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Delegate Booklet

Newton-Bhabha UK-India Researcher Links Workshop on New Electrochemical Technologies for Sustainable Fuels, Chemicals and Industrial Processes

2nd-5th December 2019

Pune, India

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About this Workshop

This workshop will bring together researchers from the UK and India who have the potential to be world-leaders in the development of new and sustainable electrochemical routes for the production of fuels, chemicals and materials, and provide an environment for developing new research programs that address these challenges.

The workshop will mostly take place in Hotel Sayaji, Pune and all delegates will be accommodated there (https://www.sayajihotels.com/sayaji-hotels/sayaji-pune/). Please note, however, that on Day 1 (2nd December), the venue for the workshop activities will be Lecture Hall Complex (LHC 101), at IISER Pune. Hotel Sayaji will arrange transfers to and from IISER Pune for workshop delegates.

The primary aim of the workshop is to facilitate the formation of networks and collaborations between the early career delegates from the UK and India. We hope that all delegates will approach the workshop with a spirit of openness to new opportunities and a willingness to forge new international links that will help to set the research agenda in electrochemistry and electrochemical technology in the coming years. Most of all, we hope that you enjoy the workshop and make some new and lasting friendships.

With very best wishes for a successful workshop,

Mark and Musthafa

Agenda

Day 1 - Monday 2nd December (LHC 101, IISER Pune)

09:00 – 09:20	Workshop opening ceremony (Srinivas Hotha)
09:20 – 09:40	British Council
09:40 – 10:00	RSC - Rajesh Parishwad
10:00 – 10:20	Workshop plan and overview
10:20 – 10:40	Tea/coffee break
10:40 – 11:05	Naga Phani B. Aetukuri
11:05 – 11:30	Alastair Lennox
11:30 – 11:55	P. Ragupathy
11:55 – 12:20	Alexander Murray
12:20 – 14:00	Lunch
14:00 – 15:00	Vijayamohanan K. Pillai
15:00 – 15:25	Mohammad Zain Khan
15:25 – 15:55	Tea/coffee break
15:55 – 16:55	Amit Paul
16:55 – 17:20	Edward Randviir
17:20 – 19:00	Networking
19:00	Dinner

Day 2 - Tuesday 3rd December (Hotel Sayaji)

09:00 – 09:05	Day 2 opening remarks
09:05 – 09:30	Eve Wildman
09:30 – 09:55	Biraj Kumar Kakati
09:55 – 10:20	
10:20 – 10:50	Tea/coffee break
10:50 – 11:15	Santoshkumar D Bhat
11:15 – 11:40	Latha Krishnan
11:40 – 12:05	Ramendra Sundar Dey
12:05 – 12:30	Ignacio Tudela-Montes
12:30 – 14:00	Lunch
14:00 – 15:00	Frank Marken
15:00 – 15:25	Moritz F. Kuehnel
15:25 – 15:55	Tea/coffee break
15:55 – 16:45	Mark Symes
16:45 – 17:10	Murali Mohan Seepana
17:10 – 17:35	Ilka Schmueser
17:35 – 19:00	Networking
19:00	Dinner

Day 3 - Wednesday 4th December (Hotel Sayaji)

09:00 – 09:05	Day 3 opening remarks
09:05 – 09:30	N. S. Venkata Narayanan
09:30 – 09:55	Madhumita Sahoo
09:55 – 10:20	Aditi Halder
10:20 – 10:50	Tea/coffee break
10:50 – 11:15	Niall Kirkaldy
11:15 – 11:40	Narayanan T. N.
11:40 – 12:05	Salvador Eslava
12:05 – 12:30	M. Ali Haider
12:30 – 14:00	Lunch
14:00 – 15:00	Sudipta Roy
15:00 – 15:25	Poulomi Roy
15:25 – 15:55	Tea/coffee break
15:55 – 16:35	Muhammed Musthafa
16:35 – 16:55	Jaishankar Natarajan (*Sponsor, Godrej & Boyce Mfg. Co. Ltd.*)
16:55 – 17:20	Surbhi Sharma
17:20 – 17:45	Kiran Vankayala
17:45 – 19:00	Networking
19:00	Dinner

Day 4 - Thursday 5th December (Hotel Sayaji)

09:00 – 09:05	Day 4 opening remarks
09:05 – 09:30	Saravana Kumar Jaganathan
09:30 – 09:55	Mohsin Ahmad Bhat
09:55 – 10:20	Maryam Bayati
10:20 – 10:50	Tea/coffee break
10:50 – 11:15	Tharamani C. Nagaiah
11:15 – 11:40	Xiaolei Fan
11:40 – 12:05	Pravin Popinand Ingole
12:05 – 12:30	Stefano Mezzavilla
12:30 – 14:00	Lunch
14:00 – 15:30	Discussion Session 1
15:30 – 16:00	Tea/coffee break
16:00 – 17:30	Discussion Session 2
17:30 – 17:45	Closing remarks

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Scientific Abstracts

Towards High Energy Density Solid-State Lithium Batteries

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Abstract: Solid-state lithium batteries that utilize metallic lithium as an anode can offer high energy density, long cycle and calendar life, enable lithium recycling and are non-flammable. Therefore, they are ideal for electric-vehicles and possibly also for stationary storage applications. However, stable cycling of lithium, especially at high current densities (>200 µA/cm^2), has been a long-standing challenge. An unstable lithium/solid-electrolyte interface has often been cited as the possible reason for the highly inhomogeneous deposition of lithium. Several research groups have worked on metallic interlayers to decrease interfacial impedance which was found to enhance dendrite growth resistance.

In this talk, we will present our recent work on understanding the correlation between interfacial resistance and the propensity for dendrite growth in Li-Li half cells. We will discuss the impact of different metallic interlayers (all less than 100 nm in thickness) on lithium dendrite growth in these half cells. We observed that the critical current density for dendrite growth could vary by as much as 2 times across different metallic interlayers. We will discuss the role of interfacial impedance, and the properties and thickness of the metallic interlayers in influencing dendrite growth. We will also touch upon possible descriptors for identifying interlayers that could further enhance critical current densities in solid-state lithium batteries and enable the practical realization of solid-state batteries.

Electrochemistry for Organic Synthesis

Alastair J. J. Lennox
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Abstract: *Current research*: Electrochemical Fluorination

Electrochemistry is becoming an increasingly important tool in the field of organic synthesis because the inherent tunability of the applied potential provides high selectivity, mild and safe conditions. It is the most sustainable way to conduct redox reactions, as there is complete control over the ultimate destination (or source) of electrons, and the waste associated with stoichiometric redox reagents is avoided.[1] The technique is practical and scalable, with a number of industrial processes in operation.[2] For these reasons the field is currently experiencing a huge resurgence of interest.[3]

Currently, we are interested in using electrochemical oxidation to incorporate fluorine into organic molecules, which is important for improving the pharmacokinetic properties, metabolism pathways and potency of bioactive molecules, such as pharmaceuticals and agrochemicals. The project that I will describe involves the generation of vicinal difluorides, which are interesting motifs for molecular design because they adopt a gauche configuration in solution. We have found a method that uses inexpensive HF salts as fluorine sources and an iodoarene as a mediator to produce a range of difluorinated compounds that are inaccessible by other means.

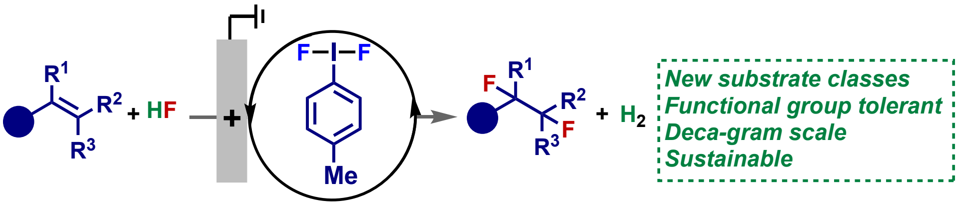

Fig. 1 Electrochemical difluorination of alkenes.

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Redox Flow Batteries for Large Scale Storage of Electricity

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Abstract: The paradigm requisite for advanced energy storage technologies catering to the need of storing intermittent energy obtained from renewable energy resources, importantly solar and wind is of great importance. The major contributor for energy production is from non-renewable energy resources in specific fossil fuels. On an average, every year tones of various substituents of fossil fuels are used for electricity production. Its impact on global climate is devastating, owing to large emission of CO_2 and other consequences leading to a greater threat to society. The smart swift from the consumption of fossil fuels to renewable resources like solar and wind is in priority among the million dollar energy producing industries. In this regard, RFBs are widely recognized as potential option for large scale storage of electricity signifying the wide application of renewable energies due to their flexibility in design to decouple the energy and power. The power of the storage devices depends on size of the cell stack (number of cells) while volume of the electrolyte determines the energy density. However, the complete utilization of conventional RFBs in broader applications has been limited to their low energy density (10 fold lower than Li-ion systems). Thus, the development of high performance, low cost and long life redox flow batteries that can outperform the state of art storage systems is highly desirable. In this talk, recent trends of redox flow batteries will be covered. Particularly, the metal halides and metal –metal hybrid redox flow batteries will be emphasized.

