspectives for the development of active and robust OER catalysts in acid are discussed.



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

Prof. WANG Xin and Dr ZHANG Hongwei

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. To boost the desired performance towards $2e^-$ ORR pathway, ideal electrocatalysts possess an optimal binding strength for OOH* such that OOH* desorption is favoured versus further dissociation.

Based on this, a molecular strategy was designed to confine anthraquinone-based molecules on the single-atom NiN_4/C catalyst. These non-covalent interactions beyond the binding site could reduce the thermodynamic barrier for OOH* desorption versus further dissociation, thus increasing the selectivity to H_2O_2 from below 55% to above 80%. Experimental characterisation in conjunction with first principles calculations reveal that aminoanthraquinone is confined on isolated MNx sites through π-π interactions, thus forming a ~3 Å wide nano-channel. Oxygen reduction intermediates (e.g. OOH*) are destabilised by confinement effects within the nano-channel, promoting the $2e^-$ pathway to H_2O_2. This project has been published in *Advanced Materials* (Adv. Mater. 2021, 2104891).

In another research project, the modified MNx sites were explored for their H_2O_2 production activity by tailing the first coordination sphere of MNx sites. Specifically, the coordinated N in MNx sites was substituted with an exotic element, so that the atom geometry and electronic structures of MNx sites could be rationally tailored, achieving the modulation of kinetic barrier of OOH* and thus enabling a flexible reaction tunability towards oxygen reduction. The introduction of S into NiNx sites was realised and experimental results showed it can greatly improve the selectivity for H_2O_2 production. Synchrotron-based X-ray absorption spectroscopy confirmed the S was embedded into the NiN_4 sites to form NiN_3S_1 moiety. The NiN_3S_1 structure shows significantly enhanced selectivity for the $2e^-$ ORR pathway, presenting a selectivity near 90% for the H_2O_2 production. Compared with NiN_4 structure, it is believed that the NiN_3S_1 moiety can optimise the binding energy of OOH*, thus achieving this high selectivity towards H_2O_2 generation. Related DFT calculation is ongoing in collaboration with Asst Prof. Tej CHOKSI, and the manuscript is under preparation now.

A new Research Fellow, Dr ZHANG Hongwei, commenced work on the project in August 2021.

In collaboration with Wang Xin (IRP2), Tej performed a first principles analysis investigating why molecule confined metal sites promote the two-electron oxygen reduction to H_2O_2 instead of the four-electron oxygen reduction to H_2O. Both simulations and experiments indicate that the organic molecule (anthraquinone amine) forms a nano-channel over the single metal (Ni) site. Dispersion effects prevalent in the nanochannel favour the desorption of OOH* species, resulting in H_2O_2 formation. Taking this study forward, Wang Xin and Tej are now investigating why sulphur modified Ni-sites enhance the selectivity of oxygen reduction to H_2O_2.

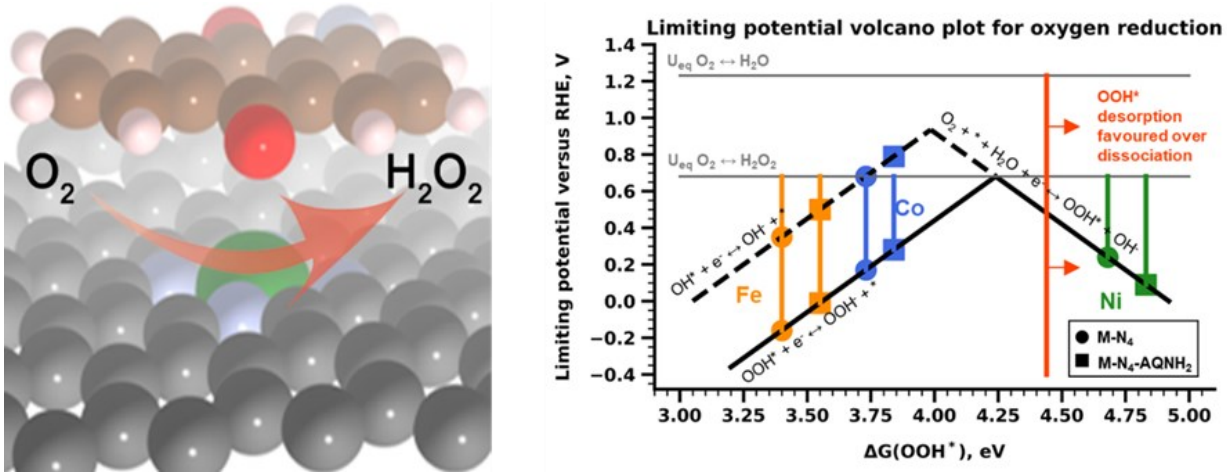


Figure 10.16: Graphical representation of a molecule confined Ni (green atom) site. (right). Volcano plot for oxygen reduction comparing single site catalysts with (squares) and without (circles) molecular confinement. Molecular confinement of Ni maintains the catalyst in the regime where OOH is desorbed, resulting in H2O2 formation. Advanced Materials, (2021), 2104891. https://doi.org/10.1002/adma.202104891*

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 and IRP 3

- Kan, Xiang, Xiaoping Chen, Ye Shen, Alexei Lapkin, Markus Kraft, and Chi-Hwa Wang. 2019. "Box-Behnken Design Based CO_2 Co-Gasification of Horticultural Waste and Sewage Sludge with Addition of Ash from Waste as Catalyst." *Applied Energy* 242 (May): 1549–61. https://doi.org/10.1016/j.apenergy.2019.03.176.

IRP 3 and IRP JPS

- Chhabra, Pulkit, Sebastian Mosbach, Iftekhar A. Karimi, and Markus Kraft. 2019. 'Practically Useful Models for Kinetics of Biodiesel Production'. *ACS Sustainable Chemistry & Engineering* 7 (5): 4983–92. https://doi.org/10.1021/acssuschemeng.8b05636.
- **Eibeck, Andreas, Daniel Nurkowski, Angiras Menon, Jiaru Bai, Jinkui Wu, Li Zhou, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2021. 'Predicting Power Conversion Efficiency of Organic Photovoltaics: Models and Data Analysis'. *ACS Omega* 6 (37): 23764–75. https://doi.org/10.1021/acsomega.1c02156.**
- Farazi, Feroz, Nenad B. Krdzavac, Jethro Akroyd, Sebastian Mosbach, Angiras Menon, Daniel Nurkowski, and Markus Kraft. 2020. 'Linking Reaction Mechanisms and Quantum Chemistry: An Ontological Approach'. *Computers & Chemical Engineering*, March, 106813. https://doi.org/10.1016/j.compchemeng.2020.106813.
- Krdzavac, Nenad, Sebastian Mosbach, Daniel Nurkowski, Philipp Buerger, Jethro Akroyd, Jacob Martin, Angiras Menon, and Markus Kraft. 2019. 'An Ontology and Semantic Web Service for Quantum Chemistry Calculations'. *Journal of Chemical Information and Modeling* 59 (7): 3154–65. https://doi.org/10.1021/acs.jcim.9b00227.
- Menon, Angiras, Nenad B Krdzavac, and Markus Kraft. 2019. 'From Database to Knowledge Graph — Using Data in Chemistry'. *Current Opinion in Chemical Engineering* 26 (December): 33–37. https://doi.org/10.1016/

j.coche.2019.08.004.

- Slavchov, Radomir I., Maurin Salamanca, Danilo Russo, Ibrahim Salama, Sebastian Mosbach, Stuart M. Clarke, Markus Kraft, Alexei A. Lapkin, and Sorin V. Filip. 2020. 'The Role of NO2 and NO in the Mechanism of Hydrocarbon Degradation Leading to Carbonaceous Deposits in Engines'. *Fuel* 267 (May): 117218. https://doi.org/10.1016/j.fuel.2020.117218.

IRP 4 and IRP JPS

- **Pan, Kang, Mei Qi Lim, Markus Kraft, and Epaminondas Mastorakos. 2021. 'Development of a Moving Point Source Model for Shipping Emission Dispersion Modeling in EPISODE–CityChem v1.3'. *Geoscientific Model Development* 14 (7): 4509–34. https://doi.org/10.5194/gmd-14-4509-2021.**

IRP 3, IRP 4 and IRP JPS

- Farazi, Feroz, Maurin Salamanca, Sebastian Mosbach, Jethro Akroyd, Andreas Eibeck, Leonardus Kevin Aditya, Arkadiusz Chadzynski, et al. 2020. 'Knowledge Graph Approach to Combustion Chemistry and Interoperability'. *ACS Omega* 5 (29): 18342–48. https://doi.org/10.1021/acsomega.0c02055.

IRP 1 and eCO_2EP

- **Liu, Guanyu, Parvathala Reddy Narangari, Quang Thang Trinh, Wenguang Tu, Markus Kraft, Hark Hoe Tan, Chennupati Jagadish, et al. 2021. 'Manipulating Intermediates at the Au–TiO_2 Interface over InP Nanopillar Array for Photoelectrochemical CO_2 Reduction'. *ACS Catalysis* 11 (18): 11416–28. https://doi.org/10.1021/acscatal.1c02043.**

C4T IRP 1: Sustainable reaction engineering

- Amar, Yehia, Artur M. Schweidtmann, Paul Deutsch, Liwei Cao, and Alexei Lapkin. 2019. 'Machine Learning and Molecular Descriptors Enable Rational Solvent Selection in Asymmetric Catalysis.' *Chemical Science* 10 (27): 6697–6706. https://doi.org/10.1039/C9SC01844A.
- Cao, Liwei, Mikhail Kabeshov, Steven V Ley, and Alexei A Lapkin. 2020. 'In Silico Rationalisation of Selectivity and Reactivity in Pd-Catalysed C–H Activation Reactions.' *Beilstein Journal of Organic Chemistry* 16 (June): 1465–75. https://doi.org/10.3762/bjoc.16.122.
- Cao, Liwei, Danilo Russo, Kobi Felton, Daniel Salley, Abhishek Sharma, Graham Keenan, Werner Mauer, Huanhuan Gao, Leroy Cronin, and Alexei A. Lapkin. 2021. 'Optimization of Formulations Using Robotic Experiments Driven by Machine Learning DoE.' *Cell Reports Physical Science*, January, 100295. https://doi.org/10.1016/j.xcrp.2020.100295.
- Cao, Liwei, Danilo Russo, and Alexei A. Lapkin. 2021. 'Automated Robotic Platforms in Design and Development of Formulations.' *AIChE Journal*, February. https://doi.org/10.1002/aic.17248.
- **Di, Andi, Yu Wang, and Hua Chun Zeng. 2021. 'TiO_2/C Tetragons with a Double-Side Concave Nanostructure and Its High Rate Performance on Na-Ion Storage.' *Applied Surface Science* 567 (November): 150756. https://doi.org/10.1016/j.apsusc.2021.150756.**
- Goyal, Prerna, Mark J. Purdue, and Shamsuzzaman Farooq. 2019. 'Adsorption and Diffusion of N_2 and CO_2 and Their Mixture on Silica Gel.' *Industrial & Engineering Chemistry Research* 58 (42): 19611–22. https://doi.org/10.1021/acs.iecr.9b02685.
- Goyal, Prerna, Mark J. Purdue, and Shamsuzzaman Farooq. 2020. 'Adsorption and Diffusion of Moisture and Wet Flue Gas on Silica Gel.' *Chemical Engineering Science* 227 (December): 115890. https://doi.org/10.1016/j.ces.2020.115890.
- Guo, Zhen, Ning Yan, and Alexei A. Lapkin. 2019. 'Towards Circular Economy: Integration of Bio-Waste into Chemical Supply Chain.' *Current Opinion in Chemical Engineering* 26 (December): 148–56. https://doi.org/10.1016/j.coche.2019.09.010.
- **Hao, Zhimian, Adrian Caspari, Artur M. Schweidtmann, Yannic Vaupel, Alexei A. Lapkin, and Adel Mhamdi. 2021. 'Efficient Hybrid Multiobjective Optimization of Pressure Swing Adsorption.' *Chemical Engineering Journal* 423 (November): 130248. https://doi.org/10.1016/j.cej.2021.130248.**
- Huang, Jijiang, Wen Liu, Wenting Hu, Ian Metcalfe, Yanhui Yang, and Bin Liu. 2019. 'Phase Interactions in Ni-Cu-Al_2O_3 Mixed Oxide Oxygen Carriers for Chemical Looping Applications.' *Applied Energy* 236

(February): 635–47. https://doi.org/10.1016/j.apenergy.2018.12.029.

