UNIVERSITY OF SURREY

TOWARDS NET-ZERO CIRCULAR ECONOMY WITH SUSTAINABLE ENERGY AND CHEMICAL CONVERSION

WORKSHOP PROGRAMME

24 June 2024

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INTRODUCTION

In the transition towards Net-Zero, there is significant interest in phasing out fossil fuels as both the energy source and precursors in the chemical sector. With a circular economy mindset, one attractive solution is getting the fossil fuel alternatives from the accumulated waste stream, such as biomass from food and agriculture waste, plastic waste and industrial pollutant water waste. Electrochemical conversion has emerged as a promising approach over the years for such application, due to its highly efficient process and low carbon emission when coupled with renewable electricity. The limitation currently is the design of efficient and stable catalyst materials, and the scaling up feasibility. Therefore, this original, multi-disciplinary research workshop aims to bring together researchers to share their cutting-edge discoveries on replacing petroleum feedstocks with waste materials in energy and chemical production.

Workshop Chair:
Dr Hui Luo, University of Surrey

Administrative support:
Louise Jones, Institute of Advanced Studies and Ellie Wang, University of Surrey

PROGRAMME

MONDAY 24 JUNE

Treetops, Wates House

(BST)

09.00 – 09.30	Registration
09.30 – 09.40	Welcome - Professor Jin Xuan and Dr Hui Luo
09.40 – 10.10	Electro-Coupling of Catalytic Hydrogen Reaction with the Alcohol/Biomass Oxidation to Maximize H2 Production – Professor Germano Tremiliosi-Filho
10.10 – 10.40	Green Hydrogen Production Technologies and Future Prospects – Dr Bahman Horri
10.40 – 11.10	Recent Advances on the Ethanol and Ammonia Electro-Oxidation Reactions on Pt, Pd, Rh, Pd-M and Rh-M Nanocatalysts: Reaction Mechanistic Studies and Electrocatalysis - Professor Joelma Perez
11.10 – 11.30	Coffee Break
11.30 – 12.00	Sustainable Batteries and Electrocatalytic Processes – Professor Magda Titirici
12.00 – 12.30	Build Biorefineries and Let the Natural World Drive the Economy - Professor Jhuma Sadhukhan
12.30 – 13.30	Lunch Break
13.30 – 14.00	Investigations of the Activity of Noble and Non-Noble Metals as Catalysts for Electrochemical Energy Conversion Processes - Professor Edson A. Ticianelli
14.00 – 14.30	Designing Dual Function Materials for Integrated Carbon Dioxide Capture and Utilisation - Dr Melis Duyar
14.30 – 15.00	AI-Enabled Data-Driven Approaches for CO2 Capture and Utilisation - Dr Lei Xing
15.00 – 15.20	Coffee Break
15.20 – 15.50	The role of kinetic instabilities in electrocatalysis - Professor Hamilton Varela
15.50 – 16.20	Operando/In-Situ Soft X-Ray Spectroscopy at the Diamond Light Source's B07 Beamline - Dr Santosh Kumar
16.20 – 16.50	Theoretical Assessment of the Delicate Interplay of the Driving Forces and the Reaction Environment in Electrocatalysis - Professor Georg Kastlunger
16.50 – 17.00	Concluding Remarks
17.00 – 18.00	Networking and Campus / Lab Tour
19.00 – 22.00	Dinner & Drinks, Guildford Town Centre

PARTICIPANTS

Dr Melis S. Duyar

Dr Melis Duyar is Senior Lecturer in the School of Chemistry and Chemical Engineering at the University of Surrey. She has a research background in heterogeneous catalysis for energy and environmental applications. Her current research interests are the development of novel adsorbent materials for CO2 capture and catalytic materials for the production of sustainable fuels and chemicals from carbon-based feedstocks. Dr Duyar received her B.Sc. (2012) in Chemical and Biological Engineering from Koç University. She obtained her M.S. (2013) and Ph.D. (2015) in Earth and Environmental Engineering from Columbia University and conducted post-doctoral research (2015-2017) in the Chemical Engineering Department at Stanford University. Prior to her academic appointment at the University of Surrey (2019), she worked at the US Department of Energy's SLAC National Accelerator Laboratory as Associate Staff Scientist at the SUNCAT Center for Interface Science and Catalysis and was also Lecturer of Chemical Engineering at Stanford University (2017-2019).