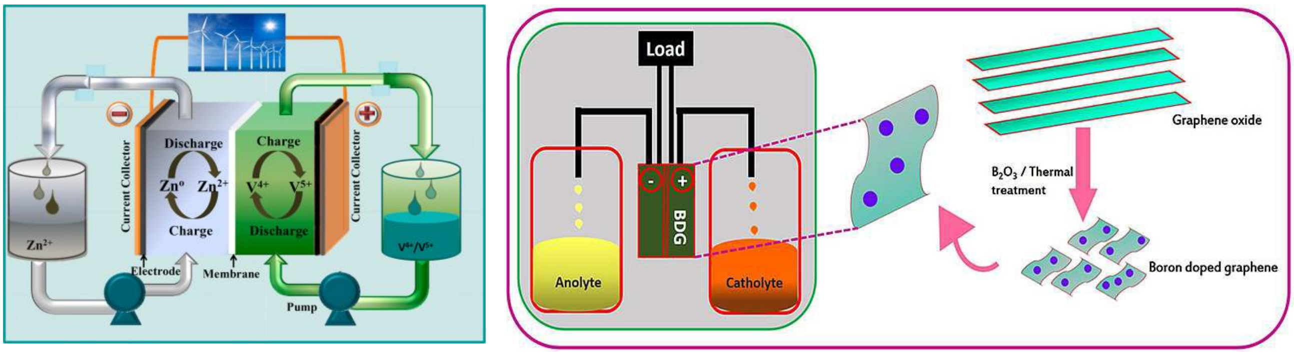

Fig. 1 Metal-metal hybrid (Zn−V) flow battery and Boron-doped graphene as electrocatalyst in metal-halide systems.

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Electrochemically active ionic mediators for organic redox flow batteries and catalysis

Alex Murray
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Abstract: Redox flow batteries (RFBs) possess huge potential for grid-scale energy storage, but suffer from the fluctuating price, poor redox kinetics and corrosivity of typical RFB platforms such as all-vanadium or zinc bromide RFBs. Organic molecules have been proposed as alternative solutions but frequently require non-renewable starting materials, long syntheses and suffer from irreversible *cross-over* of redox active molecules through an ion-selective membrane.[1]

We present initial work towards the resolution of these issues; using either 'recyclable' mediators that have thermodynamically cheap interconversion between them, or using common electrolyte systems to develop simple symmetric prototype RFBs.

Furthermore, building upon our previous work investigating the synthesis of high-value liquid products in flow using phase transfer catalysis,[2] we propose the use of such RFB mediators, possessing as they do ionic groups ideal for immiscible phase shuttling, to synthesise high-value products remote from the site of electron transfer and thus avoiding separation and/or potential degradation steps. This is a highly ambitious project which requires external collaboration in order to realise its full potential.

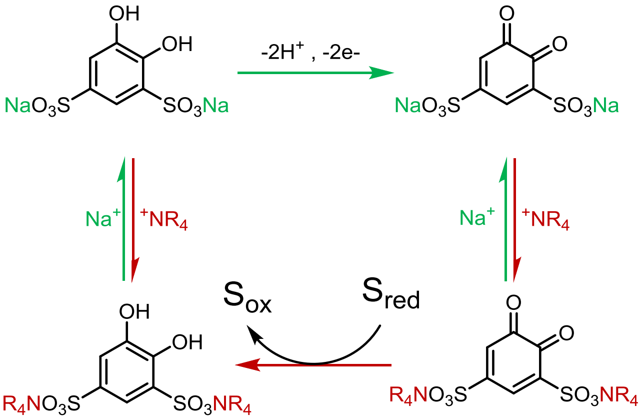

Fig 1. Proposed oxidative upgrading of high-value materials using electrochemical phase transfer catalysis

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2 A. T. Murray, S. Voskian, M. Schreier, T. A. Hatton, Y. Surendranath, *Joule*, 10.1016/j.joule.2019.09.0019

Electrocatalytic Properties of Two-Dimensional Materials

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Abstract: Many advanced materials prepared exclusively using Molecular Nanotechnology have attracted much attention recently due to the possibility of tailoring their dimensionality to facilitate a change in their fundamental properties including mechanical, electrical, optical or electrochemical behavior in comparison with similar behavior of their bulk analogues. In this lecture, I will focus on the electrocatalytic properties of 2D materials as quantum dots like graphene, molybdenum sulphide, Tungsten disulphide and phosphorene. The common aspects of elemental as well as transition metal dichalcogenides as layered materials for transformation to quantum dots and their size tuning will be discussed along with the role of ionic strength, temperature, counter ions, solvent etc. with some of the potential applications like single electron transistors, sensors, energy storage, and electrocatalysts.

References:

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2. Spotlighting graphene quantum dots and beyond: Synthesis, properties and sensing applications, Manila et al., Applied Materials Today, 9(2017), 350–371
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Bioelectrochemical Reduction of Carbon Dioxide to Biofuel by Using a diverse transition metal oxide

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Abstract: Different type of anaerobic bacteria respiration with extracellular electron acceptors requires the transport of catabolic electrons across the cell envelope. For efficient useful applications, present day artificial techniques enable us to tailor these microbial responses to enhance the desired functionality. The different mechanisms of microbe–electrode electron transfer is possible direct electron transfer or through natural nanowires (pili), mediated electron transfer by natural or artificial redox mediator and finally direct redox transformation of excreted metabolites at the electrodes. Mixed bacteria after accumulation have ability to respire with solid extracellular electron acceptors. Therefore, to improve the performance and sustainability of MECs through the functionalisation of the electrode surface. Focus has been placed on developing cost-effective cathodic materials (transition metal oxides) that are important for assembling MEC on industrial scale. In present study, cathode was coated with graphene-$W0_3$ and MnO_2 on which electroactive biofilm (acetogenic bacteria) was attached. In case of dual chamber Mn/CF-MEC achieved the production rate of acetic acid (37.9 mmol/L) that was significantly higher (43.0%) in comparison to the non-coated CF-MEC. However, in rGo-WO_3 fabricated cathode electrode chamber attained highest production rate of acetic acid (57.50 mmol/L) is 62% in contrast to non-fabricated electrode. From experimental result it was found that rGO-WO_3 is better material for enhancement of biofuel production. These modest materials when incorporated into cathodes, are believed to offer better electron transportation, or possibly equivalent performance to the generally utilized expensive counterpart like as platinum.

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Electro-organic Synthesis of Natural Products

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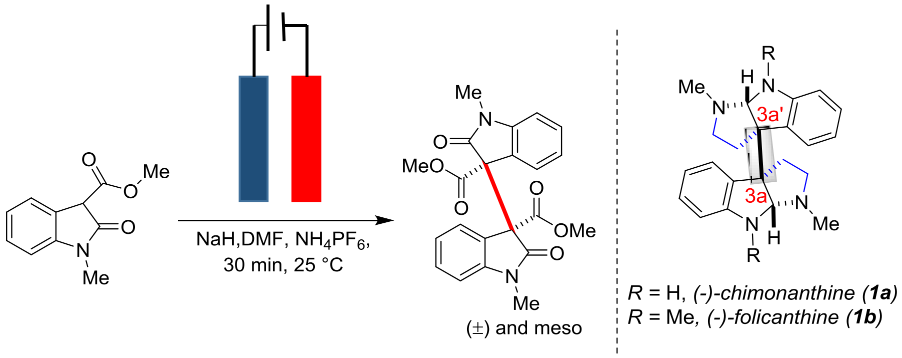
Abstract: C_2-Symmetric dimeric cyclotryptamine alkaloids which possess diverse array of biological activities,[1] puts challenge before the synthetic community due to the difficulty associated in the formation of a C−C bond containing a vicinal all-carbon quaternary center.[2] It is still more challenging to avoid the synthetic routes which includes the use of costly and toxic oxidants and reductants.[3] Electrochemistry can be seen as a green alternative to classical organic chemistry owing to the fact that it reverts solely to the electric current as an inexpensive and sustainable oxidizing or reducing agent, which minimizes the amount of waste dramatically.[4]

For that, an electrochemical oxidative coupling of 2-oxindoles has been demonstrated in an electrochemical cell using mild condition at room temperature providing a broad substrate scope with moderate to good yields which can be applied in the total synthesis of C_2-symmetric dimeric pyrroloindoline alkaloids i.e Chimonanthine (**1a**) and Folicanthine (**1b**).



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Developing New Carbon Materials from Waste Textiles

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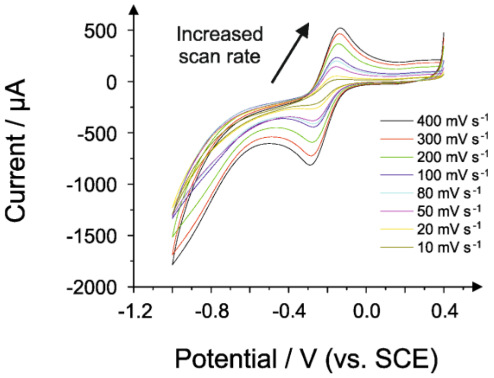
Abstract: Second to oil, the fashion industry is the largest polluting industry in the world. A combination of factors are responsible for this, from the reliance on petroleum intensive products (polyester), through to consumer behaviour in the "fast fashion" market. Around 700,000 tonnes of textile waste is unrecycled in the UK, representing around 3% of total waste to landfill. This work begins the pursuit of chemical recycling technologies to contribute towards the recycling of this waste. Using a catalyst-free hydrothermal chemical process on mixed polyester and cotton fibres, terephthalic acid is produced from polyester, while carbon materials are also recovered from the cotton component.[1] While the terepthalic acid is easily fed back into the textile production loop, the carbon is not. This research investigates the conductivity of the materials produced to examine the applicability of incorporating the materials within printed electronics. Using a carbon paste electrode approach, the as-synthesized textile materials were incorporated into electrodes and tested for their conductivity using cyclic voltammetry. Figure 1 demonstrates a scan rate study for this process, whereby a quasi-reversible system is observed for hexamine-ruthenium (III) chloride in the scan rate region of 10-400 mV s^{-1}. The work indicates potential for either co-mixing of the as-produced carbon with another conductive carbon, or further chemical treatment to maximise the utility of the carbon species produced from the reaction.



