



Electrochem

2021

Abstracts Booklet

Welcome from the Organising Committee

Welcome to Electrochem2021!

This year, Electrochem will be held entirely online and will be a single symposium event spread over two 3.5-hour sessions. In the first session, we will have the award lectures for the 2020 Faraday and 2020 Geoffrey Barker medals, as well as prize-winning student speakers from the RSC regional electrochemistry conferences and the 2020 Sheelagh Campbell award. In the second session, there will be further prize-winning student talks alongside the 2021 Faraday and Roger Parsons medal lectures, the 2021 Sheelagh Campbell award lecture and the 2021 Martin Fleischmann lecture. These talks will be supported by a Twitter poster session that is open to all comers (see information at the end of this booklet). So we have a packed schedule of electrochemistry planned!

Electrochem will be free to “attend” this year, although registration is required and we encourage you to register early to avoid disappointment.

You can register through our RSC Events webpage or using this link:

<https://register.gotowebinar.com/register/3887238012735915533>

We are very grateful both to the RSC and also to our generous sponsors (see next page) for their contributions, which have allowed us to make this event free to all and to provide poster prizes.

Finally, we would like to thank you for participating and supporting Electrochem2021. We hope you enjoy the conference!

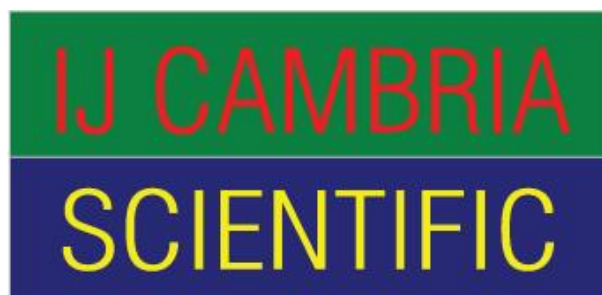
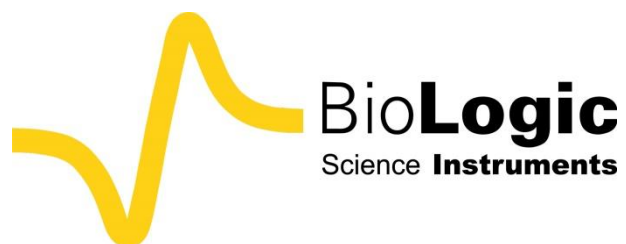
Mark Symes (University of Glasgow)

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Schedule – all times are British Summer Time

Day 1 (Monday 6th September)

13:30-13:35	Opening remarks
13:35 -14:25	2020 Barker medal and lecture - Julie Macpherson
14:25-14:40	Student regional award winner 1 - Rajesh Jethwa
14:40-14:55	Student regional award winner 2 - Franziska Boessl
14:55-15:20	2020 Sheelagh Campbell lecture - Virgil Andrei
15:20-15:55	Break
15:55-16:10	Student regional award winner 3 - Laurence Savignac
16:10-17:00	2020 Faraday medal and lecture - Shirley Meng

Day 2 (Tuesday 7th September)

13:30-13:35	Opening remarks
13:35 -14:25	Fleischmann lecture - Hubert Girault
14:25-14:55	2021 Parsons medal and lecture - Max Garcia Melchor
14:55-15:20	2021 Sheelagh Campbell lecture - Alfie Wills
15:20-15:40	Break
15:40-15:55	Student regional award winner 4 - Eric Mates Torres
15:55-16:10	Student regional award winner 5 - Matt Leech
16:10-17:00	2021 Faraday medal and lecture - Peter Strasser

Barker Medal 2020: Julie Macpherson

RSC Electrochemistry Group Geoffrey Barker Award Talk

Julie V. Macpherson

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Abstract: In this award talk, rather than focus on one research topic I will highlight the many different research avenues I have explored during my career, and the common themes that connect them. Some of the areas of research have been through choice and some very much due to serendipity. I will also reflect on both the fundamental and applied nature of the work and the many benefits to be gained by working collaboratively with academics and industrialists alike. I will highlight some of my favourite research findings and their importance in their field of electrochemistry, materials science and sensor development. I will also discuss the importance of electrochemical education. Topics covered by the talk will include high resolution electrochemical imaging (both probe development and application), carbon materials for use as electrochemical sensors, pulsed voltammetric methods of sensing (in homage to Geoffrey Barker), new electroanalysis techniques and single atom electrodeposition. As there are too many to list, I thank here all the amazing people in my group I have had the good fortune to work with over my career. Without them none of this would have been possible.