Dr Bahman Horri

Dr Bahman Horri is an Associate Professor of Energy Materials and the MSc programme leader in the School of Chemistry and Chemical Engineering at the University of Surrey. He coordinates the research studies in nanocomposite materials for Clean Energy applications (green hydrogen, solid oxide fuel cells & electrolysers (SOFCs/SOECs), and thermo-electrochemical water splitting), holding 7 US/European patents, 70+ papers in top-tiered journals, 5 book chapters, and 30+ presentations as the keynote, invited, or plenary speaker at national/international conferences. The national and international communities have recognised his research in hydrogen and fuel cells with multiple awards, including the IAAM Lecture Award (2023, Sweden), Research Supervision Award (2022, Surrey), Innovation Award in Emerging Technologies (2021, UK), Leverhulme Trust Research Fellowship Award (2021, UK), Postgraduate Publication Award (2012, Australia), etc. He is currently the PI of several research and commercialisation projects in Energy Materials and Sustainability sponsored by the EPSRC, the Royal Academy of Engineering, Innovate UK, the Royal Society, and the industrial sector. He has recently patented a hybrid water-splitting process (WO2020016580A2) combining water electrolysis hydrolysis processes for efficient green hydrogen production.

Dr Georg Kastlunger

Georg Kastlunger is a tenure track assistant professor at the Catalysis Theory Center at the Technical University of Denmark. He joined DTU in June 2019, after conducting research at the University of Vienna, in the context of his PhD project, and Brown University, Providence (USA), as postdoctoral research associate. In his 2023-founded "Interfacial chemistry" group, he focusses on improving the fundamental understanding of electrochemical processes based on quantum mechanical simulations. His current research addresses modern perspectives related to the reduction of greenhouse gases via the electrocatalytic valorization of CO2, biomass and waste, as well as improving the understanding of the electrochemical interface on the atomic-level.

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Dr Santosh Kumar

Dr Santosh is currently a beamline researcher at Diamond Light Source and a visiting researcher at Imperial College London. Before Joining Diamond, he worked as a postdoctoral research associate at Imperial College London (2019-2021), University of Bath (2018-2019) and Energy & Bioproduct Research Institute at Aston University (2015-2018).
Santosh's interdisciplinary research expertise and interests include advanced characterisation, operando/In-situ spectro-electrochemistry, (photo)electrocatalysis, and renewable energy. He published more than 45 research articles and four book chapters with over 5000 citations and 32 h-index, to date. He is a fellow of Higher Education Academy United Kingdom and a member of The People and Talent Strategy Advisory Panel (PAT SAP) of The Biotechnology and Biological Sciences Research Council (BBSRC). He is also a member of the Royal Society of Chemistry.

Professor Joelma Perez

Professor Perez obtained the B.Sc. degree in 1989 and the PhD in 1997 in Physical Chemistry at the University of São Paulo. She developed his full academic carrier at the Institute of Chemistry of São Carlos (IQSC) as a doctor professor. Scientific research publications include fifty-three scientific papers in journals listed in several indexing platforms. She collaborated on the writing of one book chapter in the electrochemistry area. She has acted as advisor of over 15 M.Sc. and Ph.D. theses in the post-graduation programs at the Institute of Chemistry of São Carlos. She is an expert in electrocatalysis in fuel cells reactions in the proton exchange membrane acid and alkaline systems.

Professor Jhuma Sadhukhan

Professor Jhuma Sadhukhan is the Director of Research & Innovation in the School of Sustainability, Civil and Environmental Engineering at the University of Surrey, UK. Jhuma obtained a PhD from UMIST, UK in 2002. Jhuma specialises in biorefineries, life cycle assessment (ISO14040-44), carbon footprinting (ISO14064-65) and life cycle sustainability assessment (ISO26000). She wrote the only authored biorefinery book "Biorefineries and Chemical Processes: Design, Integration and Sustainability", Wiley, 2014.