- **Jorayev, Perman, Danilo Russo, Joshua D. Tibbetts, Artur M. Schweidtmann, Paul Deutsch, Steven D. Bull, and Alexei A. Lapkin. 2022. 'Multi-Objective Bayesian Optimisation of a Two-Step Synthesis of p-Cymene from Crude Sulphate Turpentine.' *Chemical Engineering Science* 247 (January): 116938. https://doi.org/10.1016/j.ces.2021.116938.**
- **Jose, Nicholas A., Mikhail Kovalev, Eric Bradford, Artur M. Schweidtmann, Hua Chun Zeng, and Alexei A. Lapkin. 2021. 'Pushing Nanomaterials up to the Kilogram Scale - an Accelerated Approach for Synthesizing Antimicrobial ZnO with High Shear Reactors, Machine Learning and High-Throughput Analysis.' *Chemical Engineering Journal*, July. https://doi.org/10.1016/j.cej.2021.131345.**
- Jose, Nicholas A., Hua Chun Zeng, and Alexei A. Lapkin. 2018. 'Hydrodynamic Assembly of Two-Dimensional Layered Double Hydroxide Nanostructures.' *Nature Communications* 9 (1). https://doi.org/10.1038/s41467-018-07395-4.
- Jose, Nicholas A., Hua Chun Zeng, and Alexei A. Lapkin. 2020. 'Scalable and Precise Synthesis of Two-Dimensional Metal Organic Framework Nanosheets in a High Shear Annular Microreactor.' *Chemical Engineering Journal* 388 (May): 124133. https://doi.org/10.1016/j.cej.2020.124133.
- Jose, Nicholas, and Alexei Lapkin. 2019. 'Influence of Hydrodynamics on Wet Syntheses of Nanomaterials.' In *Advanced Nanomaterials for Catalysis and Energy*, 29–59. Elsevier. https://doi.org/10.1016/B978-0-12-814807-5.00002-4.
- **Kosari, Mohammadreza, Uzma Anjum, Shibo Xi, Alvin M. H. Lim, Abdul Majeed Seayad, Emmanuel A. J. Raj, Sergey M. Kozlov, Armando Borgna, and Hua Chun Zeng. 2021. 'Revamping SiO_2 Spheres by Core –Shell Porosity Endowment to Construct a Mazelike Nanoreactor for Enhanced Catalysis in CO_2 Hydrogenation to Methanol.' *Advanced Functional Materials*, July, 2102896. https://doi.org/10.1002/adfm.202102896.**
- Kosari, Mohammadreza, Armando Borgna, and Hua Chun Zeng. 2020. 'Transformation of Stöber Silica Spheres to Hollow Nanocatalysts.' *ChemNanoMat* 6 (6): 889–906. https://doi.org/10.1002/cnma.202000147.
- Kosari, Mohammadreza, Abdul Majeed Seayad, Shibo Xi, Sergey M. Kozlov, Armando Borgna, and Hua Chun Zeng. 2020. 'Synthesis of Mesoporous Copper Aluminosilicate Hollow Spheres for Oxidation Reactions.' *ACS Applied Materials & Interfaces* 12 (20): 23060–75. https://doi.org/10.1021/acsami.0c03052.
- Kwok, Kelvin Mingyao, Luwei Chen, and Hua Chun Zeng. 2020. 'Design of Hollow Spherical Co@hsZSM5@metal Dual-Layer Nanocatalysts for Tandem CO_2 Hydrogenation to Increase C_{2+} Hydrocarbon Selectivity.' *Journal of Materials Chemistry A* 8 (25): 12757–66. https://doi.org/10.1039/D0TA04608F.
- Kwok, Kelvin Mingyao, Sze Wei Daniel Ong, Luwei Chen, and Hua Chun Zeng. 2019. 'Transformation of Stöber Silica Spheres to Hollow Hierarchical Single-Crystal ZSM-5 Zeolites with Encapsulated Metal Nanocatalysts for Selective Catalysis.' *ACS Applied Materials & Interfaces* 11 (16): 14774–85. https://doi.org/10.1021/acsami.9b00630.
- Lapkin, Alexei. 2020. 'Rational Design of Continuous Flow Processes for Synthesis of Functional Molecules.' In *Sustainable Nanoscale Engineering*, 415–33. Elsevier. https://doi.org/10.1016/B978-0-12-814681-1.00016-3.
- **Li, Bowen, Kelvin Mingyao Kwok, and Hua Chun Zeng. 2021. 'Versatile Hollow ZSM-5 Nanoreactors Loaded with Tailorable Metal Catalysts for Selective Hydrogenation Reactions.' *ACS Applied Materials & Interfaces* 13 (17): 20524–38. https://doi.org/10.1021/acsami.1c01916.**
- Li, Bowen, and Hua Chun Zeng. 2019. 'Synthetic Chemistry and Multifunctionality of an Amorphous Ni-MOF-74 Shell on a Ni/SiO_2 Hollow Catalyst for Efficient Tandem Reactions.' *Chemistry of Materials* 31 (14): 5320–30. https://doi.org/10.1021/acs.chemmater.9b02070.
- Li, Bowen, and Hua Chun Zeng. 2020. 'Minimalization of Metallic Pd Formation in Suzuki Reaction with a Solid-State Organometallic Catalyst.' *ACS Applied Materials & Interfaces* 12 (30): 33827–37. https://doi.org/10.1021/acsami.0c09739.
- Li, Ping, and Hua Chun Zeng. 2019. 'Promoting Electrocatalytic Oxygen Evolution over Transition-Metal Phosphide-Based Nanocomposites via Architectural and Electronic Engineering.' *ACS Applied Materials & Interfaces* 11 (50): 46825–38. https://doi.org/10.1021/acsami.9b16564.
- **Li, Renhong, Zhiqi Liu, Quang Thang Trinh, Ziqiang Miao, Shuang Chen, Kaicheng Qian, Roong Jien Wong, et al. 2021. 'Strong Metal–Support Interaction for 2D Materials: Application in Noble Metal/TiB_2 Heterointerfaces and Their Enhanced Catalytic Performance for Formic Acid Dehydrogenation.' *Advanced Materials* 33 (32): 2101536. https://doi.org/10.1002/adma.202101536.**
- Li, Xian, Ye Shen, Liping Wei, Chao He, Alexei A. Lapkin, Wojciech Lipiński, Yanjun Dai, and Chi-Hwa Wang. 2020. 'Hydrogen Production of Solar-Driven Steam Gasification of Sewage Sludge in an Indirectly Irradiated Fluidized-Bed Reactor.' *Applied Energy* 261 (March): 114229. https://doi.org/10.1016/j.apenergy.2019.114229.
- **Li, Xiaogang, Shasha Tang, Shuo Dou, Hong Jin Fan, Tej S. Choksi, and Xin Wang. 2021. 'Molecule**

Confined Isolated Metal Sites Enable the Electrocatalytic Synthesis of Hydrogen Peroxide'. Advanced Materials, September, 2104891. https://doi.org/10.1002/adma.202104891.

- **Lim, Alvin M. H., and Hua Chun Zeng. 2021. 'Antisolvent Route to Ultrathin Hollow Spheres of Cerium Oxide for Enhanced CO Oxidation.' *ACS Applied Materials & Interfaces* 13 (17): 20501–10. https://doi.org/10.1021/acsami.1c01320.**
- **Liu, Wen. 2021. 'Controlling Lattice Oxygen Activity of Oxygen Carrier Materials by Design: A Review and Perspective.' *Reaction Chemistry & Engineering* 6 (9): 1527–37. https://doi.org/10.1039/D1RE00209K.**
- Mohan, Ojus, Shambhawi Shambhawi, Xu Rong, Alexei A Lapkin, and Samir Hemant Mushrif. 2021. 'Investigating CO_2 Methanation on Ni and Ru: DFT Assisted Microkinetic Analysis.' *ChemCatChem*, February, cctc.202100073. https://doi.org/10.1002/cctc.202100073.
- Neumann, Pascal, Liwei Cao, Danilo Russo, Vassilios S. Vassiliadis, and Alexei A. Lapkin. 2019. 'A New Formulation for Symbolic Regression to Identify Physico-Chemical Laws from Experimental Data.' *Chemical Engineering Journal*, November, 123412. https://doi.org/10.1016/j.cej.2019.123412.
- Qin, Runze, and Hua Chun Zeng. 2019. 'Confined Transformation of UiO-66 Nanocrystals to Yttria-Stabilized Zirconia with Hierarchical Pore Structures for Catalytic Applications.' *Advanced Functional Materials* 29 (39): 1903264. https://doi.org/10.1002/adfm.201903264.
- **Saqline, Syed, Zhen Yee Chua, and Wen Liu. 2021. 'Coupling Chemical Looping Combustion of Solid Fuels with Advanced Steam Cycles for CO_2 Capture: A Process Modelling Study.' *Energy Conversion and Management* 244 (September): 114455. https://doi.org/10.1016/j.enconman.2021.114455.**
- **Shao, Yu, and Hua Chun Zeng. 2021. 'Pt, Ir, Ru, and Rh Nanoparticles Supported on ZIF-67 Nanocubes for Evaluation of Hydrogen Spillover Ability of Noble Metals.' *ACS Applied Nano Materials*, June, acsanm.1c00871. https://doi.org/10.1021/acsanm.1c00871.**
- Shen, Ye, Chao He, Xiaoping Chen, Alexei A. Lapkin, Wende Xiao, and Chi-Hwa Wang. 2018. 'Nitrogen Removal and Energy Recovery from Sewage Sludge by Combined Hydrothermal Pretreatment and CO_2 Gasification.' *ACS Sustainable Chemistry & Engineering* 6 (12): 16629–36. https://doi.org/10.1021/acssuschemeng.8b03857.
- Sun, Bo, Lulu Ning, and Hua Chun Zeng. 2020. 'Confirmation of Suzuki–Miyaura Cross-Coupling Reaction Mechanism through Synthetic Architecture of Nanocatalysts.' *Journal of the American Chemical Society* 142 (32): 13823–32. https://doi.org/10.1021/jacs.0c04804.
- Sun, Bo, and Hua Chun Zeng. 2020. 'A Shell-by-Shell Approach for Synthesis of Mesoporous Multi-Shelled Hollow MOFs for Catalytic Applications.' *Particle & Particle Systems Characterization* 37 (6): 2000101. https://doi.org/10.1002/ppsc.202000101.
- Tan, Ying Chuan, and Hua Chun Zeng. 2019. 'Low-dimensional Metal-organic Frameworks and Their Diverse Functional Roles in Catalysis.' *ChemCatChem* 11 (14): 3138–65. https://doi.org/10.1002/cctc.201900191.
- Varghese, Jithin John, Liwei Cao, Christopher Robertson, Yanhui Yang, Lynn F. Gladden, Alexei A. Lapkin, and Samir H. Mushrif. 2019. 'Synergistic Contribution of the Acidic Metal Oxide–Metal Couple and Solvent Environment in the Selective Hydrogenolysis of Glycerol: A Combined Experimental and Computational Study Using ReO_x–Ir as the Catalyst.' *ACS Catalysis* 9 (1): 485–503. https://doi.org/10.1021/acscatal.8b03079.
- Varghese, Jithin John, and Samir H. Mushrif. 2019. 'Origins of Complex Solvent Effects on Chemical Reactivity and Computational Tools to Investigate Them: A Review.' *Reaction Chemistry & Engineering*. https://doi.org/10.1039/C8RE00226F.
- Wang, Jingjing, Wenjie Zang, Shibo Xi, Mohammadreza Kosari, Stephen J. Pennycook, and Hua Chun Zeng. 2020. 'Trimetal Atoms Confined in Openly Accessible Nitrogen-Doped Carbon Constructs for an Efficient ORR.' *Journal of Materials Chemistry A* 8 (33): 17266–75. https://doi.org/10.1039/D0TA05984F.
- Wang, Jingjing, and Hua Chun Zeng. 2019. 'A Hybrid Electrocatalyst with a Coordinatively Unsaturated Metal–Organic Framework Shell and Hollow Ni_3S_2/NiS Core for Oxygen Evolution Reaction Applications.' *ACS Applied Materials & Interfaces* 11 (26): 23180–91. https://doi.org/10.1021/acsami.9b04479.
- Wang, Jingjing, and Hua Chun Zeng. 2020. 'Hybrid OER Electrocatalyst Combining Mesoporous Hollow Spheres of N, P-Doped Carbon with Ultrafine Co_2NiO_x.' *ACS Applied Materials & Interfaces* 12 (45): 50324–32. https://doi.org/10.1021/acsami.0c12305.
- **Weber, Jana M., Zhen Guo, Chonghuan Zhang, Artur M. Schweidtmann, and Alexei A. Lapkin. 2021. 'Chemical Data Intelligence for Sustainable Chemistry.' *Chemical Society Reviews*, 10.1039.D1CS00477H. https://doi.org/10.1039/D1CS00477H.**
- Weber, Jana Marie, Pietro Lió, and Alexei A. Lapkin. 2019. 'Identification of Strategic Molecules for Future Circular Supply Chains Using Large Reaction Networks.' *Reaction Chemistry & Engineering*. https://doi.org/10.1039/C9RE00213H.
- **Xu, Tingting, Xun Wang, Bo Xiao, and Wen Liu. 2021. 'Single-Step Production of Hydrogen-Rich Syngas**