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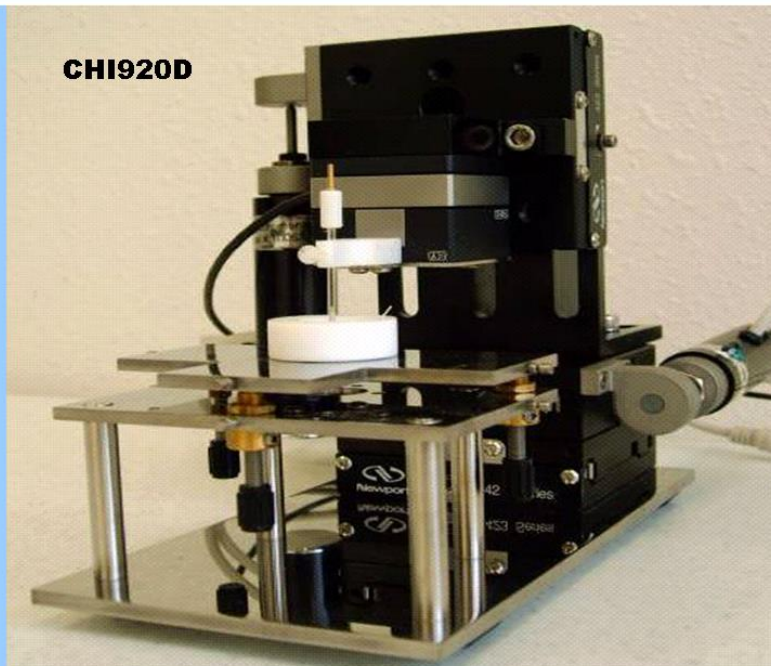
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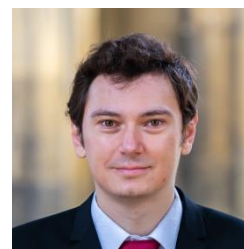
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Sheelagh Campbell Award 2020: Virgil Andrei

Photoelectrochemical Perovskite-BiVO₄ Tandem Devices for Selective CO₂ Reduction

Virgil Andrei

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Abstract: Photoelectrochemical (PEC) devices enable the light-driven conversion of small molecules like water and CO₂ into higher-value chemicals (e.g. H₂, CO). However, the photoelectrochemical CO₂ reduction remains limited by the high overpotential, low selectivity and cost of commonly employed catalysts. Here, we address those challenges by interfacing lead halide perovskite PEC devices¹ with an earth abundant molecular cobalt catalyst.² The interplay between faradaic yields, product amounts, mass transport limitations and selectivity is revealed by altering the catalyst loading, applied potential and light intensity, whereas empirical fitting of the electrochemical data helps clarify the optimal electrode selectivity at low catalyst loadings. Perovskite photocathodes employing the cobalt porphyrin catalyst maintain selective aqueous CO₂ reduction for one day at light intensities as low as 0.1 sun, providing potential pathways for maximizing daylight utilisation. The corresponding perovskite-BiVO₄ PEC tandems sustain an unprecedented bias-free syngas production for three days, operating as standalone artificial leaves in neutral pH solution. A rational design of the device structure can lead to a further increase in the device stability³ and CO₂ reduction selectivity.⁴ The overall findings are applicable to a wide range of PEC systems, with the ultimate goal of contributing towards a circular carbon economy via photoelectrocatalysis.

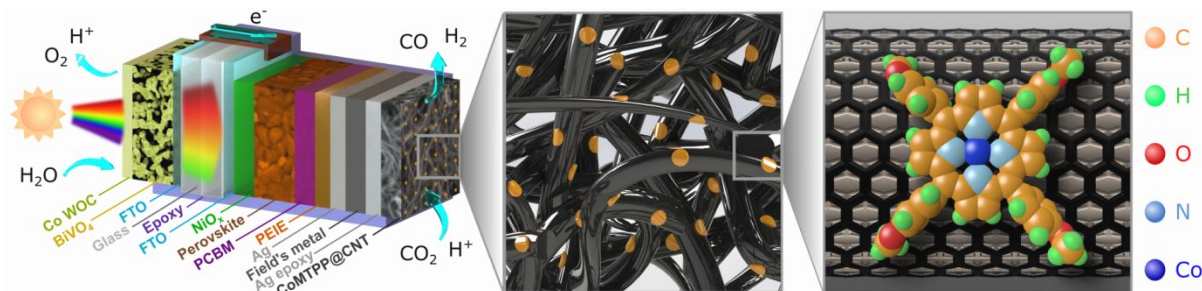


Fig. 1 Artificial leaf for syngas production: left – device structure, centre – porous CNT support, right – molecular catalyst immobilisation.