References

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New Electrolyte Materials for Fuel Cell Devices

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Abstract: Oxide ion and proton conductors, which exhibit high conductivity at intermediate temperature, are necessary to reduce the operating temperature of ceramic electrochemical conversion devices. The crystal structure plays a pivotal role in defining the ionic conduction properties and the discovery of new materials is a challenging research focus. Here we show that the cation deficient hexagonal perovskite $Ba_7Nb_4MoO_{20}$ supports pure oxygen ionic conduction. Above 300 °C, a structural transition occurs which results in significant proton conductivity in humidified atmospheres. The high bulk conductivity of $\sim$ 4 mS cm^{-1} at 500 °C is comparable with that of state-of-the-art ionic conductors [1]. The proton conductivity of $Ba_7Nb_4MoO_{20}$ is the highest observed in an oxide crystallising with a structure different from the ideal cubic perovskite and it showcases excellent chemical and electrical stability. Hexagonal perovskites form an important new family of materials for obtaining novel ionic conductors with potential applications in ceramic fuel cells and other energy-related technologies [2].

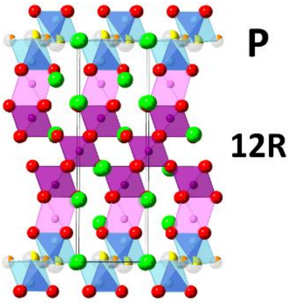

Fig. 1 Average crystal structure of $Ba_7Nb_4MoO_{20}$ composed by alternating palmierite-like and 12R perovskite layers.

The materials presented are in an early stage of characterisation. Although they have been tested in a rudimentary fuel cell set-up within an oxygen concentration cell, we aim to develop other fabrication methods (e.g. thin film) and hope to test the limits of these materials in a real-time, operating fuel cell device.

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Electrochemical Conversion of Air Pollutants Based on Data Surveyed by a Polymer Electrolyte Fuel Cell Powered Unmanned Aerial Vehicle

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Abstract: The ever-rising consumption of fossil fuels, growing industrialisation, urbanisation, and technological advancement have made ambient air pollution so serious that nine out of ten people now breathe polluted air. As reported by World Health Organisation, ambient air pollution is accounted for an estimated 4.2 million premature deaths and a total deaths of 7 million globally. Mainly particulate matter ($PM_{2.5}$ and PM_{10}), NO_x, SO_x, CO_x, and H_2S are major air pollutants with direct link to the public health[1]. There is an urgent need to keep tabs on air pollution. Monitoring the air quality data in urban areas would enable us to identify different air pollutants and their point sources, so that preventive measures can be implemented. The known traditional techniques for air quality monitoring are not sufficient enough to provide accurate data, distribution of pollutants, and their sources. A Polymer Electrolyte Fuel Cell (PEFC) powered Unmanned Ariel Vehicles (UAV), equipped with appropriate sensors, can be a useful tool to monitor spatial distribution of different pollutants and to identify their sources[2]. However, the cost of the PEFC hindering the practical implementation of such systems for these kind of application. Moreover, the durability of the PEFC in polluted atmosphere is not promising enough. For true commercialisation and widespread application, there is an urgent need to switch to a low cost catalyst which is also tolerant to the common air pollutants. In an effort to enhance the durability of the conventional Pt-group metal catalyst loaded PEFC, a rapid in-situ technique has been devised[3]. It hardly takes 300 – 900 s to revive the performance of a H_2S and/or SO_2 contaminated PEFC. In another studies, a doped graphene based catalyst has been synthesized and tested for its electrochemical activity and other relevant properties[4]. The synthesized nitrogen doped graphene catalyst shows excellent ORR activity. These kind of catalyst are relatively cheaper and tolerant to most of the common air pollutants. An extensive analysis of the pollution data collected by a PEFC powered UAV will help us to identify the spatial distribution of different pollutants and their point sources. Based on this data, electrochemical conversion of the pollutants to useful fuels and chemicals can be explored[5].

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Carbon Nanocomposite membranes for Polymer Electrolyte Fuel Cells

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Abstract: Polymer electrolyte fuel cells (PEFC) are of immense interest among the researchers because of the material challenges associated with it. Membrane electrode assembly (MEA) in fuel cell is pivotal as the reactions happen through the electrode and electrolyte interface. Membrane electrolyte acts as a physical separator that can conduct only protons. Commercially available Nafion® membranes are widely used as electrolytes for PEFC but expensive and preparation routes are complicated. Hence viable alternative electrolytes are explored such as sulfonated polyether ether ketone (sPEEK) which can mimic the characteristics of Nafion. However stability and fuel cross-over in these matrices is an important challenge which needs to be addressed. sPEEK nanocomposites are prepared with Carbon nanostructures as additive in PEFC because of its thermal and mechanical properties, low density and high surface area. Different functionalization routes are employed to the carbon nanostructures to from composite polymer membranes of better ionic conductivity. Ionic conductivity for the composite electrolyte in fuel cells is important for better PEFC performance. These additives are also used to restrict the methanol cross-over in direct methanol fuel cells (DMFC) wherein methanol chooses the tortuous path through the carbon. The impact of carbon nanostructures on electrochemical selectivity of the cell is determined by rigorous electrochemical characterization which includes cell polarization and durability. The composite polymer electrolytes show enhanced fuel cell performance and durability compared to pristine polymer membranes and also state-of-art Nafion membranes. The talk will highlight these aspects and importance of these matrices for commercializing fuel cell technology in addition to future collaboration prospects.

Electroless Copper Plating of Textile Fabrics Using Functionalized Copper Nanoparticle Catalyst

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Abstract: The MATUROLIFE project combines two different disciplines: materials innovation and creative design. The project aims to produce high value added aesthetically pleasing and comfortable assistive technology (AT) products for older people to live more independent lives. In order to achieve AT prototypes, the development of a selective metallisation (electroless copper plating) process for textiles and fabrics has been investigated to produce smart textiles where electronic circuitry becomes part of the material itself.

The electroless copper plating of textiles involves a multistep processes, 1) pre-treatment, 2) surface activation through catalysation and 3) electroless Cu plating. In general, palladium (Pd) is the most commercially used catalyst. However, the use of Pd makes the process expensive, and this metal is classified as a Critical Raw Material by the EU. In this study, an alternative, non-precious metal catalyst route is investigated namely a functionalised Cu NP catalyst whilst the standard Pd catalyst is utilised for comparison purposes. In order to produce more efficient Cu NP with better particle size distribution with reduced particle size, advanced technology (ultrasonics) was used to disperse these functionalised Cu NP. In order to achieve the optimum catalytic activity. In addition, the effect of different parameters of the Cu NP catalyst solution, such as immersion time in catalyst solution, temperature and ultrasonic power etc., were also studied.

Chemical analysis of the Cu NP catalyst was performed using X-ray Photoelectron Spectroscopy (XPS) and particle size measurements using Dynamic Light Scattering (DLS). After electroless Cu plating, the fabrics were characterised using a variety of techniques and methods including calculation of mass percentage of copper gained after electroless plating, surface morphology by Scanning Electron Microscopy (SEM) and electrical conductivity measurements using a four point probe.

The plating rate and the weight gain percentage of copper were increased noticeably with the longer immersion time (30 min) in Cu NP catalyst solution at higher temperatures (50 ^{0}C) and using high ultrasonic power (81 W) to create the Cu NP dispersion. The metallised textile fabrics produced using electroless Cu deposition with a functionalised Cu NP catalyst are shown to be highly conductive.

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Towards the development of metal-free supercapacitor for hybrid energy storage system

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Abstract: Self-sustainable integrated energy storage systems can be the most plausible solution since we are on the verge of a global energy crisis due to rapid dissolution of fossil fuels. Finding environmentally benign fossil fuel replica with a broad performance spectrum is still a very encouraging field of research.[1-2] Increasing craze of portable electronics and hybrid vehicles are raising the bar for the model energy storage systems with high specific energy and power.

Recently we have explored the synthesis of highly conductive graphene film by using laser irradiation method that shows advancement for the fabrication of metal-free robust device. The array of microsupercapacitor device was integrated with a commercial solar cell module (Fig. 1) for hybrid energy harvesting and as a storage device.[1] This study provides an effective strategy to build a metal free supercapacitor with exceptional cycle life and facilitates progress towards self-sustainable energy in the future.