from Toluene Using Multifunctional Ni-Dolomite Catalysts.' *Chemical Engineering Journal* 425 (December): 131522. https://doi.org/10.1016/j.cej.2021.131522.

- Yaseneva, Polina, Nan An, Matt Finn, Nicholas Tidemann, Nicholas Jose, Adelina Voutchkova-Kostal, and Alexei Lapkin. 2019. 'Continuous Synthesis of Doped Layered Double Hydroxides in a Meso-Scale Flow Reactor.' *Chemical Engineering Journal* 360 (March): 190–99. https://doi.org/10.1016/j.cej.2018.11.197.
- Zeng, Hua Chun. 2020a. 'Mesoporous Silica Encapsulated Metal-Organic Frameworks for Heterogeneous Catalysis.' *Matter* 3 (2): 332–34. https://doi.org/10.1016/j.matt.2020.07.013.
- Zeng, Hua Chun. 2020b. 'Hierarchy Concepts in Design and Synthesis of Nanocatalysts.' *ChemCatChem* 12 (21): 5303–11. https://doi.org/10.1002/cctc.202001003.
- Zhang, Chonghuan, Yehia Amar, Liwei Cao, and Alexei A. Lapkin. 2020. 'Solvent Selection for Mitsunobu Reaction Driven by an Active Learning Surrogate Model.' *Organic Process Research & Development* 24 (12): 2864–73. https://doi.org/10.1021/acs.oprd.0c00376.
- Zhou, Yao, and Hua Chun Zeng. 2019. 'Adsorption and On-Site Transformation of Transition Metal Cations on Ni-Doped AlOOH Nanoflowers for OER Electrocatalysis.' *ACS Sustainable Chemistry & Engineering* 7 (6): 5953–62. https://doi.org/10.1021/acssuschemeng.8b06020.

C4T IRP 2: Electrosynthetic pathways

- An, Li, Chao Wei, Min Lu, Hanwen Liu, Yubo Chen, Günther G. Scherer, Adrian C. Fisher, Pinxian Xi, Zhichuan J. Xu, and Chun-Hua Yan. 2021. 'Recent Development of Oxygen Evolution Electrocatalysts in Acidic Environment'. *Advanced Materials*, March, 2006328. https://doi.org/10.1002/adma.202006328.
- **Chen, Riccardo Ruixi, Gao Chen, Xiao Ren, Jingjie Ge, Samuel Jun Hoong Ong, Shibo Xi, Xin Wang, and Zhichuan Xu. 2021. 'SmCo$_5$ with a Reconstructed Oxyhydroxide Surface for Spin Selective Water Oxidation under Elevated Temperature'. *Angewandte Chemie International Edition*, September, anie.202109065. https://doi.org/10.1002/anie.202109065.**
- Chen, Riccardo Ruixi, Yuanmiao Sun, Samuel Jun Hoong Ong, Shibo Xi, Yonghua Du, Chuntai Liu, Ovadia Lev, and Zhichuan J. Xu. 2020. 'Antiferromagnetic Inverse Spinel Oxide $LiCoVO_4$ with Spin-Polarized Channels for Water Oxidation'. *Advanced Materials* 32 (10): 1907976. https://doi.org/10.1002/adma.201907976.
- Dai, Chencheng, Libo Sun, Jiajia Song, Hanbin Liao, Adrian C. Fisher, and Zhichuan J. Xu. 2019. 'Selective Electroreduction of Carbon Dioxide to Formic Acid on Cobalt-Decorated Copper Thin Films'. *Small Methods*, June, 1900362. https://doi.org/10.1002/smtd.201900362.
- Dai, Chencheng, Yuanmiao Sun, Gao Chen, Adrian C. Fisher, and Zhichuan Xu. 2020. 'Electrochemical Oxidation of Nitrogen towards Direct Nitrate Production on Spinel Oxides'. *Angewandte Chemie International Edition*, March. https://doi.org/10.1002/anie.202002923.
- Dou, Shuo, Jiajia Song, Shibo Xi, Yonghua Du, Jiong Wang, Zhen-Feng Huang, Zhichuan J. Xu, and Xin Wang. 2019. 'Boosting Electrochemical CO_2 Reduction on Metal–Organic Frameworks via Ligand Doping'. *Angewandte Chemie International Edition* 58 (12): 4041–45. https://doi.org/10.1002/anie.201814711.
- Duan, Yan, Jun Yan Lee, Shibo Xi, Yuanmiao Sun, Jingjie Ge, Samuel Jun Hoong Ong, Yubo Chen, et al. 2021. 'Anodic Oxidation Enabled Cation Leaching for Promoting Surface Reconstruction in Water Oxidation'. *Angewandte Chemie International Edition* 60 (13): 7418–25. https://doi.org/10.1002/anie.202015060.
- Elouarzaki, Kamal, Vishvak Kannan, Vishal Jose, Harshjyot Singh Sabharwal, and Jong-Min Lee. 2019. 'Recent Trends, Benchmarking, and Challenges of Electrochemical Reduction of CO_2 by Molecular Catalysts'. *Advanced Energy Materials* 9 (24): 1900090. https://doi.org/10.1002/aenm.201900090.
- Elouarzaki, Kamal, Vishvak Kannan, Yian Wang, Adrian C. Fisher, and Jong-Min Lee. 2021. 'Electrocatalytic Dimeric Inactivation Mechanism by a Porphyrinic Molecular-Type Catalyst: Integration in a Glucose/O_2 Fuel Cell'. *Catalysis Science & Technology*, 10.1039.D0CY02443K. https://doi.org/10.1039/D0CY02443K.
- Elouarzaki, Kamal, Yian Wang, Vishvak Kannan, Haoxiang Xu, Daojian Cheng, Jong-Min Lee, and Adrian C. Fisher. 2019. 'Hydrogenase-Like Electrocatalytic Activation and Inactivation Mechanism by Three-Dimensional Binderless Molecular Catalyst'. *ACS Applied Energy Materials* 2 (5): 3352–62. https://doi.org/10.1021/acsaem.9b00203.
- Huang, Zhen-Feng, Jiajia Song, Yonghua Du, Shibo Xi, Shuo Dou, Jean Marie Vianney Nsanzimana, Cheng Wang, Zhichuan J. Xu, and Xin Wang. 2019. 'Chemical and Structural Origin of Lattice Oxygen Oxidation in Co–Zn Oxyhydroxide Oxygen Evolution Electrocatalysts'. *Nature Energy* 4 (4): 329–38. https://doi.org/10.1038/s41560-019-0355-9.
- Kannan, Vishvak, Adrian Fisher, and Erik Birgersson. 2021. 'Monte Carlo Assisted Sensitivity Analysis of a Li-Ion Battery with a Phase Change Material'. *Journal of Energy Storage* 35 (March): 102269. https://doi.org/10.1016/j.est.2021.102269.