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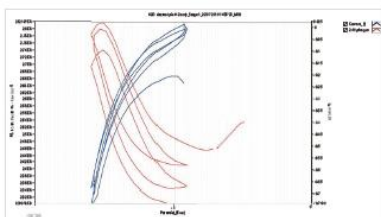


Instruments for Advanced Science

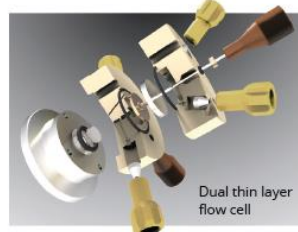
HPR-40 DEMS

A compact mass spectrometer system for analysis of dissolved species in electrochemistry, DEMS.

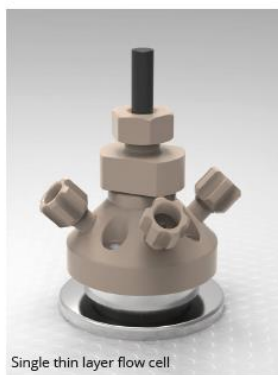
- ▶ The system is modular and adaptable, and offered with user interchangeable sampling inlets compatible with most common electrochemical cells, Redox.me and EL-CELL® for example.
- ▶ Two differential electrochemical mass spectrometry 'DEMS' cell inlets, designed for material/catalysis studies, are included as standard.
- ▶ EGAssoft – evolved gas analysis software provides for synchronous data acquisition with a coupled potentiostat, together with powerful graphical user interface.
- ▶ Mass range 200 amu is standard, a high sensitivity dual Faraday/ electron multiplier detector included.
- ▶ Data acquisition speed > 650 measurements /second.



DEMS data showing H₂ data from H₂O electrolysis in EGAssoft with I/V data from potentiostat.



Dual thin layer flow cell



Single thin layer flow cell



Faraday Medal 2020: Shirley Meng

Advanced Characterization of Electrochemical Materials and Interfaces for Better Batteries

Y. Shirley Meng

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Abstract: Lithium (Li) metal has been considered as an ideal anode for high-energy rechargeable Li batteries while Li nucleation and growth at the nano scale remains mysterious as to achieving reversible stripping and deposition. A few decades of research have been dedicated to this topic and we have seen breakthroughs in novel electrolytes in the last few years, where the efficiency of lithium deposition is exceeding 99.6%¹. Here, cryogenic-transmission electron microscopy (Cryo-TEM/Cryo-FIB) was used to reveal the evolving nanostructure of Li deposits at various transient states in the nucleation and growth process, in which a disorder-order phase transition was observed as a function of current density and deposition time. More importantly, the complementary techniques such as titration gas chromatography (TGC) reveals the important insights about the phase fraction of solid electrolyte interphases (SEI) and electrochemical deposited Li (EDLi). While cryo-EM has made significant contributions to enabling lithium metal anodes for batteries, its applications in the area of electrochemical interphases such as those in solid state batteries, beyond lithium batteries are still in the infancy, therefore, I will discuss a few new perspectives about how future advanced imaging and spectroscopic techniques can help to accelerate the innovation of novel energy storage materials and architectures.

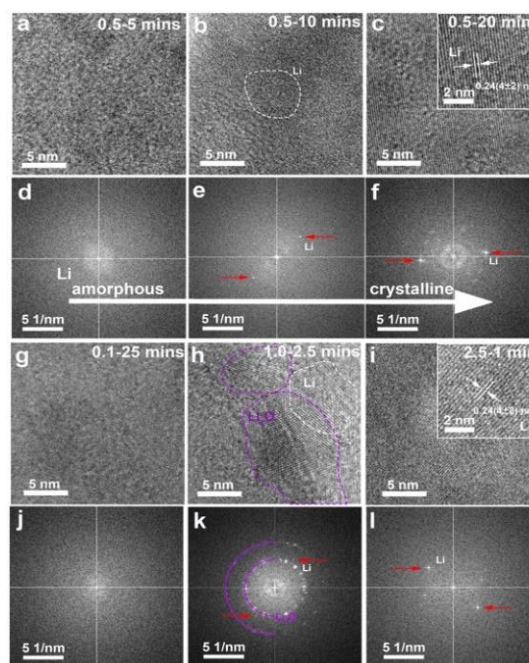


Fig. 1 Nanostructure evolution of Li deposit as a function of deposition time and current density. (from Ref. 2)

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Fleischmann Lecture: Hubert Girault

Polarised interfaces:

From ionosomes to water splitting

Hubert H. Girault

Laboratory of Physical and Analytical Electrochemistry

Ecole Polytechnique Fédérale de Lausanne – Switzerland.