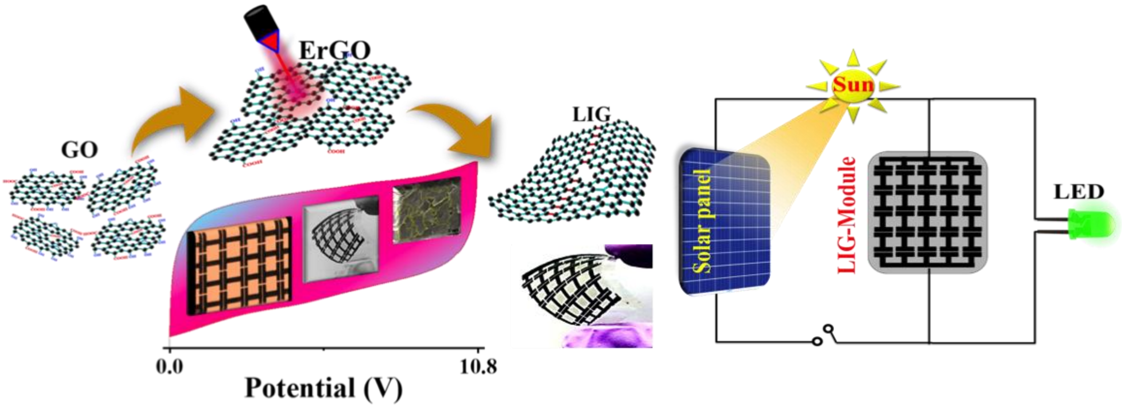

Fig. 1 Schematic representation for the synthesis of LIG film and assembled hybrid device with solar cell.

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Electrochemical Engineering at the University of Edinburgh

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Abstract: Decarbonising all economic sectors is currently major technological challenge that Industry as a whole has ever faced. But luckily for us, Electrochemistry in on our side! Electrochemical Engineering is a multidisciplinary field that can provide a broad variety of solutions to many of the different technological barriers that prevent the development of a true zero emissions economy: (i) environmentally friendly energy storage for static and movable applications (e.g. batteries), (ii) the production and/or use of hydrogen as fuel (e.g. water electrolysis, fuel cells); (iii) the decarbonisation of the chemical industry by using captured CO_2 as a chemical feedstock to produce chemicals such as methanol, ethanol, ethylene, etc.; and even the manufacturing of novel functional materials for more efficient engines, among others.

This are the same areas that our research group, Edinburgh Electrochemical Engineering Group (e3Group), is particularly interested in. In this presentation we would give a highlight of some of the work we have carried in the past, as well as current and future research we are focused on:

- Optimised design of electrochemical reactors: CFD/FEM modelling and optimisation including electrode processes (applications: fuel cells, batteries, electrolysers, etc.).
- Synthesis of materials:
  - Novel electrode materials for electrochemical applications: metal, metal/polymer, piezoelectric, (applications: electro-reduction of CO_2, water splitting, fuel cells, etc.).
  - Functional materials by electrochemical methods: coatings and thin films, particularly for applications requiring enhanced resistance to wear and higher lubricity.

Electrochemical Processes in the Presence of Polymers of Intrinsic Microporosity (PIMs)

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Abstract: Polymers of Intrinsic Microporosity (PIMs) provide a novel class of structurally rigid potentially ion-selective membrane materials with 3D nanofluidic pores of typically 1.5 nm size. For example, the PIM-EA-TB material was employed to protect nanoparticle catalysts, and in a membrane cell configuration as a pH-dependent semi-permeable anion-conductor. When deposited asymmetrically over a 20 μm diameter hole in poly-ethylene-terephthalate (PET) and investigated in a two-compartment electrochemical cell with aqueous electrolyte on both sides, ionic diode effects[1] are observed. Potential for applications in electrocatalysis[2] and in electroanalysis[3] are associated with the molecularly rigid polymer structure. Other types of PIMs such as PIM-1 and PIM-7 (see Figure 1) allow "gas management" under triphasic reaction conditions at electrocatalyst surfaces, e.g. at palladium.

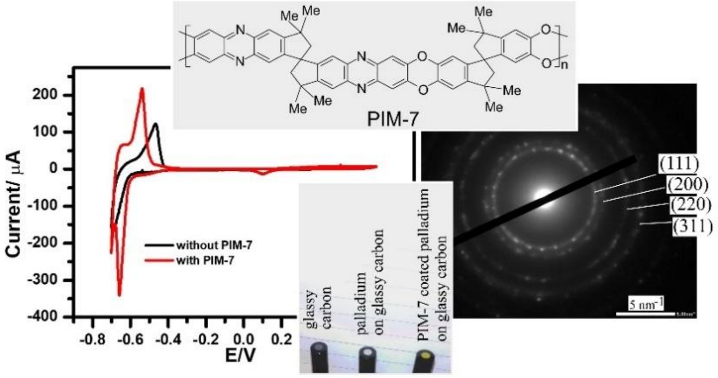

Fig. 1 Molecular structure of PIM-7 and cyclic voltammetry data for nano-palladium deposited onto glassy carbon with/without a PIM-7 coating.

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Coupling molecular electrocatalysis to light-absorbing nano-materials for solar fuel generation from CO_2, water and waste

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Abstract: Direct photochemical conversion of H_2O and CO_2 into H_2 and CO is a promising strategy to mitigate CO_2 emissions and simultaneously store solar energy in renewable fuels, but most of the currently known catalysts for this purpose are based on precious metals, require organic solvents or suffer from low stability and selectivity. We study hybrid materials that combine the photophysical properties of semiconductor nanocrystals with the selectivity of well-defined molecular electrocatalysts. Engineering the particle surface is of paramount importance to achieve efficient charge transfer in such a system. By designing material-specific surface anchors, we can attach molecular catalysts to chalcogenide quantum dots (QDs) to drive H_2 evolution and CO_2 reduction with visible light in water. Comparing different anchoring groups allows us to correlate the photocatalytic activity with the QD/catalyst interface.[1] We develop novel strategies to control the selectivity between CO_2 reduction and H_2 evolution from aqueous QDs, by modulating the capping ligand surface coverage.[2] We can further show that photocatalysis in suspension can be translated into photo-electrochemical H_2O and CO_2 reduction by immobilising molecular catalysts on photocathodes.[3,4] We have also developed new strategies to photochemically upgrade waste materials in to clean fuelsby replacing water oxidation with other oxidation reactions.[5] Photoreforming of model compounds,[6] waste biomass[7] and even plastic waste[8] over CdS-based photocatalysts allows the generation of clean hydrogen fuel using only sunlight as the energy source with simultaneous mitigation of pressing environmental risks. We are keen to expand this approach to other redox transformations such as nitrogen reduction as well as to include biological co-catalysts.

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Electrochemistry for water purification, chemical synthesis, and on the Moon

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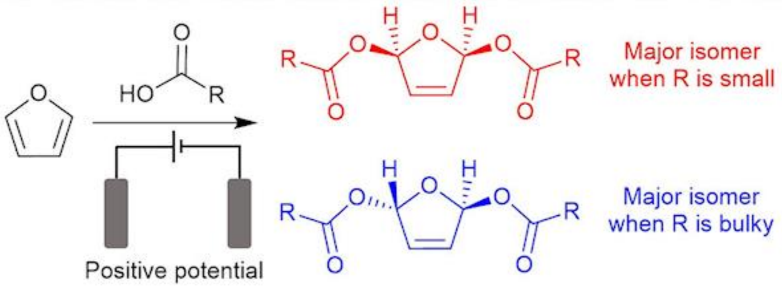
Abstract: In this talk, we will explore some of the work that my group are pursuing in the fields of sono-electrochemical water treatment, organic synthesis using electrochemistry, and the electrolysis of lunar regolith simulants. In particular, we will look at how simultaneous application of electric and ultrasonic fields might allow the treatment of industrial wastes and/or brine concentrates from water treatment technologies such as reverse osmosis and electrodialysis.[1] We will then explore some organic transformations that are catalysed or mediated by electrolysis (see figure) and discuss some of the opportunities and challenges in this field.[2] Finally, we will leave Earth far behind and explore how electrochemistry might one day underpin human habitation on the Moon.[3]



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Large Scale Electrochemical Energy Storage Technologies for Industrial Processes

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Abstract: The electrochemical energy conversion and storage plays a crucial role in the growing age of clean energy. The water electrolysis for production hydrogen fuel and photoelectron reduction of CO_2 into value added products (Solar –Syngas) is very attractive way of utilization of solar energy [1, 2, 3]. However, implementation of this technology at industrial scale is limited by because of high process cost, difficulties in storage and utilization of fuel. A Flow Battery is a better alternative to store intermittent energy and utilization [4, 5]. In recent years, continuous effort has been focused on rational material and electrode designs to improve the performance of electrochemical energy storage and conversion devices. Vanadium Redox Flow Battery (VRFB) is most promising and proven technology for large capacity electrical energy storage. But, the higher cost of VRFB system is limiting its widespread application. The first one is the high cost of membrane ($\$1400/m^2$) and second is cost of vanadium ($27/kg). The energy density of VRFB is considerably low (20-60 Wh/L) due to the low solubility of vanadium ion in the electrolyte (2.0 –3.0M) [6, 7]. The present work is focused on the both aspects of developing novel inexpensive membrane and searching for alternative active material to replace vanadium without comprising on cell efficiency. The composite membranes like PTFE-ZrP and PWA based membranes were developed which have given competent results with Nafion. Recently our team started working on alternative electro active material to replace the Vanadium. As per the literature, quinone-based materials (e.g.9,10-anthraquinone-2,7-disulphonic acid (AQDS], (1,2-benzoquinone-3,5-disulfonic acid) BQDS, carbonyl compounds (e.g. (9-fluorenone) FL, 2,5-di-tert-butyl-1,4-bis(2-methoxyethoxy)benzene (DBBB) and many other organic molecules are suitable and potential to repalce vanadium in RFBs [6]. So, we are exploring the possibility AQDS in place vanadium in the redox flow battery.