Professor Edson A. Ticianelli

Professor Ticianelli obtained the B.Sc. degree in 1976 and the PhD in 1985 in Physical Chemistry at University of São Paulo. He developed his full academic carrier at the Institute of Chemistry of São Carlos (IQSC) and in November 2003 reached the category of Full Professor. Professor Ticianelli was head of the Department of Physical Chemistry of Institute of Chemistry of São Carlos for four years and the Director of this Institute from 2006 to 2010. He is member of the São Paulo Academy of Science, the Brazilian Academy of Science, and the

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Transworld Academy of Science. He collaborated in the writing of two textbooks in the Electrochemistry area. Publication of scientific research includes two-hundred fifty scientific papers in journals listed in several indexing platforms. He has given several plenary conferences, invited lectures and keynotes in national/international scientific meetings. He has acted as advisor of over 50 M.Sc. and Ph.D. theses in the post-graduation programs at the Institute of Chemistry of São Carlos. He is an expert in electrocatalysis of water electrolysis and fuel cells reactions, particularly the proton exchange membrane alkaline systems.

Professor Magda Titirici

Magda Titirici completed her BSc in Romania and University of Bucharest followed by a PhD at the University of Dortmund, and a postdoc and Habitation at the Max Planck Institute of Colloids and Interfaces. She then moved to the UK in 2013 to take up a reader position at Queen Mary University of London being promoted to full professor in 2014. In 2019 she moved to Imperial College London as a Chair in Sustainable Energy Materials. Magda has published over 350 papers in the filed on renewable energy storage and conversion technologies being in the list of highly cited researchers since 2018. Her research was recognised by numerous awards from Royal Society of Chemistry, Institute of materials and Mines and Royal Society. Magda leads a very diverse group of 40 researchers working interdisciplinary to solve important global challenges. She also has visiting appointments at Tohoku University and University of Stockholm.

Professor Germano Tremiliosi-Filho

Professor Tremiliosi-Filho obtained the B.Sc. degree in 1977 and the PhD in Science, area: Physical Chemistry in 1986 at the University of São Paulo. He developed his academic carrier at the Institute of Chemistry of São Carlos (IQSC) and reached the category of Full Professor. In 1988-1990 he did a post-doctorate stage at the University of Ottawa, Canada and in 1997-1998 he worked as a Visiting Professor at the University of Illinois at Urbana-Champaign, USA. Professor Tremiliosi-Filho was Vice-Director (2010-2014) and Director (2014-2018) of Institute of Chemistry of São Carlos. He is among the 2 % of the Most Influenced Scientist in the World, 2023, also, among the top 10,000 Latin America Scientist, 2023 and among the top 98 Best Brazilian Chemistry, 2022. He has published 3 books, and over two-hundred scientific papers in journals listed in several indexing platforms. He has given over 10 plenary conferences, over 150 invited lectures and keynotes in national/international scientific meetings. He has acted as advisor of over 50 M. Sc. and Ph.D. theses in the post-graduation programs at the Institute of Chemistry of São Carlos. He was Associate Editor of the Electrocatalysis journal (Springer) from 2010-2022. He is expert in electrocatalysis of alcohol oxidation and hydrogen evolution reactions and he is developing the direct ethanol and glycerol fuel cells. More recently, he is also developing the electrochemical reformer of ethanol for sustainable hydrogen production.