- Kannan, Vishvak, K. Ashoke Raman, Adrian Fisher, and Erik Birgersson. 2019. 'Correlating Uncertainties of a CO_2 to CO Microfluidic Electrochemical Reactor: A Monte Carlo Simulation'. *Industrial & Engineering Chemistry Research* 58 (42): 19361–76. https://doi.org/10.1021/acs.iecr.9b04596.
- **Kannan, Vishvak, Karthik Somasundaram, Adrian Fisher, and Erik Birgersson. 2021. 'Monte Carlo-based Sensitivity Analysis of an Electrochemical Capacitor'. *International Journal of Energy Research*, May, er.6919. https://doi.org/10.1002/er.6919.**
- Kannan, Vishvak, Hansong Xue, K. Ashoke Raman, Jiasheng Chen, Adrian Fisher, and Erik Birgersson. 2020. 'Quantifying Operating Uncertainties of a PEMFC – Monte Carlo-Machine Learning Based Approach'. *Renewable Energy* 158 (October): 343–59. https://doi.org/10.1016/j.renene.2020.05.097.
- Lee, Joseph Yoon Young, Kamal Elouarzaki, Harshjyot Singh Sabharwal, Adrian C. Fisher, and Jong-Min Lee. 2020. 'A Hydrogen/Oxygen Hybrid Biofuel Cell Comprising an Electrocatalytically Active Nanoflower/Laccase-Based Biocathode'. *Catalysis Science & Technology*, 10.1039.D0CY00675K. https://doi.org/10.1039/D0CY00675K.
- Li, Haiyan, Yubo Chen, Jingjie Ge, Xianhu Liu, Adrian C. Fisher, Matthew P. Sherburne, Joel W. Ager, and Zhichuan J. Xu. 2021. 'Active Phase on $SrCo_{1-x}Fe_xO_{3-\delta}$ ($0 \le x \le 0.5$) Perovskite for Water Oxidation: Reconstructed Surface versus Remaining Bulk'. *JACS Au* 1 (1): 108–15. https://doi.org/10.1021/jacsau.0c00022.
- Nsanzimana, Jean Marie Vianney, Lanqian Gong, Raksha Dangol, Vikas Reddu, Vishal Jose, Bao Yu Xia, Qingyu Yan, Jong-Min Lee, and Xin Wang. 2019. 'Tailoring of Metal Boride Morphology via Anion for Efficient Water Oxidation'. *Advanced Energy Materials* 9 (28): 1901503. https://doi.org/10.1002/aenm.201901503.
- Pankan, Aazraa O., Kamran Yunus, and Adrian C. Fisher. 2020. 'Mechanistic Evaluation of the Exoelectrogenic Activity of Rhodopseudomonas Palustris under Different Nitrogen Regimes'. *Bioresource Technology* 300 (March): 122637. https://doi.org/10.1016/j.biortech.2019.122637.
- Pankan, Aazraa O., Kamran Yunus, Ela Sachyani, Kamal Elouarzaki, Shlomo Magdassi, Minyu Zeng, and Adrian C. Fisher. 2020. 'A Multi-Walled Carbon Nanotubes Coated 3D Printed Anode Developed for Biophotovotaic Applications'. *Journal of Electroanalytical Chemistry* 872 (January): 114397. https://doi.org/10.1016/j.jelechem.2020.114397.
- Paul, Ratul, Chitra Sarkar, Yong Yan, Quang Thang Trinh, Bolla Srinivasa Rao, Chih-Wen Pao, Jyh-Fu Lee, Wen Liu, and John Mondal. 2020. 'Porous-Organic-Polymer-Triggered Advancement of Sustainable Magnetic Efficient Catalyst for Chemoselective Hydrogenation of Cinnamaldehyde'. *ChemCatChem* 12 (14): 3687–3704. https://doi.org/10.1002/cctc.202000072.
- Ren, Xiao, Chao Wei, Yuanmiao Sun, Xiaozhi Liu, Fanqi Meng, Xiaoxia Meng, Shengnan Sun, et al. 2020. 'Constructing an Adaptive Heterojunction as a Highly Active Catalyst for the Oxygen Evolution Reaction'. *Advanced Materials* 32 (30): 2001292. https://doi.org/10.1002/adma.202001292.
- **Ren, Xiao, Tianze Wu, Yuanmiao Sun, Yan Li, Guoyu Xian, Xianhu Liu, Chengmin Shen, et al. 2021. 'Spin-Polarized Oxygen Evolution Reaction under Magnetic Field'. *Nature Communications* 12 (1): 2608. https://doi.org/10.1038/s41467-021-22865-y.**
- Rosli, Nur Farhanah, Michaela Fojtů, Adrian C. Fisher, and Martin Pumera. 2019. 'Graphene Oxide Nanoplatelets Potentiate Anticancer Effect of Cisplatin in Human Lung Cancer Cells'. *Langmuir* 35 (8): 3176–82. https://doi.org/10.1021/acs.langmuir.8b03086.
- Rosli, Nur Farhanah, Muhammad Zafir Mohamad Nasir, Nikolas Antonatos, Zdeněk Sofer, Apurv Dash, Jesus Gonzalez-Julian, Adrian C. Fisher, Richard D. Webster, and Martin Pumera. 2019. 'MAX and MAB Phases: Two-Dimensional Layered Carbide and Boride Nanomaterials for Electrochemical Applications'. *ACS Applied Nano Materials*, September, acsanm.9b01526. https://doi.org/10.1021/acsanm.9b01526.
- Rosli, Nur Farhanah, Nasuha Rohaizad, Jiri Sturala, Adrian C. Fisher, Richard D. Webster, and Martin Pumera. 2020. 'Siloxene, Germanane, and Methylgermanane: Functionalized 2D Materials of Group 14 for Electrochemical Applications'. *Advanced Functional Materials* 30 (21): 1910186. https://doi.org/10.1002/adfm.201910186.
- Song, Jiajia, Chao Wei, Zhen-Feng Huang, Chuntai Liu, Lin Zeng, Xin Wang, and Zhichuan J. Xu. 2020. 'A Review on Fundamentals for Designing Oxygen Evolution Electrocatalysts'. *Chemical Society Reviews*, March, 10.1039.C9CS00607A. https://doi.org/10.1039/C9CS00607A.
- Sun, Libo, Vikas Reddu, Adrian C. Fisher, and Xin Wang. 2020. 'Electrocatalytic Reduction of Carbon Dioxide: Opportunities with Heterogeneous Molecular Catalysts'. *Energy & Environmental Science* 13 (2): 374–403. https://doi.org/10.1039/C9EE03660A.
- **Sun, Libo, Vikas Reddu, Tan Su, Xinqi Chen, Tian Wu, Wei Dai, Adrian C. Fisher, and Xin Wang. 2021. 'Effects of Axial Functional Groups on Heterogeneous Molecular Catalysts for Electrocatalytic CO_2 Reduction'. *Small Structures*, September, 2100093. https://doi.org/10.1002/sstr.202100093.**
- Sun, Shengnan, Yuanmiao Sun, Ye Zhou, Shibo Xi, Xiao Ren, Bicheng Huang, Hanbin Liao, Luyuan Paul Wang, Yonghua Du, and Zhichuan J. Xu. 2019. 'Shifting Oxygen Charge Towards Octahedral Metal: A Way

to Promote Water Oxidation on Cobalt Spinel Oxides'. *Angewandte Chemie International Edition* 58 (18): 6042–47. https://doi.org/10.1002/anie.201902114.

- Sun, Yuanmiao, Hanbin Liao, Jiarui Wang, Bo Chen, Shengnan Sun, Samuel Jun Hoong Ong, Shibo Xi, et al. 2020. 'Covalency Competition Dominates the Water Oxidation Structure–Activity Relationship on Spinel Oxides'. *Nature Catalysis* 3 (7): 554–63. https://doi.org/10.1038/s41929-020-0465-6.
- Sun, Yuanmiao, Shengnan Sun, Haitao Yang, Shibo Xi, Jose Gracia, and Zhichuan J. Xu. 2020. 'Spin-Related Electron Transfer and Orbital Interactions in Oxygen Electrocatalysis'. *Advanced Materials*, August, 2003297. https://doi.org/10.1002/adma.202003297.
- Tham, Guo Xiong, Adrian C. Fisher, and Richard D. Webster. 2019. 'A Vitamin-Based Voltammetric PH Sensor That Functions in Buffered and Unbuffered Media'. *Sensors and Actuators B: Chemical* 283 (March): 495–503. https://doi.org/10.1016/j.snb.2018.12.036.
- Tham, Guo Xiong, Adrian C. Fisher, and Richard D. Webster. 2020. 'Voltammetric Studies on Surface-Modified Electrodes with Functionalised Carbon Nanotubes under Different Dispersion Conditions'. *Electrochimica Acta* 357 (October): 136880. https://doi.org/10.1016/j.electacta.2020.136880.
- Tham, Guo Xiong, Arnold Subrata, Adrian C. Fisher, and Richard D. Webster. 2021. 'Properties of Electrochemically Copolymerized Aniline and Melamine on Functionalized Multiwalled-carbon Nanotube Film Electrodes'. *Electrochemical Science Advances*, May. https://doi.org/10.1002/elsa.202100021.
- Wang, Jiarui, Ye Zhou, Libo Sun, Jingjie Ge, Jingxian Wang, Chencheng Dai, and Zhichuan Xu. 2020. 'Ir-Skinned Ir-Cu Nanoparticles with Enhanced Activity for Oxygen Reduction Reaction'. *Chemical Research in Chinese Universities* 36 (3): 467–72. https://doi.org/10.1007/s40242-020-0087-1.
- Wang, Jiong, Liyong Gan, Qianwen Zhang, Vikas Reddu, Yuecheng Peng, Zhichao Liu, Xinghua Xia, Cheng Wang, and Xin Wang. 2019. 'A Water-Soluble Cu Complex as Molecular Catalyst for Electrocatalytic CO_2 Reduction on Graphene-Based Electrodes'. *Advanced Energy Materials* 9 (3): 1803151. https://doi.org/10.1002/aenm.201803151.
- Wang, Jiong, Xiang Huang, Shibo Xi, Jong-Min Lee, Cheng Wang, Yonghua Du, and Xin Wang. 2019. 'Linkage Effect in the Heterogenization of Cobalt Complexes by Doped Graphene for Electrocatalytic CO_2 Reduction'. *Angewandte Chemie International Edition* 58 (38): 13532–39. https://doi.org/10.1002/anie.201906475.
- Wang, Xin, Shuo Dou, Libo Sun, Shibo Xi, Xiaogang Li, Tan Su, and Hong Jin Fan. 2021. 'Enlarging the Π-conjugation of Cobalt Porphyrin for Highly Active and Selective CO_2 Electroreduction'. *ChemSusChem*, March, cssc.202100176. https://doi.org/10.1002/cssc.202100176.
- Wang, Xin, Libo Sun, Zhenfeng Huang, Vikas Reddu, Tan Su, and Adrian C. Fisher. 2020. 'A Planar, Conjugated N4-macrocyclic Cobalt Complex for Heterogeneous Electrocatalytic CO_2 Reduction with High Activity'. *Angewandte Chemie International Edition*, July, anie.202007445. https://doi.org/10.1002/anie.202007445.
- Wei, Chao, Reshma R. Rao, Jiayu Peng, Botao Huang, Ifan E. L. Stephens, Marcel Risch, Zhichuan J. Xu, and Yang Shao-Horn. 2019. 'Recommended Practices and Benchmark Activity for Hydrogen and Oxygen Electrocatalysis in Water Splitting and Fuel Cells'. *Advanced Materials* 31 (31): 1806296. https://doi.org/10.1002/adma.201806296.
- Wei, Chao, Shengnan Sun, Daniel Mandler, Xun Wang, Shi Zhang Qiao, and Zhichuan J. Xu. 2019. 'Approaches for Measuring the Surface Areas of Metal Oxide Electrocatalysts for Determining Their Intrinsic Electrocatalytic Activity'. *Chemical Society Reviews* 48 (9): 2518–34. https://doi.org/10.1039/C8CS00848E.
- Wei, Jumeng, Min Zhou, Anchun Long, Yanming Xue, Hanbin Liao, Chao Wei, and Zhichuan J. Xu. 2018. 'Heterostructured Electrocatalysts for Hydrogen Evolution Reaction Under Alkaline Conditions'. *Nano-Micro Letters* 10 (4). https://doi.org/10.1007/s40820-018-0229-x.
- Wu, Tianze, Shengnan Sun, Jiajia Song, Shibo Xi, Yonghua Du, Bo Chen, Wardhana Aji Sasangka, et al. 2019. 'Iron-Facilitated Dynamic Active-Site Generation on Spinel $CoAl_2O_4$ with Self-Termination of Surface Reconstruction for Water Oxidation'. *Nature Catalysis* 2 (9): 763–72. https://doi.org/10.1038/s41929-019-0325-4.
- Xu, Zhichuan J. 2019. 'Transition Metal Oxides for Water Oxidation: All about Oxyhydroxides?' *Science China Materials*, September. https://doi.org/10.1007/s40843-019-9588-5.
- Xu, Zhichuan J., and Xun Wang. 2020. 'Electrocatalysis: A Core Technique for a Sustainable Future'. *Chemistry – A European Journal*, March, chem.202000909. https://doi.org/10.1002/chem.202000909.
- Zhang, Shengliang, Sheng Cao, Tianran Zhang, and Jim Yang Lee. 2020. 'Plasmonic Oxygen-Deficient TiO_{2-x} Nanocrystals for Dual-Band Electrochromic Smart Windows with Efficient Energy Recycling'. *Advanced Materials* 32 (43): 2004686. https://doi.org/10.1002/adma.202004686.
- Zhang, Shengliang, Sheng Cao, Tianran Zhang, Qiaofeng Yao, Haibin Lin, Adrian Fisher, and Jim Yang Lee. 2019. 'Overcoming the Technical Challenges in Al Anode–Based Electrochromic Energy Storage Windows'. *Small Methods*, September, 1900545. https://doi.org/10.1002/smtd.201900545.
- Zhang, Shengliang, Yang Li, Tianran Zhang, Sheng Cao, Qiaofeng Yao, Haibin Lin, Hualin Ye, Adrian C.