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Electrochemical Sensors for Process Development and Optimisation

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Abstract: Electrochemical sensors are useful tools for the development and, once implemented, monitoring of industrial processes. The knowledge about local changes in a system allows for the highly targeted process adjustments, fault detection and failure analysis in a larger process, leading to higher yield and product quality. Among electrochemical sensors, micro- and nanoscale devices offer highly desirable qualities, including low susceptibility to natural or forced convection and high signal to noise ratios. This makes miniaturised devices well-suited to integration into a process flow with some advantages over also considered optical sensors.

In metal extraction processes such as used in the PUREX (Plutonium Uranium Redox Extraction) process, nitric acid of varying concentrations up to 7 M is used as the aqueous phase in a liquid-liquid extraction process.[1] The dependence of the process on the solution pH and quality of the nitric acid (presence of decomposition products) means accurate knowledge of these and other parameters is critical in the safe and efficient running of the process.

In this talk, I will describe the development of custom devices targeting the specific challenges of measurements in harsh environments, such as strong acids, to enable improved process control and efficiency and thus achieve a more sustainable system.

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Hydrogen Fuel Exhaling Zn-Ferricyanide Redox Flow Battery

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Abstract: Electrochemical water splitting reaction provides a reaction pathway for green fuel synthesis which in turn offers a carbon-neutral energy platform for stabilizing global mean temperatures. However, it is a thermodynamically unfavorable reaction often requiring substantial electrical driving force. Secondly, the concurrent generation of hydrogen and oxygen in close proximity in state-of-the-art water electrolyzer may pose potentially dangerous consequences. We offer a unique approach for fuel synthesis and report a hydrogen fuel synthesizing Zn-ferricyanide battery by exploiting the concept of dual electrolytes, where exclusive hydrogen fuel synthesis is spontaneously coupled with electric power production. The key to our approach[1] is short-circuited electrodes housed in dual electrolytes without ionic communication where oxidative Zn dissolution and reductive hydrogen fuel synthesis are spontaneously driven at the two poles during electric power generation. This battery chemistry eventually amplifies the voltage output of Zn-ferricyanide battery from 1.7 V to 3 V and boost the energy density from 9.5 Wh/L to 16 Wh/L while concomitantly synthesizing 932 micro-mol/h of clean hydrogen fuel. We believe that coupling hydrogen fuel synthesis with electric power harnessing distinctly integrates an extra dimension to battery functionality and articulates a pathway towards balancing mean global temperatures.

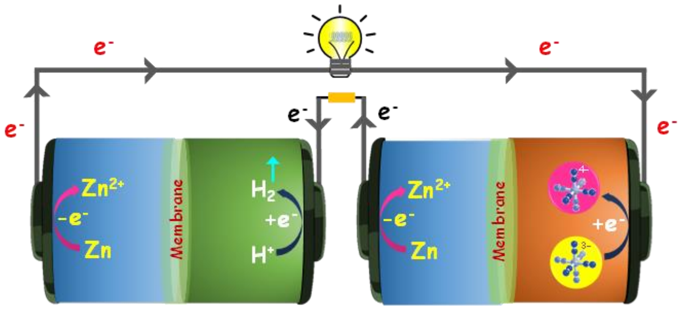

Fig. 1 Schematic representation of hydrogen fuel synthesizing zinc ferricyanide battery (HSZFB) by connecting a Zn-H_2O battery and a Zn ferricyanide battery in tandem.

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Efficient Electrochemical Energy Conversion and Storage devices - Harnessing Engineered Carbon Nanomaterials

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Abstract: The efficient interconversion of chemical and electrical energy in the electrochemical processes holds a huge prospect towards a green and sustainable world. Multi-functional carbon nanomaterials (e.g. carbon nanotube, graphene, and their derivatives) play a major role in these processes by providing the required surface area, porosity, electrical and thermal conductivity, etc. Hybrid carbon nanostructures (HCNS) have a huge impact on the performance and stability of the electrochemical systems on the basis of their constituent elements, structure, surface morphology and interfacial interaction. Here, I will discuss my research towards understanding and developing HCNS for Li-ion batteries (LIBs) and proton exchange membrane fuel cells (PEMFCs). Higher performance LIB anode materials with more Li/C ratio than LiC_6 of graphite are desirable for achieving high and reversible specific capacity to meet the present energy demand of the market[1]. I will first discuss the effect of doping and hybridization of HCNS[2-4] towards their electrochemical performance as potential anode material for LIB. Then, I will present my research efforts to the cost-effective solutions of PEMFC by reducing the Pt amount[5, 6] or employing metal free[7] HCNS electrocatalysts. Finally, I will discuss our latest and novel approach to use the single-layer graphene[8, 9] as a cheaper alternative for Nafion (the most commonly used expensive PEM) with respect to graphene coverage and membrane thickness for hydrogen fuel cells.

Acknowledgments: Graphene-based membranes (EP/K016946/1) and 2-D materials as the next generation membranes in hydrogen generation and low temperature fuel cells (EP/N013670/1)

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Performance Enhancement Using Different Crystallographic Orientation and Dopant Concentration of MnO_2 for Energy Storage

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Abstract: The catalytic properties and the energy storage capability of the materials depends often on the crystalline phases and presence of dopant incorporated within it. The focus of our study is to comparatively investigate the catalytic properties of different crystal phases of MnO_2 along with the different concentration of dopant within it for electrochemical conversion and storage. Our experimental observation states that the conversion and storage properties varies with the crystal phase of MnO_2. α-MnO_2 exhibits better energy conversion properties whereas δ- MnO_2 shows better energy storage property. The rod shaped α- MnO_2 with tunnel structure exhibits superior bifunctional properties for oxygen reduction and oxygen evolution reaction which is comparable to commercial Pt/C and RuO_2 respectively. On the other hand, 2D layers of δ-MnO_2 shows remarkable properties as supercapacitor (587.23 F/g). We used both the materials for Zn air battery application and for the assembled Zn air battery, δ-MnO_2 shows better performance. Also in this work we will show how presence of different concentration of dopant influences its energy storage property for zinc air battery application.[1]

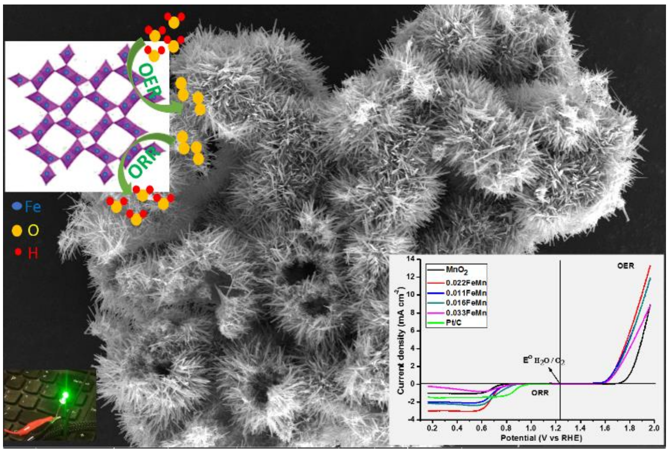

Fig. 1 Fe-doped MnO_2 for Zn-air battery application

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Combined H_2 Production and Battery Storage using a Hybrid Aqueous Flow System

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Abstract: Giving up fossil fuels requires new ways of storing energy. H_2 is often viewed as the ideal sustainable fuel, forming a clean, closed energy cycle with H_2O and electricity. However, dangers exist in both the production and storage of H_2 due to its explosive nature in the presence of O_2. The use of redox mediators to break up water splitting into two separate steps (one which produces O_2 and a second for H_2) provides an inherently safer approach to H_2 production, since the two gases are formed at completely different times and/or places.[1]

Here, this decoupled approach to water splitting is demonstrated on a practical scale, using a dual-cell PEM electrolyser.[2] This system was shown to be able to operate at current densities of over 3 $A\cdot cm^{-2}$, matching the capabilities of the state of the art in PEM water splitting, whilst providing benefits on safety and gas purity. Furthermore, by a simple adjustment to the system, it can also be used as a form of battery storage. This was achieved through using the redox mediator as a negative electrode alongside the O_2/H_2O redox couple as the positive electrode, thereby acting as a hybrid between a redox flow battery and a fuel cell. This device can therefore act as both a H_2 generator and a battery, giving the user a choice of an electrical energy output or a clean, sustainable fuel.

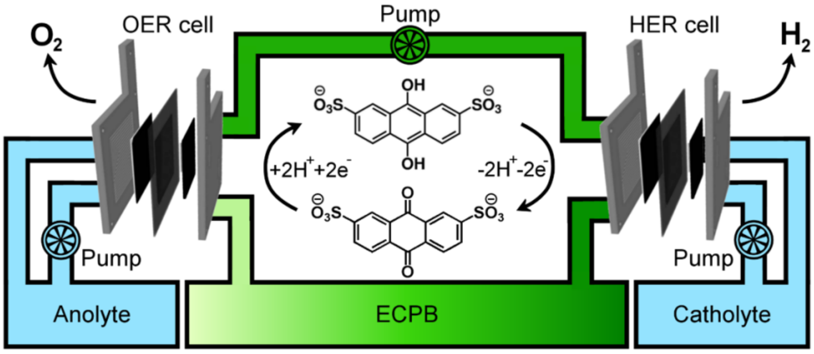

Fig. 1 Schematic representation of the dual-cell PEM electrolyser for decoupled H_2 production from water splitting. The two gas evolution reactions take place at entirely separate times/locations, thanks to the use of a highly reversible redox mediator which is pumped between the two cells.