Professor Hamilton Varela

Hamilton Varela (1973) graduated in Chemical Engineering from Universidade Federal do Rio Grande do Norte (Natal, Brazil) in 1997. He then obtained his master's degree in physical chemistry from the São Carlos Institute of Chemistry at the University of São Paulo (IQSC/USP, São Carlos, Brazil) in 2000. From 2000 to 2003, he pursued his PhD with Professor K. Krischer at the Physical Chemistry Department (headed by Professor G. Ertl, Nobel Laureate in Chemistry, 2007) at Fritz Haber Institut der Max Planck Gesellschaft (Berlin, Germany). His thesis titled 'Spatiotemporal Pattern Formation during Electrochemical Oxidation of Hydrogen on Platinum' was presented in 2003 at the Freie Universität Berlin, where he received a final mark magna cum laude. After spending eight months as a postdoctoral Max Planck Fellow at the Physics Department of the Technical University Munich, he returned to Brazil. Between 2005 and 2007, he worked as a Group Leader (Jovem Pesquisador FAPESP) at IQSC/USP. In 2007, he was appointed Assistant Professor at the Physical Chemistry Department of the same institution. In 2012, he became an Associate Professor and in 2017 a Full Professor of Physical Chemistry at IQSC/USP. Dr Varela is currently interested in several topics including the interconversion between chemical and electrical energies, electrocatalysis, kinetic instabilities in electrocatalysis, and complex systems. He helped establish the Ertl Center for Electrochemistry and Catalysis in Gwangju, South Korea and since 2010 has been one of the three Managing Scientists there. In 2023, Professor Varela was listed among the top 2% most influential researchers in the sub-field of energy. Professor Varela is currently the Director of the IQSC/USP, Deputy Director of the Bioenergy with Carbon Capture and Storage (BECCS) program and member of the Executive Committee of the Research Center for Greenhouse Gas Innovation (RCGI/USP).

Dr Lei Xing

Dr Lei Xing is a Lecturer in Digital Chemical Engineering at the University of Surrey, UK. His research aims to propel the sustainable growth of the chemical and energy sectors through industrial decarbonisation and AI-driven digitalisation, all within the framework of the circular economy. Dr Xing's work predominantly focuses on pioneering next-generation processes and systems in carbon capture and utilisation, fuel cells, flow batteries, metal-air batteries, and electrolysis. Currently, his research delves into the multi-scale modelling and multi-criteria optimisation of CO2 utilisation and renewable nexus, that integrate advanced carbon capture and utilisation techniques with intermittent renewable energy sources, employing AI-based adaptive optimisation, techno-economic analysis, and life cycle assessment to contribute significantly towards achieving the Net Zero target. Dr Xing's interdisciplinary work has led to national and international collaborations with experts in chemistry, mechanical engineering, electrical engineering, and computer science. He is a Chartered Member of IChemE and holds positions on the editorial boards of Energy and AI, Frontiers in Energy Research, and Energies. Additionally, he serves as a Guest Editor, Topic Editor, and Review Editor for several journals. Dr Xing's scholarly output includes 4 book chapters, 100+ journal papers with 3500+ citations.

ABSTRACTS

Electro-Coupling of Catalytic Hydrogen Reaction with the Alcohol/Biomass Oxidation to Maximize H2 Production

Professor Germano Tremiliosi-Filho, University of São Paulo, Institute of Chemistry of Sao Carlos

The water electrolysis process combines the favorable hydrogen evolution reaction with the thermodynamically unfavorable oxygen evolution reaction demanding high energy consumption. However, in the advent of substituting the kinetically slow oxygen evolution reaction for a more favorable reaction, as the alcohol/biomass oxidation, turns this electro-coupled process with a combination of two synergistic electrocatalytic systems for the co-production of high-purity H2 and valuable products (from the alcohol/biomass oxidation) with a low energy consumption and high Faradaic efficiency.
In this context, this seminar will describe the development of non-noble metal catalysts for hydrogen evolution reaction (HER) and ethanol electro-oxidation, operating in alkaline medium (1 - 4 mole L-1 KOH in presence and absence of 1 M ethanol at 25 – 85 []C). Two class of materials were developed as catalysts for hydrogen reaction: (i) MoS2 and (ii) Ni/B intermetallic compounds. The activity of MoS2 for the HER is similar to the Pt electrode and showed insensibility for ethanol reduction. The Ni2B intermetallic showed an improvement for the HER in presence of ethanol, while the HER on Ni3B was inhibited in presence of ethanol. Regarding the ethanol oxidation reaction, electrocatalysts of low-cost oxides were developed, the most promising material were Pd/Fe3O4/C and Pd/Fe3O4SnO2/C, with low load of palladium.