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Abstract: A reaction is defined as electrochemical if its Gibbs energy depends on a potential difference. Hence, it is of fundamental importance to apprehend the potential distribution and the charge distribution at interfaces. Beyond the classical Gouy-Chapman model, the presence of a discrete charge distribution, especially at molecular or biointerfaces, influences the polarisation. We shall first discuss the so-called “Discrete Helmholtz model” [1] and related charge transfer reactions, and then present the ionosomes which are nanosized water droplets stabilised by an ionic bilayer [2].

We shall then discuss water splitting using two approaches:

- Using a Vanadium-Manganese Redox Flow Battery and redox electrocatalysis
- Using a molecular biphasic photosystem based on tetrathiafulvalene assemblies.

References

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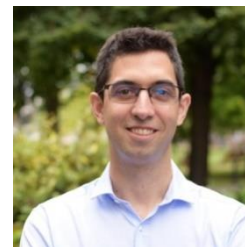
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Parsons Medal 2021: Max García-Melchor

Computational Rational Design to Drive Discovery in Molecular Water Oxidation Catalysis



Dr. Max García-Melchor

School of Chemistry, CRANN and AMBER Research Centres, Trinity College
Dublin, College Green, Dublin 2, Ireland.
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Abstract: Although fossil fuels have brought forth the dawn of civilization as we know it, they have also left an enduring effect on the Earth's climate. To address this, it is imperative that we devise energy storage and conversion technologies using renewable energy sources to establish a carbon-neutral energy cycle. For example, one could envision using sunlight to drive photoelectrochemical water splitting devices to produce hydrogen, a highly energy-dense fuel when compressed and stored. A major roadblock in realizing this, however, is the lack of highly efficient and cost-effective catalysts for the oxygen evolution reaction (OER).^{1,2}

In this talk, I will present our recent advances towards the accelerated rational design of molecular OER catalysts. Firstly, I will present our theoretical findings³ which demonstrate that molecular complexes obey the same OER scaling relations observed for heterogeneous systems. Yet, we have identified a mechanism by which the most active homogeneous catalysts seem to circumvent the “overpotential wall” of 370 mV imposed by scaling relations,^{4,5} opening a promising avenue for the design of “ideal” molecular OER catalysts.

In the second part of my talk, I will present a set of design principles that we put forward using the above insights and their application for the high-throughput screening of over 400 molecular OER catalysts using well-known ligand scaffolds and six different transition metals (Cr, Mn, Fe, Ru, Co, and Ni).⁶ Importantly, this screening has led to the discovery of 17 complexes with a predicted overpotential within 300 mV, of which 14 are based only on abundant and non-critical elements. After filtering these catalysts on the basis of refined design principles incorporating pH-dependence, we have identified 3 novel Cr-based systems as promising OER catalysts for experimental realization. In addition, using this dataset, we have very recently developed a machine learning algorithm that allows the prediction of the OER activity at almost no computational cost and with a mean absolute error of 0.10 eV. These investigations are expected to contribute to advancing the development of commercial water splitting technologies.

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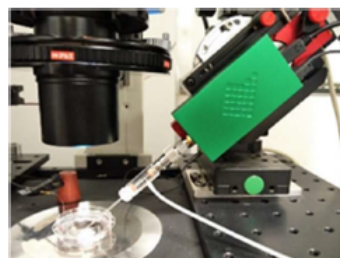
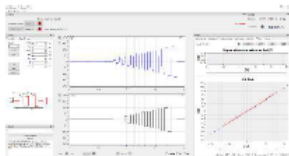


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Sheelagh Campbell Award 2021: Alfie Wills

Switching Sides? A case study on the use of alternating potential electrolysis in synthetic organic electrochemistry