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Importance of Interfaces in Catalysis

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Abstract: Engineering nanostructures has paramount importance in different fields, particularly in the field of catalysis. Mesoscopic structures of interconnected nanostructures are of great interest in this category. Recently we have identified different molecular junctions of structured nanomaterials where different types of interfaces namely, metal-insulator, metal-semiconductor, and metal-semiconductor-metal are designed and developed [1-3]. These molecular interfaces have interesting catalytic properties, particularly towards the hydrogen evolution reaction (HER).

In the second part, our recent efforts on the transient modification of polycrystalline metallic surfaces towards their engineered heterogeneous electro-catalytic activities will be discussed [4,5]. In one such work, the inherent HER activities of polycrystalline platinum (Pt) and gold (Au) electrodes were altered by different lithium salts. The HER activity of Pt is found to be suppressed by increasing the Li^+ ion concentration while inverse effect is observed in Au, and this is verified in different pH (2−13) conditions and also with different counter-ions (such as Li , Na , ClO_4^-, Cl^-, and bis(trifluoromethanesulfonyl)-imide) ion) [4]. A mechanistic insight is provided for this observed phenomenon, which has paramount importance in other electro-catalytic processes as well, such as carbon dioxide reduction and nitrogen reduction reactions. Following to this, ambient condition electrochemical N_2 reduction is shown with aqueous electrolyte using polycrystalline copper using Li+ ions as supporting. While having these encouraging results, an *in situ* evidence towards the role of Li^+ is lacking and such collaborative opportunities will be discussed at the end of the talk.

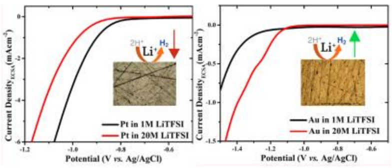

Fig. 1 Engineering the electro-catalytic HER of polycrystalline Pt and Au in different manner using Li^+ ions [4].

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Engineering photoanodes for photoelectrochemical solar water splitting

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Abstract: Photoelectrochemical solar water splitting offers a clean solution to the world energy requirements of a sustainable future. Achieving its full potential depends on developing inexpensive photoanodes that can efficiently evolve oxygen from aqueous electrolytes, the most kinetically demanding step in water splitting. Here I present recent developments we have achieved in the preparation of inexpensive photoanodes: a nanostructured TiO_2 with exposed {0 1 0} facets, an α-Fe_2O_3 self-coated with FeOx electrocatalyst and with an electrodeposited $CoFeO_x$, and a novel all-inorganic halide perovskite $CsPbBr_3$.[1-4] The nanostructured TiO_2 photoanodes are prepared using $Ti_7O_4(OEt)_{20}$ clusters as a precursor and resulting photoanodes show a unique morphology resembling desert roses, pure anatase phase and high exposure of the very active {0 1 0} facet, achieving remarkable ☐100% IPCE efficiency at 350 nm wavelength.[1] α-Fe_2O_3 photoanodes simultaneously coated with FeO_x electrocatalyst are prepared using precursors whose morphology and crystallinity is tuned with lactic acid additive, boosting photoanode photocurrents from 0.32 to 1.39 mA cm^{-2} at 1.23 V_{RHE}.[2] An extended electrochemical characterisation also shows that the charge transfer to electrolyte at α-Fe_2O_3 interfaces can be boosted by an extremely thin layer of $CoFeO_x$, unlike less thin $CoFeO_x$ layers that just reduces surface recombination due to self-oxidation.[3] Finally, all-inorganic halide perovskite $CsPbBr_3$ photoanodes are prepared using carbon as a hole transport layer.[4] This type of semiconductor is revolutionising the field of solar cells due to their high efficiencies and inexpensive preparation but remain practically unexplored in applications using aqueous electrolytes. However, our developed inexpensive carbon layers effectively protect the halide perovskite for more than 30 h directly immersed in water, evolving oxygen with a Faradaic efficiency of 82% and achieving photocurrents above 2 mA cm^{-2} at 1.23 V_{RHE}.

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Opportunities and Challenges in Rational Design of Materials for Renewable Energy

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Abstract: In search for a sustainable supply of fuels and chemicals, development of green and renewable processes is desirable for mitigating climate change. Towards fulfilling this goal, design of nanoscale materials with desirable level of catalytic or electrocatalytic properties, essentially holds the key to success. In our efforts, a bottom-up approach is adopted, wherein quantum mechanical *ab initio* density functional theory (DFT) simulations of reactions occurring on the material surface are guiding the rational design of the catalyst materials. The inherent design ideas vary and depend on the problem at hand. Overall, the *ab initio* level theoretical simulations provide us a mechanistic insight into the reaction, which in-turn offers us an opportunity to engineer the material itself. This is often implemented in experiments by changing the material surface, morphology and the characteristic length scales.

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Electrochemical Processes for a Circular Economy

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Abstract: Electrochemical effluent treatment can provide a route to recover precious and strategic metals such as gold, copper and nickel transforming traditional linear extraction methods to a circular one that can substantially reduce human impact on the environment. These processes employ electrons instead of chemicals and can use renewables as the energy source. Deploying such zero-discharge decarbonised processes rely on an in-depth analysis of thermodynamic and kinetic behaviour of the reaction system. This presentation will examine how chemical thermodynamics, kinetics and reactor design could be optimised to recover metals from industrial effluents. In particular, copper recovery from Tin-Strip waste solutions[1] and plating sludge[2] as well as gold recovery[3] from rinse water from the electronics manufacturers are used as exemplars. Issues arising from differences between simulated conditions and those from industry partners will be elaborated using different reaction models. The Strathclyde research group welcomes collaboration on materials recovery and recycling from other participants.

Fig. 1 Shows the zero discharge alongside green chemistry concepts where no new chemicals are added to the system. Electrochemical processes use electricity as energy source that can be sourced from renewables.

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Metal Oxide Nanoarchitectures as Efficient Catalysts for Electrochemical Oxygen Evolution Reaction

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Abstract: To address the ever-increasing energy demand, electrochemical water splitting has attracted tremendous attention these days for the production of hydrogen as clean fuel avoiding environmental pollution. The role of catalyst for oxygen evolution reaction (OER) cannot be ignored as the kinetics can be modulated not only by choosing the materials with their intrinsic catalytic properties, electronic structure but also by designing the morphology in nanoscale level offering large number of active sites.[1] While the number of active sites is important, easy diffusion of electrolytes and access to the active sites is also crucial for exhibiting high activity. Furthermore, insertion of catalytically active foreign elements enhances the catalytic activity into many folds. Therefore, manipulation of intrinsic properties of material is highly desirable by designing different nanoarchitectures as well as by optimum doping with transition metals.[2] Even though conventional OER catalysts are available; their extensive use in industrial application has been limited due to their expensive nature. Cobalt oxide (Co_3O_4) has been identified as a potential material to be considered as OER catalyst. The effective doping with Mn in Co_3O_4 nanoflakes not only reduces the charge transfer resistance significantly but also improves the OER kinetics, resulting significant enhancement in electrocatalytic activity.[3] The studies indicate that the presence of metallic Mn along with Mn^{2+} species and its subsequent strain generation during Mn doping are responsible for such a remarkable performance. In another attempt, bismuth molybdenum oxide in its different morphologies has been identified as an emerging electrocatalysts other than its well-known photocatalytic activities. The detailed electrocatalytic analysis shows almost two fold enhancement in OER activity compared to bare Ni foam, used as substrate, and also better than conventional RuO_2 or IrO_2. The presentation will discuss about the material, modification of their intrinsic properties and detailed electrochemical analyses in terms of performance parameters, like, overpotential, Tafel slope calculation and EIS characteristics, mass activities etc.

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Hydrogen Economy with Electrochemical Energy Devices

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Abstract: Hydrogen economy is the sustainable production and utilization of hydrogen and shifting to hydrogen economy has the potential to reduce the carbon footprint substantially. The production of hydrogen, the first part of hydrogen economy is typically achieved by electrochemical and photoelectrochemical water splitting reactions. These reactions are energy demanding catalytic reactions and enormous efforts are dedicated across the globe to invent new catalysts and combinations to reduce the overpotential to economically accessible levels. The fact remains that hydrogen production is still an expensive electrochemical reaction and we aim to realize the hydrogen economy in energy devices by tailoring electrochemical interfaces. Fuel generation with concomitant organic synthesis can be induced in energy devices by harvesting the heat of reaction as well as heat from the surroundings. Hydrogen generation as well as utilization or hydrogen economy can be realized in rechargeable batteries by utilizing the proton coupled electron transfer in hydrogen storage molecules.

Tailoring Surface Chemistry of Graphene: Electrochemical and Energy Applications

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Abstract: Graphene materials have displayed tremendous scope for their use in the field of electrochemical and energy applications. Their diverse potential is particularly enhanced when synthesised *via* the graphene oxide (GO) route, which offers immense potential for tailoring the chemical structure by introducing variable levels of oxygen groups allowing the tuning of hydrophilicity, electronic and protonic conductivity, and photo-electrochemistry without significantly affecting mechanical strength. With the tunability of these oxygen functional groups, GO and its reduced/partially reduced variants, make an ideal support for the nucleation and growth of metal nanostructures, tailoring of catalyst properties and even for enhancing water uptake and retention to allow better proton conduction. The graphene-based materials have thus been particularly explored for low temperature Polymer Electrolyte Membrane Fuel Cells (PEMFC) electrocatalysts and more recently in proton conducting membranes. This presentation will provide an overview of my recent work on the use of GO in electrochemical energy devices, from tailoring and boosting of carbon monoxide (CO) tolerance of Pt supported on partially reduced GO to developing GO based composite[1] and multi-layered membranes for PEMFCs[2] to their use for enhancing the sulfur and lithium polysulfide immobilization in lithium-sulfur (Li-S) batteries[3]. The talk will also touch upon i) combining microbial interactions of GO and precious metal reclamation for the development of catalyst-reduced GO systems[4] and ii) partially reduced GO-ceramic composites, and their scope for electrochemical device applications.