Fisher, and Jim Yang Lee. 2019. 'Dual-Band Electrochromic Devices with a Transparent Conductive Capacitive Charge-Balancing Anode'. *ACS Applied Materials & Interfaces*, December, acsami.9b17678. https://doi.org/10.1021/acsami.9b17678.

- Zhang, Tianran, Shengliang Zhang, Sheng Cao, Qiaofeng Yao, and Jim Yang Lee. 2018. 'A Self-Templating Redox-Mediated Synthesis of Hollow Phosphated Manganese Oxide Nanospheres as Noble-Metal-like Oxygen Electrocatalysts'. *Chemistry of Materials* 30 (22): 8270–79. https://doi.org/10.1021/acs.chemmater.8b03681.
- Zhang, Tianran, Shengliang Zhang, Sheng Cao, Qiaofeng Yao, and Jim Yang Lee. 2020. 'Bridging the Energy Efficiency Gap between Quasi-Neutral and Alkaline Rechargeable Zinc-Air Batteries by an Efficient Hybrid Battery Design'. *Energy Storage Materials* 33 (December): 181–87. https://doi.org/10.1016/j.ensm.2020.08.019.
- Zhou, Ye, Shengnan Sun, Chao Wei, Yuanmiao Sun, Pinxian Xi, Zhenxing Feng, and Zhichuan J. Xu. 2019. 'Significance of Engineering the Octahedral Units to Promote the Oxygen Evolution Reaction of Spinel Oxides'. *Advanced Materials*, July, 1902509. https://doi.org/10.1002/adma.201902509.

C4T IRP 3: Combustion for cleaner fuels and better catalysts

- Boje, Astrid, Jethro Akroyd, and Markus Kraft. 2019. 'A Hybrid Particle-Number and Particle Model for Efficient Solution of Population Balance Equations'. *Journal of Computational Physics* 389 (July): 189–218. https://doi.org/10.1016/j.jcp.2019.03.033.
- Botero, Maria L., Jethro Akroyd, Dongping Chen, Markus Kraft, and John R. Agudelo. 2021. 'On the Thermophoretic Sampling and TEM-Based Characterisation of Soot Particles in Flames'. *Carbon* 171 (January): 711–22. https://doi.org/10.1016/j.carbon.2020.09.074.
- Bowal, Kimberly, Peter Grančič, Jacob W. Martin, and Markus Kraft. 2019. 'Sphere Encapsulated Monte Carlo: Obtaining Minimum Energy Configurations of Large Aromatic Systems'. *The Journal of Physical Chemistry A* 123 (33): 7303–13. https://doi.org/10.1021/acs.jpca.9b04821.
- Bowal, Kimberly, Jacob W. Martin, and Markus Kraft. 2019. 'Partitioning of Polycyclic Aromatic Hydrocarbons in Heterogeneous Clusters'. *Carbon* 143 (March): 247–56. https://doi.org/10.1016/j.carbon.2018.11.004.
- **Bowal, Kimberly, Jacob W. Martin, and Markus Kraft. 2021. 'Self-Assembly of Curved Aromatic Molecules in Nanoparticles'. *Carbon* 182 (September): 70–88. https://doi.org/10.1016/j.carbon.2021.05.013.**
- Bowal, Kimberly, Jacob W. Martin, Alston J. Misquitta, and Markus Kraft. 2019. 'Ion-Induced Soot Nucleation Using a New Potential for Curved Aromatics'. *Combustion Science and Technology* 191 (5–6): 747–65. https://doi.org/10.1080/00102202.2019.1565496.
- Bowal, Kimberly, Laura Pascazio, Hongyu Wang, Dongping Chen, and Markus Kraft. 2020. 'Surface Properties of Heterogeneous Polycyclic Aromatic Hydrocarbon Clusters'. *Proceedings of the Combustion Institute*, October, S1540748920301905. https://doi.org/10.1016/j.proci.2020.06.123.
- Dreyer, Jochen A. H., Radomir I. Slavchov, Eric J. Rees, Jethro Akroyd, Maurin Salamanca, Sebastian Mosbach, and Markus Kraft. 2019. 'Improved Methodology for Performing the Inverse Abel Transform of Flame Images for Color Ratio Pyrometry'. *Applied Optics* 58 (10): 2662. https://doi.org/10.1364/AO.58.002662.
- Dreyer, Jochen A.H., Eric J. Bringley, Manoel Y. Manuputty, Jethro Akroyd, and Markus Kraft. 2020. 'Temperature and CH* Measurements and Simulations of Laminar Premixed Ethylene Jet-Wall Stagnation Flames'. *Proceedings of the Combustion Institute*, September, S154074892030167X. https://doi.org/10.1016/j.proci.2020.06.106.
- Dreyer, Jochen A.H., Maximilian Poli, Nick A. Eaves, Maria L. Botero, Jethro Akroyd, Sebastian Mosbach, and Markus Kraft. 2019. 'Evolution of the Soot Particle Size Distribution along the Centreline of an N-Heptane/Toluene Co-Flow Diffusion Flame'. *Combustion and Flame* 209 (November): 256–66. https://doi.org/10.1016/j.combustflame.2019.08.002.
- Hou, Dingyu, Qingzhao Chu, Dongping Chen, Laura Pascazio, Markus Kraft, and Xiaoqing You. 2020. 'Atomic Insights into the Sintering Process of Polycyclic Aromatic Hydrocarbon Clusters'. *Proceedings of the Combustion Institute*, September, S1540748920304648. https://doi.org/10.1016/j.proci.2020.06.368.
- Hou, Dingyu, Casper S. Lindberg, Manoel Y. Manuputty, Xiaoqing You, and Markus Kraft. 2019. 'Modelling Soot Formation in a Benchmark Ethylene Stagnation Flame with a New Detailed Population Balance Model'. *Combustion and Flame* 203 (May): 56–71. https://doi.org/10.1016/j.combustflame.2019.01.035.
- Hou, Dingyu, Casper S. Lindberg, Mengda Wang, Manoel Y. Manuputty, Xiaoqing You, and Markus Kraft. 2020. 'Simulation of Primary Particle Size Distributions in a Premixed Ethylene Stagnation Flame'. *Combustion and Flame* 216 (June): 126–35. https://doi.org/10.1016/j.combustflame.2020.02.028.

- **Hou, Dingyu, Laura Pascazio, Jacob Martin, Yuxin Zhou, Markus Kraft, and Xiaoqing You. 2022. 'On the Reactive Coagulation of Incipient Soot Nanoparticles'. *Journal of Aerosol Science* 159 (January): 105866. https://doi.org/10.1016/j.jaerosci.2021.105866.**
- Hou, Dingyu, Diyuan Zong, Casper S. Lindberg, Markus Kraft, and Xiaoqing You. 2020. 'On the Coagulation Efficiency of Carbonaceous Nanoparticles'. *Journal of Aerosol Science* 140 (February): 105478. https://doi.org/10.1016/j.jaerosci.2019.105478.
- Kächele, Rebecca, Daniel Nurkowski, Jacob Martin, Jethro Akroyd, and Markus Kraft. 2019. 'An Assessment of the Viability of Alternatives to Biodiesel Transport Fuels'. *Applied Energy* 251 (October): 113363. https://doi.org/10.1016/j.apenergy.2019.113363.
- Lao, Chung Ting, Jethro Akroyd, Nickolas Eaves, Alastair Smith, Neal Morgan, Daniel Nurkowski, Amit Bhave, and Markus Kraft. 2020. 'Investigation of the Impact of the Configuration of Exhaust After-Treatment System for Diesel Engines'. *Applied Energy* 267 (June): 114844. https://doi.org/10.1016/j.apenergy.2020.114844.
- **Lao, Chung Ting, Jethro Akroyd, Alastair Smith, Neal Morgan, Kok Foong Lee, Daniel Nurkowski, and Markus Kraft. 2021. 'Modelling Investigation of the Thermal Treatment of Ash-Contaminated Particulate Filters'. *Emission Control Science and Technology*, September. https://doi.org/10.1007/s40825-021-00197-z.**
- Leon, Gustavo, Nick Eaves, Jethro Akroyd, Sebastian Mosbach, and Markus Kraft. 2019. 'A New Methodology to Calculate Process Rates in a Kinetic Monte Carlo Model of PAH Growth'. *Combustion and Flame* 209 (November): 133–43. https://doi.org/10.1016/j.combustflame.2019.07.032.
- **Leon, Gustavo, Jacob W. Martin, Eric J. Bringley, Jethro Akroyd, and Markus Kraft. 2021. 'The Role of Oxygenated Species in the Growth of Graphene, Fullerenes and Carbonaceous Particles'. *Carbon*, June, S0008622321005558. https://doi.org/10.1016/j.carbon.2021.05.052.**
- Leon, Gustavo, Angiras Menon, Laura Pascazio, Eric J. Bringley, Jethro Akroyd, and Markus Kraft. 2020. 'Kinetic Monte Carlo Statistics of Curvature Integration by HACA Growth and Bay Closure Reactions for PAH Growth in a Counterflow Diffusion Flame'. *Proceedings of the Combustion Institute*, October, S1540748920304454. https://doi.org/10.1016/j.proci.2020.06.352.
- **Li, Jie, Lanjia Pan, Manu Suvarna, and Xiaonan Wang. 2021. 'Machine Learning Aided Supercritical Water Gasification for H_2-Rich Syngas Production with Process Optimization and Catalyst Screening'. *Chemical Engineering Journal* 426 (December): 131285. https://doi.org/10.1016/j.cej.2021.131285.**
- Lindberg, Casper S., Manoel Y. Manuputty, Jethro Akroyd, and Markus Kraft. 2019. 'A Two-Step Simulation Methodology for Modelling Stagnation Flame Synthesised Aggregate Nanoparticles'. *Combustion and Flame* 202 (April): 143–53. https://doi.org/10.1016/j.combustflame.2019.01.010.
- Lindberg, Casper S., Manoel Y. Manuputty, Philipp Buerger, Jethro Akroyd, and Markus Kraft. 2019. 'Numerical Simulation and Parametric Sensitivity Study of Titanium Dioxide Particles Synthesised in a Stagnation Flame'. *Journal of Aerosol Science* 138 (December): 105451. https://doi.org/10.1016/j.jaerosci.2019.105451.
- Lindberg, Casper S., Manoel Y. Manuputty, Edward K.Y. Yapp, Jethro Akroyd, Rong Xu, and Markus Kraft. 2019. 'A Detailed Particle Model for Polydisperse Aggregate Particles'. *Journal of Computational Physics* 397 (November): 108799. https://doi.org/10.1016/j.jcp.2019.06.074.
- Lu, Haichang, Yuzheng Guo, Jacob W. Martin, Markus Kraft, and John Robertson. 2019. 'Atomic Structure and Electronic Structure of Disordered Graphitic Carbon Nitride'. *Carbon* 147 (June): 483–89. https://doi.org/10.1016/j.carbon.2019.03.031.
- Lu, Yan, Haojing Wang, Pengfei Yu, Yifei Yuan, Reza Shahbazian-Yassar, Yuan Sheng, Shuyang Wu, et al. 2020. 'Isolated Ni Single Atoms in Nitrogen Doped Ultrathin Porous Carbon Templated from Porous G-C_3N_4 for High-Performance CO_2 Reduction'. *Nano Energy* 77 (November): 105158. https://doi.org/10.1016/j.nanoen.2020.105158.
- Manuputty, Manoel Y., Jochen A. H. Dreyer, Yuan Sheng, Eric J. Bringley, Maria L. Botero, Jethro Akroyd, and Markus Kraft. 2019. 'Polymorphism of Nanocrystalline TiO_2 Prepared in a Stagnation Flame: Formation of the TiO_2-II Phase'. *Chemical Science* 10 (5): 1342–50. https://doi.org/10.1039/C8SC02969E.
- Manuputty, Manoel Y., Casper S. Lindberg, Maria L. Botero, Jethro Akroyd, and Markus Kraft. 2019. 'Detailed Characterisation of TiO_2 Nano-Aggregate Morphology Using TEM Image Analysis'. *Journal of Aerosol Science* 133 (July): 96–112. https://doi.org/10.1016/j.jaerosci.2019.04.012.
- **Manuputty, Manoel Y., Casper S. Lindberg, Jochen A.H. Dreyer, Jethro Akroyd, John Edwards, and Markus Kraft. 2021. 'Understanding the Anatase-Rutile Stability in Flame-Made TiO_2'. *Combustion and Flame* 226 (April): 347–61. https://doi.org/10.1016/j.combustflame.2020.12.017.**
- Martin, Jacob W., Dingyu Hou, Angiras Menon, Laura Pascazio, Jethro Akroyd, Xiaoqing You, and Markus Kraft. 2019. 'Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Implications of Localized π-Radicals on Rim-Based Pentagonal Rings'. *The Journal of Physical Chemistry C* 123 (43): 26673–82. https://

