

University of
St Andrews

The 7th Meeting of the Energy Materials Discovery Characterisation and Application Group 2022



3rd—5th May 2022

Ben Wyvis Strathmore Hotel

Strathpeffer

Program

3rd May 2022

12:00-13:00

Lunch

Session A: Exsolution (Jair G. Triana-Pequeno)

Time	Speaker	Title
13:00-13:05	John T. S. Irvine	Welcome and Opening Remarks
13:05-13:50	Brian Rosen Tel Aviv University	Co-exsolution of unalloyed metals and multiphase particles
13:50-14:10	Shreyasi Chattopadhyay	Exsolution of Transition Metal Nanoparticles Towards Multifunctional Electrocatalyst for Alkaline Water Electrolysis
14:10-14:30	Selda Ozkan	Noble - transition metal exsolved perovskite oxides and their activity for oxygen reduction reaction
14:30-14:50	Shangshang Zuo	Cobalt doped $\text{La}_x\text{Ca}_{0.9-x}\text{Ti}_{1-y}\text{Co}_y\text{O}_3$ perovskites for OER
14:50-15:20	<i>Coffee Break</i>	
Session B: Batteries (Chair: Atia Azad)		
15:30-15:50	Matthew H. Friskey	Investigations into Cobalt-Doped Manganese Niobate as a Battery Material
15:50-16:10	Chinnasamy Murugesan	Addressing the initial coulombic inefficiency of SnP_2O_7 negative electrode material for Na-ion batteries
16:10-16:30	Abhinav Tripathi	Sn based negatives for Na-ion batteries
16:30-16:50	Shuoshuo Zhang	Study on Improving Resistance of Silicon Carbide Elements to Degradation During Lithium Battery Materials Formation
16:50-17:10	Xin Chen	Future Positive Electrode Materials for Potassium Ion Batteries
Poster Session I (Flash presentations: 5 min)		
17:10-17:30	Roxana N. Murgu	Understanding the crystal chemistry of phosphate cathode materials
	Andrea Veronese	Integrated biomass gasification catalyst and support for tubular SOFCs: Synthesis and forming by extrusion
	Hong Zhang	Photocatalytic Degradation of Methyl Orange by Ag Modified $\text{La}_2\text{Ti}_2\text{O}_7$
	Xiaoxia Yang	Enhancing electrocatalytic CO_2 reduction in solid oxide electrolysis cell with LCTM-based cathode
17:30-19:30	<i>Free time</i>	
19:30-20:30	<i>Dinner</i>	
20:30-21:30	<i>Pub Quiz</i>	

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7:30-9:00 <i>Breakfast</i>		
Session C: Solid-State Batteries (Chair: Katy Bateman)		
Time	Speaker	Title
9:00-09:45	Venkataraman Thangadurai University of Calgary	Materials for solid state batteries and solid oxide fuel cells
09:45-10:05	Mihkel Vestli	$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ – electrolyte for solid state Li-ion battery
10:05-10:25	Cameron Bathgate	Optimising the interface of solid-state oxide batteries
10:25-10:55	<i>Coffee Break</i>	
10:55-11:15	Zipei Wan	The study of $\text{Li}_{7-x}\text{La}_3\text{Ce}_{2-x}\text{Ta}_x\text{O}_{12}$ garnet solid-state electrolyte
11:15-11:35	Ioanna Maria Pateli	Microscopical and spectroscopical investigation of the stability of garnet Ta/Nb doped $\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}/\text{Nb}_{0.6}\text{O}_{12}$ electrolyte
11:35-11:55	Colm Boyle	Ca-doped LiYO_2 as a Solid State Electrolyte Candidate
12:00-13:00	<i>Lunch</i>	
Session D: Catalysis and Photocatalysis (Chair: Nouxi Zhang)		
13:00-13:20	Aida Fuente Cuesta	Turquoise Hydrogen – An Exploration of Catalysts for Methane Pyrolysis
13:20-13:40	Chayopas Tupberg	Integrating Photoelectrochemical Charging into Lithium Batteries for Use as a Single Multifunctional Device
13:40-14:00	Nikoletta Gkoulemani	Reactor development for photocatalytic applications
14:20-14:20	Yuan Liao	Doped strontium niobate titanates $\text{Sr}_m\text{Ti}_x\text{Nb}_{1-x}\text{Cr}_{1-x}\text{O}_{3-6}$ ($m \leq 1$) for photocatalytic hydrogen production
14:20-14:40	Mengyuan Guo	Research on bio-mass ashes collected from the Eden campus boiler
14:40-14:55	<i>Group Photograph</i>	
15:00-15:30	<i>Coffee Break</i>	
Poster Session II (Flash presentations: 5 min)		
15:30-16:00	Minjian Ma	Development of $(\text{PrBa})_{1.8}\text{Fe}_{2-x}\text{Ti}_x\text{O}_{5+6}$ perovskite anodes for direct carbon fuel cells with waste as the fuel
	Andrea Paris	New hybrid bismuth halide perovskites for photovoltaic applications
	SeoJim Kim	Characterising $(\text{La},\text{Sr})(\text{Ni},\text{Ti})\text{O}_3$ perovskite oxide with EDS and WDS analysis.
	Yuri Hirano	Bismuth Halide Materials for Photovoltaic Applications
	Chengzhi Sun	Probing oxygen vacancy effect on oxygen reduction reaction of the $\text{NdBaCo}_2\text{O}_{5+6}$ cathode for solid oxide fuel cells
	Josin Jose	Scale- up of Thermal Batteries for flight applications
16:30-18:30	<i>Walk to Touchstone Maze/Blackmuir Wood</i>	
18:30-19:30	<i>Free time</i>	
19:30-20:30	<i>Dinner</i>	
20:30-22:00	<i>Explore Town</i>	