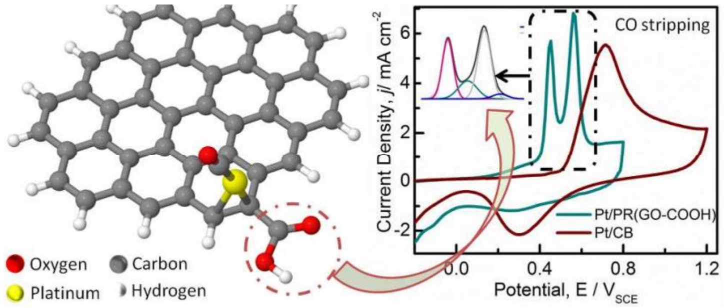

Fig. 1 Most stable configuration from DFT suggesting that -COOH may facilitate Pt nucleation on an edge in its vicinity and further facilitate reduced CO-Pt interactions as shown by CO stripping studies.[1]

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Approaches for Enhanced Photosplitting of Water

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Abstract: The establishment of clean and sustainable hydrogen economy powered by renewable energy sources like solar energy can be one of the most promising approaches. However, the production of hydrogen through water splitting in a photoelectrochemical cell suffers from high overpotential that limits the efficiencies. In this talk, the new attributes of chiral molecules that help in enhancing photosplitting of water by utilizing spin filtering ability offered by chiral molecules, will be presented. The spin selective charge transport through chiral molecule[1,2] modified catalyst favour the parallel alignment of electrons' spin of oxygen atoms during water oxidation that reduces the overpotential required for oxygen evolution and enhanced performance was achieved.[3,4] The talk also discusses how improved selectivity towards water oxidation can be achieved by chiral systems as compared to non-chiral ones.[3] These findings shed new light on our understanding of the underlying mechanism in multiple electron-transfer reactions and pave the way for designing efficient photoelectrochemical cells.

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Electrospun materials for engineering applications

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Abstract: Scaffolds are used in tissue engineering application to support cell attachment and growth. Materials in medical application need to be compatible with surrounding tissues besides its intended function. To achieve this, electrospun scaffold mimicking native human extracellular matrix structure seems to be a viable option. Electrospun scaffolds renders appropriate porosity, fibre dimension and surface area suitable for the new tissue growth. Electrospun polyurethane scaffold supplemented with nickel oxide particles have been experimented for cardiac tissue engineering[1]. It was found to render necessary physiochemical cues and mechanical properties relevant to cardiac tissue engineering. Further, *in vitro* and blood compatibility test promoted their feasibility for the cardiac tissue engineering applications. Field emission scanning electron microscope images of polyurethane and polyurethane decorated with nickel oxide is shown in Figure 1. I am currently looking to advance this product for further trials to steer them as promising candidates. From this workshop, I would love to collaborate with the partners who seek material characterization and testing for medical and other engineering applications. Also, I am keen on learning the use of electrospun products for other engineering applications like air filtration, energy and food packing.

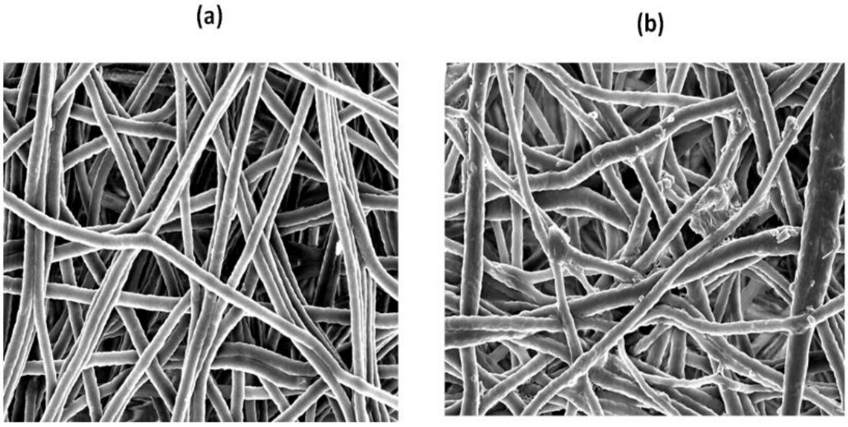

Fig. 1 FESEM image of electrospun (a) polyurethane and (b) polyurethane/nickel oxide fibres

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The life and work of Mohsin Ahmad Bhat

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Nitrogen-doped Carbon Nanofiber Supported MoO2/Ni Composite: An Efficient Catalyst for Green Hydrogen Generation

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Abstract: The depletion of fossil fuel resources, global warming and carbon emission are three major issues of our contemporary society. Although advances in renewable energies reduce our dependency to fossil fuel in power generation, but it necessitates the surplus electricity conversion to chemicals and fuels in an efficient manner. Hydrogen is considered to not only address this issue but also be a promising alternative to replace fossil fuels. Currently fossil fuels are the main sources of hydrogen production which contribute heavily into emission of green house gases. To achieve industrial scale production of high-purity green hydrogen with low cost and zero emission, electrochemical water splitting is an attractive way. So far platinum based family of metals and their alloys are considered as the most active hydrogen evolution reaction (HER) catalysts. However, the scarcity and high cost of Pt limits its application and rises up the cost of the green hydrogen. Therefore, efficient noble-metal-free electrocatalysts are required for the widespread application of electrochemical water splitting. Herein, we synthesized N-doped carbon nano-fiber supported Ni/MoO2 ,NiMoNCNT, (Figure 1) using a hydrothermal method for hydrogen generation with high efficiency and low-overpotential in acid media (figure 2).

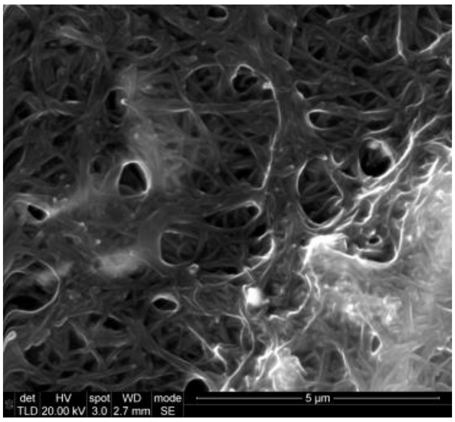

Fig. 1. SEM image of synthesised NiMoNCNT catalyst.

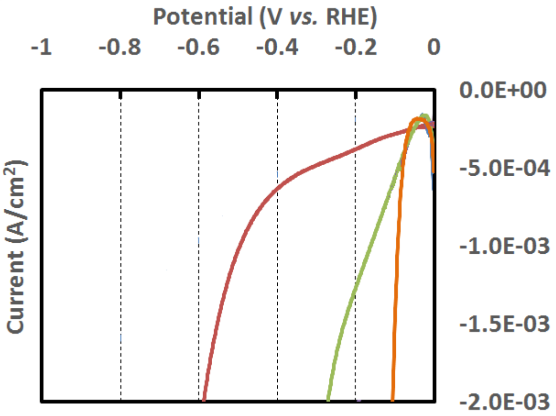

Fig. 2. Linear swept voltammogram of Pt (Orange colour), NiMoNCNT (Green colour) and Ni NCNT(brown colour).

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Recovery of chlorine from waste industrial Hydrochloric acid by electrocatalysis

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Abstract: Chlorine is a highly reactive element, which practically does not exist as Cl_2 naturally and act as a key building element for manufacturing important industrial chemicals and engineering materials. The requirement of chlorine has risen appreciably in the last few decades, owing to its increased demand for healthcare, textile and preparation of chlorine-free products like polyurethanes (PU), polycarbonates (PC) and chlorinated polymers (e.g. PVC) which are produced using chlorine chemistry. The production of these chlorine free material yields HCl and chloride salts as a by-product during the course of their manufacturing. However, this waste HCl can be put to useful end by recovering high purity chlorine gas using an energy efficient electrolysis process, which renders these industrial process sustainable.

Recycling of chlorine from HCl is still challenging due to high cost, inadequate activity and long term instability of noble-metal based catalysts commonly employed for HCl electrolysis. We are extensively working towards design and development a bifunctional electrocatalyst capable of both evolving chlorine and simultaneous oxygen reduction on the cathode under the highly corrosive condition prevalent in HCl electrolysis.

The talk addresses, several strategies pursued to replace noble-metal free electrocatalysts and use of scanning electrochemical microscopy (SECM) for the development of stable catalytic for HCl electrolysis.