doi.org/10.1021/acs.jpcc.9b07558.

- Martin, Jacob W., Angiras Menon, Chung Ting Lao, Jethro Akroyd, and Markus Kraft. 2019. 'Dynamic Polarity of Curved Aromatic Soot Precursors'. *Combustion and Flame* 206 (August): 150–57. https://doi.org/10.1016/j.combustflame.2019.04.046.
- Martin, Jacob W., Leonard Nyadong, Caterina Ducati, Merilyn Manley-Harris, Alan G. Marshall, and Markus Kraft. 2019. 'Nanostructure of Gasification Charcoal (Biochar)'. *Environmental Science & Technology* 53 (7): 3538–46. https://doi.org/10.1021/acs.est.8b06861.
- **Martin, Jacob W., Laura Pascazio, Angiras Menon, Jethro Akroyd, Katharina Kaiser, Fabian Schulz, Mario Commodo, Andrea D'Anna, Leo Gross, and Markus Kraft. 2021. 'π-Diradical Aromatic Soot Precursors in Flames'. *Journal of the American Chemical Society* 143 (31): 12212–19. https://doi.org/10.1021/jacs.1c05030.**
- **Martin, Jacob W., Maurin Salamanca, and Markus Kraft. 2022. 'Soot Inception: Carbonaceous Nanoparticle Formation in Flames'. *Progress in Energy and Combustion Science* 88 (January): 100956. https://doi.org/10.1016/j.pecs.2021.100956.**
- Martin, Jacob W., Carla de Tomas, Irene Suarez-Martinez, Markus Kraft, and Nigel A. Marks. 2019. 'Topology of Disordered 3D Graphene Networks'. *Physical Review Letters* 123 (11): 116105. https://doi.org/10.1103/PhysRevLett.123.116105.
- Menon, Angiras, Jochen A. H. Dreyer, Jacob W. Martin, Jethro Akroyd, John Robertson, and Markus Kraft. 2019. 'Optical Band Gap of Cross-Linked, Curved, and Radical Polyaromatic Hydrocarbons'. *Physical Chemistry Chemical Physics* 21 (29): 16240–51. https://doi.org/10.1039/C9CP02363A.
- Menon, Angiras, Gustavo Leon, Jethro Akroyd, and Markus Kraft. 2020. 'A Density Functional Theory Study on the Kinetics of Seven-Member Ring Formation in Polyaromatic Hydrocarbons'. *Combustion and Flame* 217 (July): 152–74. https://doi.org/10.1016/j.combustflame.2020.03.032.
- Menon, Angiras, Jacob Martin, Gustavo Leon, Dingyu Hou, Laura Pascazio, Xiaoqing You, and Markus Kraft. 2020. 'Reactive Localized π-Radicals on Rim-Based Pentagonal Rings: Properties and Concentration in Flames'. *Proceedings of the Combustion Institute*, September, S1540748920304740. https://doi.org/10.1016/j.proci.2020.07.042.
- Menon, Angiras, Jacob W. Martin, Jethro Akroyd, and Markus Kraft. 2020. 'Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Kinetics and Equilibria'. *The Journal of Physical Chemistry A* 124 (48): 10040–52. https://doi.org/10.1021/acs.jpca.0c07811.
- Pascazio, Laura, Jacob W. Martin, Maria L. Botero, Mariano Sirignano, Andrea D'Anna, and Markus Kraft. 2019. 'Mechanical Properties of Soot Particles: The Impact of Crosslinked Polycyclic Aromatic Hydrocarbons'. *Combustion Science and Technology*, September, 1–21. https://doi.org/10.1080/00102202.2019.1668380.
- Pascazio, Laura, Jacob W. Martin, Kimberly Bowal, Jethro Akroyd, and Markus Kraft. 2020. 'Exploring the Internal Structure of Soot Particles Using Nanoindentation: A Reactive Molecular Dynamics Study'. *Combustion and Flame* 219 (September): 45–56. https://doi.org/10.1016/j.combustflame.2020.04.029.
- Pascazio, Laura, Jacob W. Martin, Angiras Menon, Dingyu Hou, Xiaoqing You, and Markus Kraft. 2020. 'Aromatic Penta-Linked Hydrocarbons in Soot Nanoparticle Formation'. *Proceedings of the Combustion Institute*, October, S1540748920306908. https://doi.org/10.1016/j.proci.2020.09.029.
- Salamanca, Maurin, Maria L. Botero, Jacob W. Martin, Jochen A.H. Dreyer, Jethro Akroyd, and Markus Kraft. 2020. 'The Impact of Cyclic Fuels on the Formation and Structure of Soot'. *Combustion and Flame* 219 (September): 1–12. https://doi.org/10.1016/j.combustflame.2020.04.026.
- Slavchov, Radomir I., Maurin Salamanca, Danilo Russo, Ibrahim Salama, Sebastian Mosbach, Stuart M. Clarke, Markus Kraft, Alexei A. Lapkin, and Sorin V. Filip. 2020. 'The Role of NO2 and NO in the Mechanism of Hydrocarbon Degradation Leading to Carbonaceous Deposits in Engines'. *Fuel* 267 (May): 117218. https://doi.org/10.1016/j.fuel.2020.117218.
- **Tan, Yong Ren, Maurin Salamanca, Jiaru Bai, Jethro Akroyd, and Markus Kraft. 2021. 'Structural Effects of C3 Oxygenated Fuels on Soot Formation in Ethylene Coflow Diffusion Flames'. *Combustion and Flame* 232 (October): 111512. https://doi.org/10.1016/j.combustflame.2021.111512.**
- Tan, Yong Ren, Maurin Salamanca, Laura Pascazio, Jethro Akroyd, and Markus Kraft. 2021. 'The Effect of Poly(Oxymethylene) Dimethyl Ethers (PODE3) on Soot Formation in Ethylene/PODE3 Laminar Coflow Diffusion Flames'. *Fuel* 283 (January): 118769. https://doi.org/10.1016/j.fuel.2020.118769.
- Vo, Chi Hung, Nishu Goyal, Iftekhar A Karimi, and Markus Kraft. 2020. 'First Observation of an Acetate Switch in a Methanogenic Autotroph (*Methanococcus Maripaludis* S2)'. *Microbiology Insights* 13 (January): 117863612094530. https://doi.org/10.1177/1178636120945300.
- Wu, Shaohua, Jethro Akroyd, Sebastian Mosbach, George Brownbridge, Owen Parry, Vivian Page, Wenming Yang, and Markus Kraft. 2020. 'Efficient Simulation and Auto-Calibration of Soot Particle Processes in Diesel Engines'. *Applied Energy* 262 (March): 114484. https://doi.org/10.1016/j.apenergy.2019.114484.
- Wu, Shaohua, Chung Ting Lao, Jethro Akroyd, Sebastian Mosbach, Wenming Yang, and Markus Kraft. 2020.

'A Joint Moment Projection Method and Maximum Entropy Approach for Simulation of Soot Formation and Oxidation in Diesel Engines'. *Applied Energy* 258 (January): 114083. https://doi.org/10.1016/j.apenergy.2019.114083.