Green Hydrogen Production Technologies and Future Prospects

Dr Bahman Horri, School of Chemistry and Chemical Engineering, University of Surrey

As a non-toxic, renewable, transportable and emission-free energy carrier, hydrogen is becoming a more popular alternative fuel in the energy sector. Green hydrogen is a generic term referring to the technical pathways applied to producing carbon-free hydrogen, which will be briefly summarised in this talk. Electrochemical water splitting is currently the most common route to produce green hydrogen at the commercial scale, which is associated with a minimum energy consumption of about 4.3 kWh/Nm3, at ~70% efficiency. At Surrey, we have recently patented a hybrid water-splitting process, the so-called SurreyH2 technology, for sustainable hydrogen production by combining the thermochemical and electrochemical routes. SurreyH2 process is comprised of a modified alkaline electrolyser operating at room temperature as the reduction zone and a water-splitting reactor using a transition metal as the oxidation zone, which will be discussed in this talk in more detail.

Recent Advances on the Ethanol and Ammonia Electro-Oxidation Reactions on Pt, Pd, Rh, Pd-M and Rh-M Nanocatalysts: Reaction Mechanistic Studies and Electrocatalysis

Professor Joelma Perez, University of São Paulo, Institute of Chemistry of Sao Carlos

A deep understanding of the reactions involved in noble metals nanocatalysts for fuel cell anodes may facilitate their use as a source for energy storage and conversion. We can highlight the study

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of the ethanol and ammonia oxidation reactions on surfaces such as Pt, Pt-Pd, Pd, Pd-M, Rh, and Rh-M (M =Fe, Ru, and Cu) dispersed in high-area carbon surfaces. Ethanol is a biomass fuel with low toxicity and high energy density; on the other hand, ammonia is a carbon-free energy storage and conversion source. Therefore, using an experimental approach of combining online electrochemical mass spectrometry (OLEMS), ion chromatography (IC), and high-performance liquid chromatography (HPLC) with high-area electrode surfaces, many products of these oxidation reactions can be simultaneously detected, and the variation in oxidation reaction selectivity depending on the surface conditions can be demonstrated. In the ethanol oxidation reaction (EOR) combining the OLEMS and HPLC analyses, it was possible to identify the presence of products such as acetaldehyde, acetic acid, CO, methane, ethyl acetate, acetaldol, crotonaldehyde, and CO2 depending on the applied potential and surface conditions. For example, the ammonia oxidation reaction (AOR) in Pt/C the real-time identification of seven gaseous products, viz., nitrogen, nitric oxide, hydrazine, hydroxylamine, hydrogen azide, and nitrous oxide, and two solution-phase products, nitrite, and nitrate, enabled us to propose AOR mechanistic pathways, opening more possibilities for the electrochemical generation of high-value-added nitrogenated products depending on Pt surface conditions. The contributions to mechanism comprehension of the EOR and AOR over noble metal surfaces are essential for future studies on these reactions, which is essential for using ethanol or ammonia for energy storage and conversion.

Sustainable Batteries and Electrocatalytic Processes

Professor Magda Titirici, Department of Chemical Engineering, Imperial College London

To mitigate the climate change and reach a carbon neutral society before it is too late, a mix of sustainable energy technologies are needed. In this talk I will present research from my group in the area of sustainable batteries beyond Li ion, green H2 from the electrolysis of biomass derivatives as well as fuel cells free of Pt electrocatalysts for the cathodic reaction.
Batteries will continue to play a vital role in decarbonising transportation as well as in storing the intermittent renewable energy. Li ion batteries have revolutionised the electrification of transportation and contributed significantly to grid storage. However, there are increasing concerns with the availability of the minerals currently used in Li-ion batteries today, especially looking at the predicted growth of batteries demand. Diversification of battery technologies with more sustainable options in mind, not only for the raw minerals used in future batteries but also for more sustainable manufacturing practices for cells and packs are needed. In my talk I will touch on some of these sustainable practices needed to be implemented today while showing the 12 principles of “green batteries” inspired from “green chemistry” my research group introduced. I will than focus on Na-ion batteries, the next battery technology in line for commercialisation in 2024, with emphasis on our research on hard carbon anodes on understanding the fundamentals on Na ion storage using mischaracterisation techniques coupled with electrochemistry. I will also discuss the importance and complexity of solid electrolyte interfaces and some perspectives on commercialisation from our group.