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7:30-9:00	<i>Breakfast</i>	
Session E: Solid Oxide Cells (Chair: Nouxi Zhang)		
Time	Speaker	Title
9:00-9:45	John Hansen Haldor Topsoe	Power to X from a Topsoe perspective
9:45-10:05	Kamil Nowicki	Direct Ammonia Protonic Solid Oxide Fuel Cell
10:05-10:25	Xuefa Xia	An electrochemical membrane reactor for reaction-separation coupling: to produce pure hydrogen
10:25-10:45	Xiaoqiang Zhang	Investigation of microstructure impact on SOFC using CFD simulation
10:45-11:05	Xinyu Liu	Waste to energy direct carbon fuel cell development with lanthanum strontium calcium titanate based anode
11:05-11:15	<i>Winning Poster Announcement</i>	
11:15-11:30	John T. S. Irvine	Concluding Remarks
12:00-13:00	<i>Lunch</i>	
13:00	<i>Departure</i>	

Posters	
Speaker	Title
Roxana N. Murgu	Understanding the crystal chemistry of phosphate cathode materials
Andrea Veronese	Integrated biomass gasification catalyst and support for tubular SOFCs: Synthesis and forming by extrusion
Hong Zhang	Photocatalytic Degradation of Methyl Orange by Ag Modified $\text{La}_2\text{Ti}_2\text{O}_7$
Xiaoxia Yang	Enhancing electrocatalytic CO_2 reduction in solid oxide electrolysis cell with LCTM-based cathode
Minjian Ma	Development of $(\text{PrBa})_{1.8}\text{Fe}_{2-x}\text{Ti}_x\text{O}_{5+\delta}$ perovskite anodes for direct carbon fuel cells with waste as the fuel
Andrea Paris	New hybrid bismuth halide perovskites for photovoltaic applications
SeoJim Kim	Characterising $(\text{La,Sr})(\text{Ni,Ti})\text{O}_3$ perovskite oxide with EDS and WDS analysis.
Yuri Hirano	Bismuth Halide Materials for Photovoltaic Applications
Chengzhi Sun	Probing oxygen vacancy effect on oxygen reduction reaction of the $\text{NdBaCo}_2\text{O}_{5+\delta}$ cathode for solid oxide fuel cells
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Exsolution

**Exsolution of Transition Metal Nanoparticles Towards Multifunctional
Electrocatalyst for Alkaline Water Electrolysis**

Shreyasi Chattopadhyay¹, John Irvine¹

¹*School of Chemistry, University of St Andrews, Scotland, UK*

Abstract: The ever-increasing demand of global energy consumption associated with the depletion of fossil fuel and environmental challenges have stimulated the research on renewable green energy conversion technologies. Recently, low-temperature alkaline water electrolysis for oxygen evolution reaction (OER), oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER) is grabbing significant interest as a green, environmentally friendly way leading to a sustainable energy cycle with zero carbon emission. With this view, exsolution of transition metal nanoparticles on doped lanthanum strontium titanate has been attempted to design efficient low-cost electrocatalyst with multifunctional activity.