- Wu, Shaohua, Casper Lindberg, Jethro Akroyd, Wenming Yang, and Markus Kraft. 2019. 'Bivariate Extension of the Moment Projection Method for the Particle Population Balance Dynamics'. *Computers & Chemical Engineering* 124 (May): 206–27. https://doi.org/10.1016/j.compchemeng.2018.12.011.
- Wu, Shuyang, Manoel Y. Manuputty, Yuan Sheng, Haojing Wang, Yong Yan, Markus Kraft, and Rong Xu. 2020. 'Flame Synthesized Blue TiO_{2-x} with Tunable Oxygen Vacancies from Surface to Grain Boundary to Bulk'. *Small Methods*, December, 2000928. https://doi.org/10.1002/smtd.202000928.
- Wu, Shuyang, Weijing Wang, Wenguang Tu, Shengming Yin, Yuan Sheng, Manoel Y. Manuputty, Markus Kraft, and Rong Xu. 2018. 'Premixed Stagnation Flame Synthesized TiO_2 Nanoparticles with Mixed Phases for Efficient Photocatalytic Hydrogen Generation'. *ACS Sustainable Chemistry & Engineering* 6 (11): 14470–79. https://doi.org/10.1021/acssuschemeng.8b03142.
- Yu, Wenbin, Yichen Zong, Qinjie Lin, Kunlin Tay, Feiyang Zhao, Wenming Yang, and Markus Kraft. 2020. 'Experimental Study on Engine Combustion and Particle Size Distributions Fueled with Jet A-1'. *Fuel* 263 (March): 116747. https://doi.org/10.1016/j.fuel.2019.116747.
- **Zhu, Qiren, Yichen Zong, Wenbin Yu, Wenming Yang, and Markus Kraft. 2021. 'Understanding the Blending Effect of Polyoxymethylene Dimethyl Ethers as Additive in a Common-Rail Diesel Engine'. *Applied Energy* 300 (October): 117380. https://doi.org/10.1016/j.apenergy.2021.117380.**

C4T IRP BB: Pathways to industrial decarbonisation

- **Huang, Kenneth Guang-Lih, Can Huang, Huijun Shen, and Hao Mao. 2021. 'Assessing the Value of China's Patented Inventions'. *Technological Forecasting and Social Change* 170 (September): 120868. https://doi.org/10.1016/j.techfore.2021.120868.**
- **Lezak, Emil, Enrico Ferrera, and Steve Evans. 2019. 'Towards Industry 4.0: Efficient and Sustainable Manufacturing Leveraging MTEF – MTEF-MAESTRI Total Efficiency Framework'. In *Technological Developments in Industry 4.0 for Business Applications*. Advances in Logistics, Operations, and Management Science. IGI Global. https://doi.org/10.4018/978-1-5225-4936-9.**

C4T IRP JPS: The J-Park Simulator

- **Akroyd, Jethro, Sebastian Mosbach, Amit Bhave, and Markus Kraft. 2021. 'Universal Digital Twin - A Dynamic Knowledge Graph'. *Data-Centric Engineering* 2: e14. https://doi.org/10.1017/dce.2021.10.**
- **Atherton, John, Wanni Xie, Leonardus Kevin Aditya, Xiaochi Zhou, Gourab Karmakar, Jethro Akroyd, Sebastian Mosbach, Mei Qi Lim, and Markus Kraft. 2021. 'How Does a Carbon Tax Affect Britain's Power Generation Composition?' *Applied Energy* 298 (September): 117117. https://doi.org/10.1016/j.apenergy.2021.117117.**
- **Devanand, Aravind, Gourab Karmakar, Nenad Krdzavac, Feroz Farazi, Mei Qi Lim, Y.S. Foo Eddy, Iftekhar A. Karimi, and Markus Kraft. 2021. 'ElChemo: A Cross-Domain Interoperability between Chemical and Electrical Systems in a Plant'. *Computers & Chemical Engineering*, October, 107556. https://doi.org/10.1016/j.compchemeng.2021.107556.**
- Devanand, Aravind, Gourab Karmakar, Nenad Krdzavac, Rémy Rigo-Mariani, Y.S. Foo Eddy, Iftekhar A. Karimi, and Markus Kraft. 2020. 'OntoPowSys: A Power System Ontology for Cross Domain Interactions in an Eco Industrial Park'. *Energy and AI* 1 (August): 100008. https://doi.org/10.1016/j.egyai.2020.100008.
- Devanand, Aravind, Markus Kraft, and Iftekhar A Karimi. 2019. 'Optimal Site Selection for Modular Nuclear Power Plants'. *Computers & Chemical Engineering* 125 (June): 339–50. https://doi.org/10.1016/j.compchemeng.2019.03.024.
- Eibeck, Andreas, Arkadiusz Chadzynski, Mei Qi Lim, Kevin Aditya, Laura Ong, Aravind Devanand, Gourab Karmakar, et al. 2020. 'A Parallel World Framework for Scenario Analysis in Knowledge Graphs'. *Data-Centric Engineering* 1: e6. https://doi.org/10.1017/dce.2020.6.
- Eibeck, Andreas, Mei Qi Lim, and Markus Kraft. 2019. 'J-Park Simulator: An Ontology-Based Platform for Cross-Domain Scenarios in Process Industry'. *Computers & Chemical Engineering* 131 (December): 106586. https://doi.org/10.1016/j.compchemeng.2019.106586.
- **Eibeck, Andreas, Daniel Nurkowski, Angiras Menon, Jiaru Bai, Jinkui Wu, Li Zhou, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2021. 'Predicting Power Conversion Efficiency of Organic**

Photovoltaics: Models and Data Analysis'. *ACS Omega* 6 (37): 23764–75. https://doi.org/10.1021/acsomega.1c02156.

- **Hofmeister, Markus, Sebastian Mosbach, Jörg Hammacher, Martin Blum, Gerd Röhrig, Christoph Dörr, Volker Flegel, Amit Bhave, and Markus Kraft. 2022. 'Resource-Optimised Generation Dispatch Strategy for District Heating Systems Using Dynamic Hierarchical Optimisation'. *Applied Energy* 305 (January): 117877. https://doi.org/10.1016/j.apenergy.2021.117877.**
- Inderwildi, Oliver, Chuan Zhang, Xiaonan Wang, and Markus Kraft. 2020. 'The Impact of Intelligent Cyber-Physical Systems on the Decarbonization of Energy'. *Energy Environ. Sci.* 13 (3): 744–71. https://doi.org/10.1039/C9EE01919G.
- Liu, Zuming, Mei Qi Lim, Markus Kraft, and Xiaonan Wang. 2020. 'Simultaneous Design and Operation Optimization of Renewable Combined Cooling Heating and Power Systems'. *AIChE Journal* 66 (12). https://doi.org/10.1002/aic.17039.
- Liu, Zuming, Shukun Wang, Mei Qi Lim, Markus Kraft, and Xiaonan Wang. 2021. 'Game Theory-Based Renewable Multi-Energy System Design and Subsidy Strategy Optimization'. *Advances in Applied Energy*, March, 100024. https://doi.org/10.1016/j.adapen.2021.100024.
- Mosbach, Sebastian, Angiras Menon, Feroz Farazi, Nenad Krdzavac, Xiaochi Zhou, Jethro Akroyd, and Markus Kraft. 2020. 'Multiscale Cross-Domain Thermochemical Knowledge-Graph'. Journal *of Chemical Information and Modeling* 60 (12): 6155–66. https://doi.org/10.1021/acs.jcim.0c01145.
- Rigo-Mariani, Remy, Chuan Zhang, Alessandro Romagnoli, Markus Kraft, K. V. Ling, and Jan M. Maciejowski. 2019. 'A Combined Cycle Gas Turbine Model for Heat and Power Dispatch Subject to Grid Constraints'. *IEEE Transactions on Sustainable Energy*, January, 1–1. https://doi.org/10.1109/TSTE.2019.2894793.
- Sikorski, Janusz J., Oliver Inderwildi, Mei Qi Lim, Sushant S. Garud, Johannes Neukäufer, and Markus Kraft. 2019. 'Enhanced Procurement and Production Strategies for Chemical Plants: Utilizing Real-Time Financial Data and Advanced Algorithms'. *Industrial & Engineering Chemistry Research* 58 (8): 3072–81. https://doi.org/10.1021/acs.iecr.8b02925.
- Yu, Changmin, Marko Seslija, George Brownbridge, Sebastian Mosbach, Markus Kraft, Mohammad Parsi, Mark Davis, Vivian Page, and Amit Bhave. 2020. 'Deep Kernel Learning Approach to Engine Emissions Modeling'. *Data-Centric Engineering* 1: e4. https://doi.org/10.1017/dce.2020.4.
- Zhou, Xiaochi, Andreas Eibeck, Mei Qi Lim, Nenad B. Krdzavac, and Markus Kraft. 2019. 'An Agent Composition Framework for the J-Park Simulator - A Knowledge Graph for the Process Industry'. Computers *& Chemical Engineering* 130 (November): 106577. https://doi.org/10.1016/j.compchemeng.2019.106577.
- Zhou, Xiaochi, Mei Qi Lim, and Markus Kraft. 2020. 'A Smart Contract-Based Agent Marketplace for the J-Park Simulator - a Knowledge Graph for the Process Industry'. *Computers & Chemical Engineering* 139 (August): 106896. https://doi.org/10.1016/j.compchemeng.2020.106896.
- **Zhou, Xiaochi, Daniel Nurkowski, Sebastian Mosbach, Jethro Akroyd, and Markus Kraft. 2021. 'Question Answering System for Chemistry'. *Journal of Chemical Information and Modeling* 61 (8): 3868–80. https://doi.org/10.1021/acs.jcim.1c00275.**

CLIC: Centre for Lifelong Learning and Individualised Cognition

- **Friedman, Naomi P., and Trevor W. Robbins. 2021. 'The Role of Prefrontal Cortex in Cognitive Control and Executive Function'. *Neuropsychopharmacology*, August. https://doi.org/10.1038/s41386-021-01132-0.**

eCO$_2$EP: Carbon capture and utilisation

- Ager, Joel W., and Alexei A. Lapkin. 2018. 'Chemical Storage of Renewable Energy'. *Science* 360 (6390): 707–8. https://doi.org/10.1126/science.aat7918.
- Amaniampong, P. N., N. Y. Asiedu, E. Fletcher, D. Dodoo-Arhin, O. J. Olatunji, and Q. T. Trinh. 2020. 'Conversion of Lignocellulosic Biomass to Fuels and Value-Added Chemicals Using Emerging Technologies and State-of-the-Art Density Functional Theory Simulations Approach'. In *Valorization of Biomass to Value-Added Commodities*, edited by Michael O. Daramola and Augustine O. Ayeni, 193–220. Green Energy and Technology Book Series (GREEN). Cham: Springer International Publishing. https://doi.org/10.1007/978-3-030-38032-8_10.
- Amaniampong, Prince N., Quang Thang Trinh, Karine De Oliveira Vigier, Duy Quang Dao, Ngoc Han Tran, Yingqiao Wang, Matthew P. Sherburne, and François Jérôme. 2019. 'Synergistic Effect of High-Frequency

Ultrasound with Cupric Oxide Catalyst Resulting in a Selectivity Switch in Glucose Oxidation under Argon'. *Journal of the American Chemical Society* 141 (37): 14772–79. https://doi.org/10.1021/jacs.9b06824.