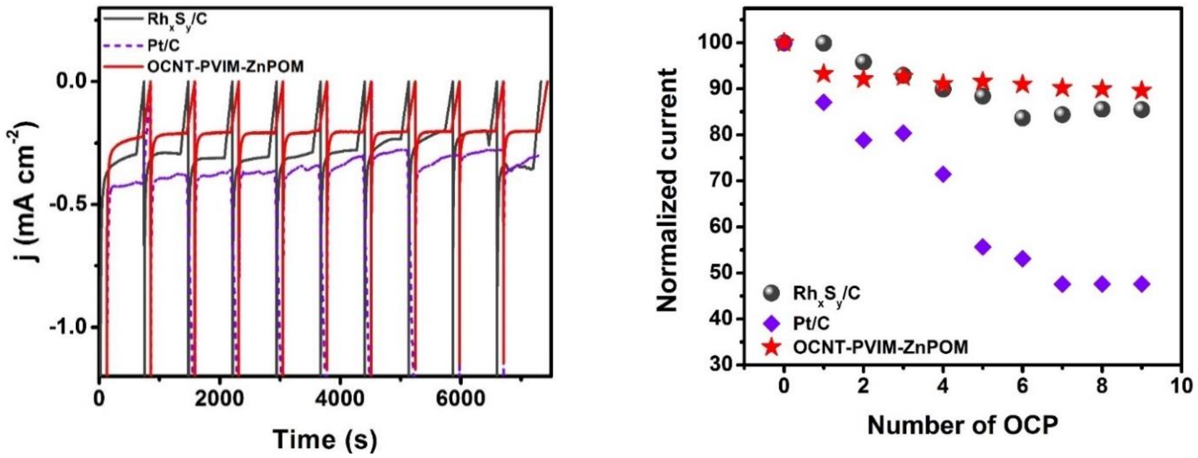

Fig. 1. Electrocatalytic stability test by chronoamperometric experiments of OCNT-PVIM-ZnPOM, RhxSy/C (30%) and Pt/C (20%) catalyst in O_2 saturated 0.4 M HCl electrolyte at a potential of -150 mV with 10 min of operation and 2 min of interruption to open-circuit potential (left); and their normalized current vs. interruption cycles derived from (a). CE: Pt mesh; RE: Ag/AgCl/3 M KCl (right).

Porous materials for catalysis and adsorption

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Abstract: Porous materials are at the heart of heterogeneous catalysis, both as the catalysts and catalyst supports (e.g. zeolites). As the world moves towards more sustainable technologies and feedstocks to ensure a cleaner future, heterogeneous catalysts based on porous materials will have an even bigger role to play. This opens the door to new next generation porous materials such as metal-organic frameworks (MOFs), or even requires looking to the past for the more traditional zeolite based catalysts (concerning their modification and functionalisation) to be redesigned for the new challenges regardless their applications in emerging reactions or more efficient traditional reactions. My research group focuses specifically on the development and characterisation of porous materials, ranging from microporous zeolites/MOFs, through zeolites and carbons with mesoporosity, to macroporous cellular foams, for gas adsorption and catalytic applications. Recently, we have developed the invention of novel post-synthesis microwave-assisted modification protocols (MWAC) for producing zeolites (e.g. FAU Y and MFI ZSM-5) with tunable physical and chemical properties (e.g. mesoporosity), more importantly, significantly reduced energy and cost.[1] The resultant zeolites are intrinsically sustainable and should find applications at electrochemical interfaces, utilising their size/shape selectivity combined with the improved accessibility, ion exchange capacity and catalytic properties of both intrinsic and extrinsic sites of zeolites.

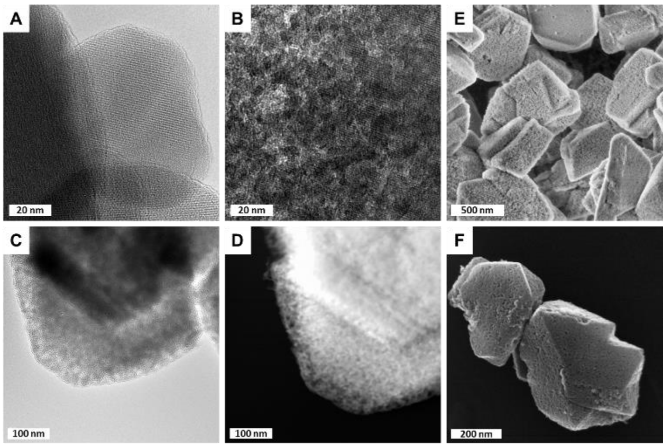

Fig. 1 S/TEM (A-D), low voltage SEM (E) and GFIS-FIB electron imaging of the developed hierarchical FAU Y zeolites.

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Metal Oxide-based Composite Nanostructures for Supercapacitor and Water Splitting Applications

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Abstract: Today, energy crisis due to depleting fossil fuel supply and their negative impact on environment like global warming is probably the world's biggest problem. Efforts have been made to develop abundant, inexpensive and environment friendly renewable resources of energy among which water splitting using solar light is considered as one of the most potential approach. Besides, the need for the technologies related to energy storage devices is also high on demand. Especially, flexible, light weight energy storage devices have emerged as the most promising devices and becoming more and more popular because of their high-performance, non-flammability, non-toxicity, and easier device fabrication techniques. In the present talk, I shall discuss about our recent research activities related to the metal oxide based composite nanostructures for electrochemical and photo-electrochemical water splitting and electrochemical supercapacitor applications. Particularly, I shall focus on electro-spun one-dimensional carbon nanostructure-metal oxide based composites for electrochemical supercapacitor applications. The fabricated electrode shows much higher specific capacitance, an excellent cyclic stability.

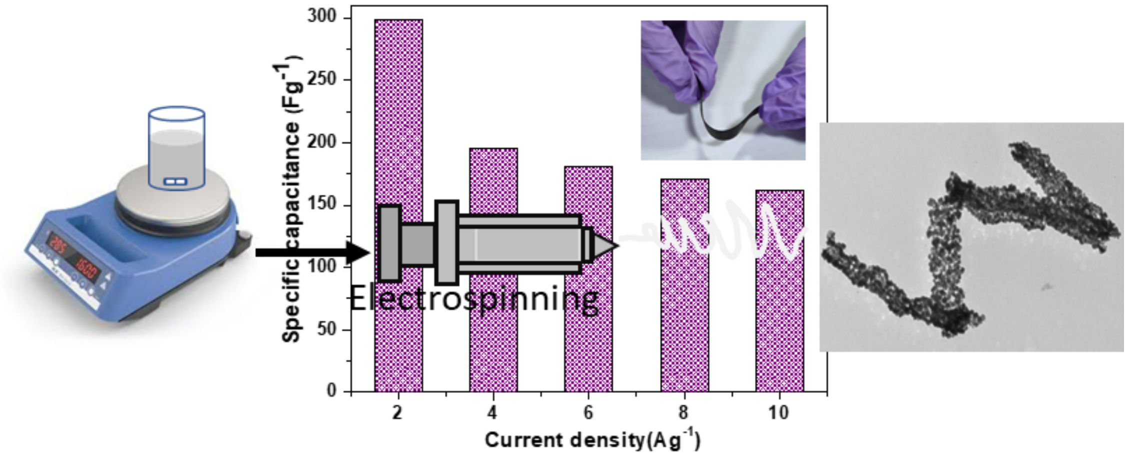

Fig. 1 Electrospun metal oxide composites for flexible, high performance electrochemical supercapacitor.

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Electrochemical Reduction of CO_2 on Gold Surfaces – a Structure-Sensitivity Study

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The electrocatalytic reduction of CO_2 to CO and syngas, which underpin multi-million tons scale chemical processes, and it is a promising strategy to electrify the chemical industry. Gold is the most active electrocatalysts capable to produce CO at low overpotentials and with excellent selectivity.[1] Many strategies, such as nanostructuring[2] and grafting with organic ligands, have been proposed to further enhance its performance. However, the fundamental knowledge of how the atomistic structure of the catalyst surface influences reaction rates and selectivity remains a very important missing fundamental insight. In the first part of the talk I will present a recent work where we experimentally established – for the first time – that atomic steps and undercoordinated sites control the activity of Au for CO_2 reduction.[3] We performed a thorough experimental investigation of gold single crystals having well-defined surface orientations. Low-index single crystals, such as (111), (100) and (110), were compared to a steps-rich (211) surface. The electrochemical reduction of CO_2 to CO was found to exhibit a pronounced structure sensitivity: the CO partial current density registered with the most active catalysts (i.e., (110) and (211)) is ca. 20-fold higher than the one measured with Au (100), see Figure 1. We further established the dominance of steps by selective poisoning experiments. These findings offer elements to optimize the theoretical description of the electrochemical interface and reaction kinetics, which in turn may strengthen the prediction accuracy of future screening investigations. In the second part of the talk I will shortly summarize my research vision for CO_2 electroreduction (and beyond) and I will identify areas where possible collaborations can be established.

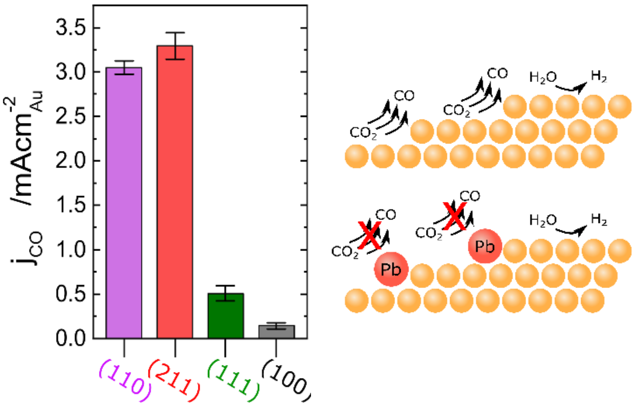

Figure 1. (left) CO partial current densities measured with Au single crystals in CO_2 sat. 0.1 M $KHCO_3$ at -0.6 V_{RHE}. (right) schematic representation of the Pb poisoning experiments.

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