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In addition to batteries, green H2 is also a key energy vector helping our transition to net zero. Green H2 is commonly obtained from water electrolysis using various membranes such as alkaline, proton conductive, anion exchange or solid oxides. While the cathodic hydrogen evolution reaction happens with a minimum amount of Pt (0.05 mg/cm2) and with a low overpotential (ηHER ~ 0.01V at 1.4 V), the anodic oxygen evolution reaction is sluggish and requires large amounts of IrOx, a critical mineral, (0.3mg/cm2) at high overpotentials (ηOER ~ 0.4V). The search for new electrocatalysts for PEM electrolysis with a minimal amount of Ir is crucial. I will briefly present our high throughput approach towards fundamental understanding of what controls the activity of IrOx in the search for such new catalysts using robotic platforms coupled with machine learning. I will also present our research on new substates for electrocatalytic H2 production based on biomass/plastic waste derivatives such as glycerol, ethylene glycol or 5-hydroxymethylfurfural with advantages in terms of lower potentials where the biomass/waste oxidation reactions occur and the advantages of producing other high value chemicals in addition to green H2, helping a circular economy.
Finally, I will touch on the use of H2 in fuel cells for zero carbon electricity production. The sluggish reaction here is the oxygen reduction reaction happening at the cathodes requiring Pt catalysts which are scarce and expensive. I will present research on bioinspired catalysts based on Fe single atoms coordinated to nitrogen atoms doped on a conductive carbon matrix and their activity emphasising the importance of determining the number of active sites, turnover frequency and understanding the issues hindering the stability of such catalysts.
I will finish the talk by drawing some parallels on what we can learn in the field of electrocatalysis from batteries and the other way around exemplifying briefly with two reactions: N2 reduction to ammonia and CO2 to reduction to ethylene.

Build Biorefineries and Let the Natural World Drive the Economy

Professor Jhuma Sadhukhan, School of Sustainability, Civil and Environmental Engineering, University of Surrey

We can save our planet by building biorefineries powered by the natural world. We need a country-wide bioeconomy plan to optimise renewable and bio-based resources (biomass) to produce products from food and pharmaceuticals through consumer chemicals to biofuel and bioenergy. In the drive of net-zero, it is easy to fixate on growing crops to power our homes or cars. However, we can do so much more with alternative resources. Around the world, businesses are turning biomass into shoe soles or skin creams. With the right investment and the right plan, a country can grow its economy sustainably based on renewables and biomass. There are plenty of reasons to prefer biological material from agricultural, forestry or municipal waste over fossil fuels. Plants are renewable and absorb carbon dioxide while they grow. The key is to build biorefineries – large plants that turn organic matter into chemicals. The more products made in the same facility, the better for the environment and the economy. Even better – they could generate energy and heat at the same time. A biorefinery producing 220 kilotonnes per annum costs about the same as a petrochemical facility: $750 million. The research is published in the Journal of Cleaner Production, and helps promote UN Sustainable Development Goals 8 (decent work and economic growth), 9 (industry, innovation and infrastructure), and 12 (responsible consumption and production).

Investigations of the Activity of Noble and Non-Noble Metals as Catalysts for Electrochemical Energy Conversion Processes

Professor Edson A. Ticianelli, University of São Paulo, Institute of Chemistry of Sao Carlos

The ever-increasing world demand for clean electrical energy requires the development of more efficient, environmentally sustainable, and diversified energy conversion systems. Among these, photovoltaic solar, wind turbines and hydraulic power systems appear to be the most promising sustainable energy sources, together with biomass related systems. However, the intermittency of some these sources requires developing energy conversion systems and energy carriers for the periods of peak consumption or low production. In this context, electrochemical energy conversion devices, comprising different types of electrolyzers and fuel cells, together with different kinds of batteries, will have central importance, since they can efficiently convert the electrical energy into chemical energy and vice-versa, and also produce different energy carrier species such as molecular hydrogen, formic acid, syngas, ammonia, etc. Considering this scenario, a number of electrochemical processes are nowadays investigated in our group and this presentation we will discuss the performance of noble and non-noble electrocatalysts for electrochemical reactions involved energy in different conversion processes: (i) reduction of protons or water for hydrogen generation and water oxidation for oxygen production in water eletrolyzers; (ii) reduction of oxygen for electrical energy production from hydrogen in fuel cells; (iii) reduction of carbon dioxide, mostly aimed to syngas syntheses. In these cases, different types of nanostructured electrocatalysts and compositions of the electrolyte are investigated, aiming at determining the parameters governing the electrocatalytic activity and stability and to construct innovative electrolyzers, fuel cells, production different energy carriers.