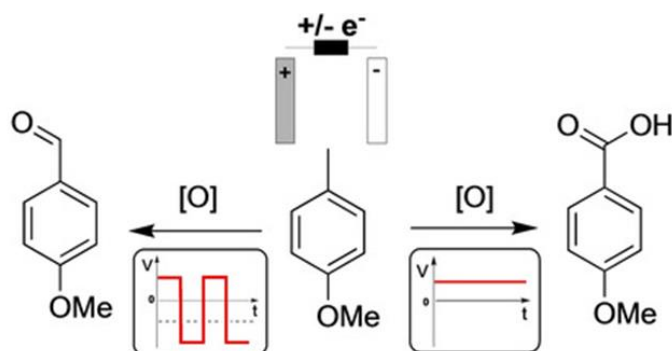


Alfie Wills^{1,2}

¹Medicinal Chemistry, GSK, Stevenage, ²Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow
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Abstract: Synthetic organic electrochemistry has experienced a resurgence in recent years as it enables access to unique reactivity that is more environmentally benign than traditional chemical synthesis.^{1,2} However, the widespread adoption of electrochemistry has been slowed by the requirement for specialist equipment, as well as concerns over reproducibility.³ The IKA ElectraSyn 2.0 is a standardised electrochemistry set-up that has been developed to combat these issues by providing a more accessible alternative to a potentiostat and external cell for organic electrosynthesis.

The IKA ElectraSyn 2.0 has a function that periodically alternates the potential. This is generally used to prevent fouling and passivation of the electrodes during electrolysis.⁴ Whilst investigating the electrochemical oxidation of benzylic methyl groups, the use of this function inverted the selectivity for aldehyde and carboxylic acid products. Further study revealed an unexpected mode of action that leads to an uncontrolled increase in anodic potential.⁵ The mode of action for the alternating potential function is described and the mechanism by which it causes the observed change in selectivity is proposed. Because one of the principle advantages of electrochemistry is the ability to precisely control the oxidative or reductive potential of a transformation, this study holds important information for all users of the IKA ElectraSyn 2.0.



**Constant or alternating current?
Mechanisms?
Implications for organic electrochemistry?**

References

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Faraday Medal 2021: Peter Strasser

The Electrocatalytic Dark Side of Solar Fuels and Solar Chemicals

Peter Strasser

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Abstract: The rising share of renewable electricity is testament to the increasing importance of solar-electric routes – largely photo-absorption or Faradaic induction - to harvest sun light directly or indirectly in form of potential differences and free electrons. While some electricity is used directly or stored capacitively, an increasing portion calls for direct conversion into valuable molecular solar fuels or chemicals. This conversion in the dark is made possible by heterogeneous electrocatalysis on the surface of solid electrodes. Electrocatalysis at the electrode surface orchestrates the stepwise making or breaking of molecular chemical bonds by means of electronic charge transfer across the electrified solid electrode/electrolyte interface. Kinetic barriers of elementary reaction steps – associated with suboptimal chemisorption or stabilization of intermediates - control the efficiency of the overall reaction process. Fundamental understanding of the origin of the kinetic barriers arising along the reaction coordinate aids in the design of more efficient, tailor-made electrochemical interfaces.

In this presentation, I will report on recent advances in our understanding of “dark” electrocatalytic materials, interfaces and mechanisms relevant to the conversion of solar energy into value-added molecular compounds, using in-situ/operando X-ray spectroscopic, microscopic, scattering or spectrometric techniques. Examples include the electrochemistry of small molecules as they occur in low-temperature water- and CO₂ electrolyzers, electrosynthetic processes, as well as low-temperature PEM fuel cells.

Twitter poster session details

The poster competition for Electrochem 2021 will take place on Twitter. The Poster competition will begin the day before the conference starts (5th of Sept 2021) and will last for approximately 48 hours. This is to allow for discussion over twitter and to accommodate the time differences of the conference attendees from all over the globe.

There are prizes for the Twitter Poster competition (thanks to our sponsors!), and the winners of these prizes will be announced at the closing of the conference on the 7th of September.

How to participate:

- No need to send an abstract. All posters welcome from everyone.
- Prepare your poster and upload to Twitter from 2 pm (GMT/London time) on the 5th of September 2021 (you will need a twitter account to participate).
- In the tweet, please include the **title of the poster**, the hashtag **#Electrochem21Poster** and include the twitter handle **@RSCElectrochem**. The RSC Electrochemistry committee will retweet your post for maximum exposure once the @RSCElectrochem handle is added. Feel free to add any other information, hashtags and twitter handles to your tweet.
- During the conference, answer questions asked by the community posted on your poster tweet and interact with other posters by asking questions. The judges of the poster competition could be anyone, much like in a person-to-person poster competition.