- An, Li, Chao Wei, Min Lu, Hanwen Liu, Yubo Chen, Günther G. Scherer, Adrian C. Fisher, Pinxian Xi, Zhichuan J. Xu, and Chun-Hua Yan. 2021. 'Recent Development of Oxygen Evolution Electrocatalysts in Acidic Environment'. *Advanced Materials*, March, 2006328. https://doi.org/10.1002/adma.202006328.
- Barecka, Magda H., Joel W. Ager, and Alexei A. Lapkin. 2021a. 'Economically Viable CO_2 Electroreduction Embedded within Ethylene Oxide Manufacturing'. *Energy & Environmental Science* 14 (3): 1530–43. https://doi.org/10.1039/D0EE03310C.
- **Barecka, Magda H., Joel W. Ager, and Alexei A. Lapkin. 2021b. 'Carbon Neutral Manufacturing via On-Site CO_2 Recycling'. *iScience* 24 (6): 102514. https://doi.org/10.1016/j.isci.2021.102514.**
- **Barecka, Magda H., Joel W. Ager, and Alexei A. Lapkin. 2021c. 'Techno-Economic Assessment of Emerging CO_2 Electrolysis Technologies'. *STAR Protocols* 2 (4): 100889. https://doi.org/10.1016/j.xpro.2021.100889.**
- **Chen, Gao, Yuanmiao Sun, Riccardo Ruixi Chen, Chiara Biz, Adrian C. Fisher, Matthew Sherburne, Joel W Ager III, Jose Gracia, and Zhichuan J Xu. 2021. 'A Discussion on the Possible Involvement of Singlet Oxygen in Oxygen Electrocatalysis'. *Journal of Physics: Energy* 3 (3): 031004. https://doi.org/10.1088/2515-7655/abe039.**
- Chen, Yubo, Haiyan Li, Jingxian Wang, Yonghua Du, Shibo Xi, Yuanmiao Sun, Matthew Sherburne, Joel W. Ager, Adrian C. Fisher, and Zhichuan J. Xu. 2019. 'Exceptionally Active Iridium Evolved from a Pseudo-Cubic Perovskite for Oxygen Evolution in Acid'. *Nature Communications* 10 (1). https://doi.org/10.1038/s41467-019-08532-3.
- Do, Ha Huu, Dang Le Tri Nguyen, Xuan Cuong Nguyen, Thu-Ha Le, Thang Phan Nguyen, Quang Thang Trinh, Sang Hyun Ahn, Dai-Viet N. Vo, Soo Young Kim, and Quyet Van Le. 2020. 'Recent Progress in TiO_2-Based Photocatalysts for Hydrogen Evolution Reaction: A Review'. *Arabian Journal of Chemistry* 13 (2): 3653–71. https://doi.org/10.1016/j.arabjc.2019.12.012.
- Huynh, Kim Anh, Dang Le Tri Nguyen, Van-Huy Nguyen, Dai-Viet N. Vo, Quang Thang Trinh, Thang Phan Nguyen, Soo Young Kim, and Quyet Van Le. 2020. 'Halide Perovskite Photocatalysis: Progress and Perspectives'. *Journal of Chemical Technology & Biotechnology*, February, jctb.6342. https://doi.org/10.1002/jctb.6342.
- Li, Haiyan, Yubo Chen, Jingjie Ge, Xianhu Liu, Adrian C. Fisher, Matthew Sherburne, Joel W. Ager, and Zhichuan J. Xu. 2021. 'Active Phase on $SrCo_{1-x}Fe_xO_{3-\delta}$ ($0 \le x \le 0.5$) Perovskite for Water Oxidation: Reconstructed Surface versus Remaining Bulk'. *JACS Au* 1 (1): 108–15. https://doi.org/10.1021/jacsau.0c00022.
- Li, Haiyan, Shengnan Sun, Shibo Xi, YuBo Chen, Ting Wang, Yonghua Du, Matthew Sherburne, Joel W. Ager, Adrian C. Fisher, and Zhichuan J. Xu. 2018. 'Metal-Oxygen Hybridization Determined Activity in Spinel-Based Oxygen Evolution Catalysts: A Case Study of $ZnFe_{2-x}Cr_xO_4$'. *Chemistry of Materials* 30 (19): 6839–48. https://doi.org/10.1021/acs.chemmater.8b02871.
- Liu, Guanyu, Yuan Sheng, Joel W. Ager, Markus Kraft, and Rong Xu. 2019. 'Research Advances towards Large-Scale Solar Hydrogen Production from Water'. *EnergyChem* 1 (2): 100014. https://doi.org/10.1016/j.enchem.2019.100014.
- **Liu, Guanyu, William S. Y. Wong, Markus Kraft, Joel W. Ager, Doris Vollmer, and Rong Xu. 2021. 'Wetting-Regulated Gas-Involving (Photo)Electrocatalysis: Biomimetics in Energy Conversion'. *Chemical Society Reviews*, 10.1039.D1CS00258A. https://doi.org/10.1039/D1CS00258A.**
- Malkhandi, Souradip, and Boon Siang Yeo. 2019. 'Electrochemical Conversion of Carbon Dioxide to High Value Chemicals Using Gas-Diffusion Electrodes'. *Current Opinion in Chemical Engineering* 26 (December): 112–21. https://doi.org/10.1016/j.coche.2019.09.008.
- Mohan, Ojus, Quang Thang Trinh, Arghya Banerjee, and Samir H. Mushrif. 2019. 'Predicting CO_2 Adsorption and Reactivity on Transition Metal Surfaces Using Popular Density Functional Theory Methods'. *Molecular Simulation* 45 (14–15): 1163–72. https://doi.org/10.1080/08927022.2019.1632448.
- Ngo, Thi Chinh, Quang Thang Trinh, Nguyen Thi Thai An, Nguyen Ngoc Tri, Nguyen Tien Trung, Dinh Hieu Truong, Bui The Huy, Minh Tho Nguyen, and Duy Quang Dao. 2020. 'SERS Spectra of the Pesticide Chlorpyrifos Adsorbed on Silver Nanosurface: The Ag 20 Cluster Model'. The *Journal of Physical Chemistry C*, September, acs.jpcc.0c06078. https://doi.org/10.1021/acs.jpcc.0c06078.
- Nguyen, Van-Huy, Ba-Son Nguyen, Chao-Wei Huang, Thi-Thu Le, Chinh Chien Nguyen, Thi Thanh Nhi Le, Doyeon Heo, et al. 2020. 'Photocatalytic NOx Abatement: Recent Advances and Emerging Trends in the Development of Photocatalysts'. *Journal of Cleaner Production* 270 (October): 121912. https://doi.org/10.1016/j.jclepro.2020.121912.
- Raman, K. Ashoke, Erik Birgersson, Yi Sui, and Adrian Fisher. 2020. 'Electrically Induced Droplet Ejection Dynamics under Shear Flow'. *Physics of Fluids* 32 (3): 032103. https://doi.org/10.1063/1.5143757.
- Sarkar, Chitra, Saikiran Pendem, Abhijit Shrotri, Duy Quang Dao, Phuong Pham Thi Mai, Tue Nguyen

Ngoc, Dhanunjaya Rao Chandaka, et al. 2019. 'Interface Engineering of Graphene-Supported Cu Nanoparticles Encapsulated by Mesoporous Silica for Size-Dependent Catalytic Oxidative Coupling of Aromatic Amines'. *ACS Applied Materials & Interfaces* 11 (12): 11722–35. https://doi.org/10.1021/acsami.8b18675.

- Tekalgne, Mahider Asmare, Khiem Van Nguyen, Dang Le Tri Nguyen, Van-Huy Nguyen, Thang Phan Nguyen, Dai-Viet N. Vo, Quang Thang Trinh, et al. 2020. 'Hierarchical Molybdenum Disulfide on Carbon Nanotube–Reduced Graphene Oxide Composite Paper as Efficient Catalysts for Hydrogen Evolution Reaction'. *Journal of Alloys and Compounds* 823 (May): 153897. https://doi.org/10.1016/j.jallcom.2020.153897.
- Trinh, Quang Thang, Arghya Banerjee, Khursheed B. Ansari, Duy Quang Dao, Asmaa Drif, Nguyen Thanh Binh, Dang Thanh Tung, et al. 2020. 'Upgrading of Bio-Oil from Biomass Pyrolysis: Current Status and Future Development'. In *Biorefinery of Alternative Resources: Targeting Green Fuels and Platform Chemicals*, edited by Sonil Nanda, Dai-Viet N. Vo, and Prakash Kumar Sarangi, 317–53. Singapore: Springer Singapore. https://doi.org/10.1007/978-981-15-1804-1_14.
- Trinh, Quang Thang, Kartavya Bhola, Prince Nana Amaniampong, François Jérôme, and Samir H. Mushrif. 2018. 'Synergistic Application of XPS and DFT to Investigate Metal Oxide Surface Catalysis'. The *Journal of Physical Chemistry C* 122 (39): 22397–406. https://doi.org/10.1021/acs.jpcc.8b05499.
- Van Hien, Pham, Nguyen Si Hoai Vu, Lai Xuan Bach, Ngoc Quyen Tran, Vinh Ai Dao, Quang Thang Trinh, and Nguyen Dang Nam. 2019. 'Capability of Aganonerion Polymorphum Leaf-Water Extract in Protecting Hydrochloric Acid Induced Steel Corrosion'. *New Journal of Chemistry*. https://doi.org/10.1039/C9NJ04079J.
- Wei, Chao, Yuanmiao Sun, Günther G. Scherer, Adrian C. Fisher, Matthew Sherburne, Joel W. Ager, and Zhichuan J. Xu. 2020. 'Surface Composition Dependent Ligand Effect in Tuning the Activity of Nickel–Copper Bimetallic Electrocatalysts toward Hydrogen Evolution in Alkaline'. *Journal of the American Chemical Society* 142 (17): 7765–75. https://doi.org/10.1021/jacs.9b12005.
- **Wu, Tianze, Xiao Ren, Yuanmiao Sun, Shengnan Sun, Guoyu Xian, Günther G. Scherer, Adrian C. Fisher, et al. 2021. 'Spin Pinning Effect to Reconstructed Oxyhydroxide Layer on Ferromagnetic Oxides for Enhanced Water Oxidation'. *Nature Communications* 12 (1): 3634. https://doi.org/10.1038/s41467-021-23896-1.**
- Xing, Weinan, Shengming Yin, Wenguang Tu, Guanyu Liu, Shuyang Wu, Haojing Wang, Markus Kraft, Guangyu Wu, and Rong Xu. 2019. 'Rational Synthesis of Amorphous Iron-Nickel Phosphonates for Highly Efficient Photocatalytic Water Oxidation with Nearly 100% Yield'. *Angewandte Chemie International Edition*, November. https://doi.org/10.1002/anie.201912552.

CKG: Cities Knowledge Graph

- **Chadzynski, Arkadiusz, Nenad Krdzavac, Feroz Farazi, Mei Qi Lim, Shiying Li, Ayda Grisiute, Pieter Herthogs, Aurel von Richthofen, Stephen Cairns, and Markus Kraft. 2021. 'Semantic 3D City Database — An Enabler for a Dynamic Geospatial Knowledge Graph'. *Energy and AI* 6 (December): 100106. https://doi.org/10.1016/j.egyai.2021.100106.**

Other publications

- **Jeraal, Mohammed I., Simon Sung, and Alexei A. Lapkin. 2021. 'A Machine Learning-Enabled Autonomous Flow Chemistry Platform for Process Optimization of Multiple Reaction Metrics'. *Chemistry–Methods* 1 (1): 71–77. https://doi.org/10.1002/cmtd.202000044. [PIPS]**
- Jose, Nicholas, Mikhail Kovalev, Eric Bradford, Artur Schweidtmann, Hua Chun Zeng, and Alexei Lapkin. 2020. 'Pushing Nanomaterials Past the Kilogram Scale—a Targeted Approach Integrating Scalable Microreactors, Machine Learning and High-Throughput Analysis'. Preprint. https://doi.org/10.26434/chemrxiv.12732914.v1. [SMART—former project]
- Schmidt, Hugo. 2019. 'Explosive Precursor Safety: An Application of the Deming Cycle for Continuous Improvement'. *Journal of Chemical Health and Safety* 26 (1): 31–36. https://doi.org/10.1016/j.jchas.2018.09.005. [Lab safety]
- Schmidt, Hugo G. 2019. 'Use of Lean Six Sigma Methods to Eliminate Fume Hood Disorder'. *Journal of Chemical Health and Safety*, April, S1871553219300222. https://doi.org/10.1016/j.jchas.2019.03.006. [Lab safety]

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