Designing Dual Function Materials for Integrated Carbon Dioxide Capture and Utilisation

Dr Melis S. Duyar, School of Chemistry and Chemical Engineering, University of Surrey

Carbon dioxide capture and utilisation (CCU) technologies will play an essential role in decarbonising all sectors to reach a net zero emission future. In particular there is an urgent need to replace fossil derived carbon in the chemical industry as well as in fuels supplied to “hard-to-decarbonise” sectors such as transportation and residential heating. Dual function materials (DFMs) for integrated CCU are materials designed with both adsorbent and catalytic capabilities (hence “dual function”) that can capture and subsequently directly convert dilute streams of CO2 (from stationary emissions or the atmospheric air) to useful chemicals. In a typical cycle of operation, the DFMs are first exposed to a source of CO2 to achieve capture, then switched to a stream of co-reactant such as hydrogen or hydrocarbons to achieve the in-situ conversion of captured CO2. The chemical transformation of captured CO2 regenerates the adsorbent while releasing a concentrated stream of desired end product. In combining CO2 capture and utilisation, DFMs can achieve unique synergies that can improve energy efficiency. For example, exothermic hydrogenations of CO2 such as the methanation reaction can supply heat that then drives CO2 on adsorbent sites to spill over to catalytic sites during DFM operation. This allows reaction heat to be directly used in the energy intensive process of sorbent regeneration, while maintaining isothermal conditions to promote CO2 conversion on catalytic sites. This seminar will discuss approaches to develop novel adsorbent materials for CO2 capture, catalytic materials for the production of

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sustainable chemicals and present strategies to effectively combine these approaches to yield an integrated CCU system. A rational design approach based on fundamental understanding of structure-function relationships is needed to accelerate materials discovery for CCU in a diverse set of scenarios, and recent developments in this area will also be presented.

AI-Enabled Data-Driven Approaches for CO2 Capture and Utilisation
Dr Lei Xing, School of Chemistry and Chemical Engineering, University of Surrey

CO2 stands as the foremost greenhouse gas contributing to global warming. There has been a concerted global effort among researchers to focus on the capture/storage and conversion of CO2 into value-added chemicals, employing notable techniques such as direct air capture (DAC) and electrochemical CO2 reduction (eCO2R). These innovative methods of CO2 capture and utilisation hold immense potential to transition from the traditional linear manufacturing processes to a circular economy, thereby closing the carbon loop. The advent of machine learning and AI has further augmented the promise of digitalising the CO2 capture and utilisation processes and systems. Through the amalgamation of data-driven and physics-based modelling, alongside the integration of AI-based adaptive control strategies, there is a substantial enhancement in the efficiency and performance of these processes. This presentation will delve into CO2 capture via enhanced weathering and CO2 utilisation through electrochemical conversion as prime examples of the efficacy of data-driven approaches within a circular CO2 economy framework. It will cover the fundamentals and mechanistic models of CO2 capture and conversion processes, the implementation of various data-driven surrogate models in our research, and the AI models designed to predict the availability of carbon sources and renewable energy. Conclusively, it will highlight the AI-based model for adaptive optimisation of the CO2 capture and utilisation process, underscoring the significant strides being made in this critical field.

The Role of Kinetic Instabilities in Electrocatalysis
Professor Hamilton Varela, FRSC, São Carlos Institute of Chemistry of the University of São Paulo

Electrocatalytic systems are often characterized by kinetic instabilities, which manifest as multi-stability and potential/current oscillations within certain parameter regions. Notably, the electrochemical oxidation of small organic molecules — such as formic acid, methanol, ethanol, ethylene glycol, and glycerol — can exhibit spontaneous oscillations in reaction rates under certain conditions. These oscillations are not just curiosities; they can reveal critical kinetic features of the system and may enhance both its activity and long-term operational stability. This seminar will present various examples of complex dynamics observed in electrocatalytic systems. Through a combination of experimental data, modeling, and numerical simulations, we will discuss these phenomena with a particular focus on the mechanistic aspects. The aim is to demonstrate how fundamental studies of such dynamics can inform and improve the electrocatalysis of small organic molecule oxidation.

Operando/In-Situ Soft X-Ray Spectroscopy at the Diamond Light Source's B07 Beamline
Dr Santosh Kumar, B07 beamline, Diamond Light Source

By encouraging knowledge-based design and operation of catalytic processes rather than trial-

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and-error experimental or synthetic approaches, understanding structure-activity links is a difficult but essential step in building more effective and stable catalysts.[1] In-situ and operando characterisation have become established as crucial ideas for obtaining such structure-activity relations in catalysis over the years. [2] In particular, soft X-ray spectroscopies (including X-ray photoelectron spectroscopy (XPS) and Near-edge X-ray absorption fine structure (NEXAFS)) are powerful element selective techniques that help understand the electronic and geometric structure of (photo)electrocatalysts under operating conditions. [1-3]
Suitable reaction cells are critical for operando near ambient pressure (NAP) XPS and NEXAFS studies. [2] They enable tracking the chemical state and structural properties of catalytically active materials under realistic reaction conditions, and thus allow a better understanding of charge transfer at the liquid-solid interface, activation of reactant molecules, and surface intermediate species. [4] In order to facilitate such studies at the Diamond Light Source's B07 Beamline, we have designed and commissioned a spectro-electrochemical flow cell, which allows user-friendly operation for synchrotron-based soft X-ray photoelectron and absorption spectroscopy measurements. The reaction cell design also allows simultaneous measurements of total electron yield (TEY), Auger electron yield (AEY) and total fluorescence-yield (TFY) to vary the depth-sensitivity of the measurements. A few case studies will be presented to demonstrate the capabilities of the spectro-electrochemical flow cell at the Versatile Soft X-ray (VerSoX) B07 beamline. [3,5] More importantly, the spectro-electrochemical flow cell is available for user community of Diamond Light Source.

[1] Science, 355 (2017), 4998; [2] Journal of The Electrochemical Society, 167 (2020), 054509; [3] Synchrotron Radiation News, 35 (2022), 39; [4] Chemical Reviews, 120 (2020), 4056. [5] J. Synchrotron Rad., (2024), 31.

Theoretical Assessment of the Delicate Interplay of the Driving Forces and the Reaction Environment in Electrocatalysis
Dr Georg Kastlunger and Dr Sihang Liu, Technical University of Denmark, Fysikvej, Kongens Lyngby, Denmark

The atomistic understanding of complex reaction mechanisms in electrocatalysis aids not only the discovery of improved catalytic materials but also the choice an ideal reaction environment for tailored products. In my talk, I will present density functional theory-based studies on electrocatalytic reaction mechanisms with a special focus on electrochemical CO(2) reduction and biomass valorization. I will describe how the combination of constant-potential DFT approaches and transition state theory-based considerations allow us to explicitly study the potential, pH and electrolyte dependence of multistep reaction networks relevant for the green transition.[1,2] Further, I will discuss general trends in the kinetic characteristics of the competing elementary reactions in electrocatalytic reductions and their consequences on the potential and pH response of the product selectivity.[3,4]

1. Kastlunger, G. et al. Using pH Dependence to Understand Mechanisms in Electrochemical CO Reduction. ACS Catal 12, 4344–4357 (2022).
2. Liu, S. et al. Solvation of furfural at metal–water interfaces: Implications for aqueous phase hydrogenation reactions. J Chem Phys 159, 84702 (2023).

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3. Kastlunger, G., Heenen, H. H. & Govindarajan, N. Combining First-Principles Kinetics and Experimental Data to Establish Guidelines for Product Selectivity in Electrochemical CO 2 Reduction. ACS Catal 13, 5062–5072 (2023).
4. Liu, S. et al. Unraveling the reaction mechanisms for furfural electroreduction on copper. EES Catalysis 1, 539–551 (2023).

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