**Noble - transition metal exsolved perovskite oxides and their activity for
oxygen reduction reaction**

Selda Ozkan¹, John T. S. Irvine¹

¹*School of Chemistry, University of St Andrews, St Andrews KY16 9ST, United Kingdoms*

Abstract: The main challenges with the catalysts used for low-temperature fuel cell applications are poor stability of carbon supports, weak catalyst-carbon support interaction, high cost and poor utilization of noble metals that are prepared by conventional deposition techniques. Here, we report the exsolution of transition and noble metal nanoparticles (Ni, Co, Fe, Pt, Ru) from perovskite oxides and assess them for low-temperature fuel cell applications, particularly for oxygen reduction and oxygen evolution reactions. The embedded nanoparticles obtained by exsolution process renders strong catalyst-support interaction, enhanced stability, and good control over the amount of catalyst loading.

Cobalt doped $\text{La}_x\text{Ca}_{0.9-x}\text{Ti}_{1-y}\text{Co}_y\text{O}_3$ perovskites for OER

Shangshang Zuo¹, John Irvine¹

¹*School of Chemistry, University of St Andrews, St Andrews KY16 9ST, United Kingdoms*

Abstract: A series of cobalt doped $\text{La}_x\text{Ca}_{0.9-x}\text{Ti}_{1-y}\text{Co}_y\text{O}_3$ perovskites have been synthesised by the sol-gel method. Their structures have been investigated by the PXRD and SEM. Their OER catalytic performance have been researched on a three-electrode setup by LSV, CV, EIS, etc.

To further enhance their OER performance, they have been reduced in a tubular furnace with 5% H_2/Ar atmosphere at a series of temperatures and times. Co nanoparticles anchored on the perovskite surface have been successfully prepared by this procedure. LSV and tafel slope show that Co exsolved perovskite exhibit significant improvement of the OER activity.

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Batteries

Investigations into Cobalt-Doped Manganese Niobate as a Battery Material

Matthew H. Friskey, Julia L. Payne

Abstract: Developing materials to improve the performance of energy storage devices is essential as new technology demands better capacities, lifetimes, and power. Columbite materials ($M\text{Nb}_2\text{O}_6$ where M = transition metals) have been studied for their photocatalytic and magnetic properties but more recently have gained interest as potential electrode materials in batteries and supercapacitors.¹ Through a simple solid-state synthesis phase-pure MnNb_2O_6 has been produced.² A series of samples with the composition $\text{Mn}_{1-x}\text{Co}_x\text{Nb}_2\text{O}_6$ have been prepared. Electrochemical characterisation is currently underway, in order to investigate the optimal voltage operating window for these materials in order to obtain both good capacities and cycle life.

References

- G. Yang, X. Zhao, F. Liao, Q. Cheng, L. Mao, H. Fa, and L. Chen, *Sustainable Energy Fuels*, 2021, **5**, 3039
F. Garcia-Alvarado, A. Orera, J. Canales-Vazquez and J. T. S. Irvine, *Chem. Mater.*, 2006, **18**, 3827-3834

Addressing the initial coulombic inefficiency of SnP_2O_7 negative electrode material for Na-ion batteries

Chinnasamy Murugesan¹, Abhinav Tripathi, Robert Armstrong, John T. S. Irvine¹

¹School School of Chemistry, University of St Andrews, SCOTLAND, KY16 9ST
*cm465@st-andrews.ac.uk

Abstract: Tin compounds have superior electrochemical properties in terms of energy density when used as negatives in a Na-ion battery. Their cost and environmental benignity makes them even more attractive. However, they offer low initial coulombic efficiency (ICE) of ~50% in the first cycle, leading to the wastage of more than 50% positive electrode capacity in a full cell. To address this issue, presodiation is considered to be an effective method that can be achieved in a few ways, such as i) pre-charging and discharging half cells and making full cells ii) proper selection of electrolyte with additives (sacrificial salts) iii) surface modification iv) adding extra Na to compensate for the loss iv) chemical presodiation methods. Among all presodiation methods, using organic reagents with low redox potential such as Na-Biphenyl, Na-Naphthalene was found to be the most suitable method. Since this composition is liquid, it penetrates homogeneously throughout the electrode surface, enabling uniform presodiation of the electrode surface, which improves the initial coulombic efficiency by over 90%. Also, the handling of such chemicals is safer than handling Na metal. The electrochemical performance of presodiated SnP_2O_7 and its improved coulombic efficiency will be presented in detail.

Sn based negatives for Na-ion batteries
Abhinav Tripathi, Chinnasamy Murugesan, John T. S. Irvine¹

¹School School of Chemistry, University of St Andrews, SCOTLAND, KY16 9ST
*cm465@st-andrews.ac.uk

Abstract: Sn based anodes are explored as negatives for Na-ion batteries. Sn as negative can deliver capacities of around 700-800 mAh/g, however 400-450% volume changes from Sn to Na_xSn leads to poor cycling and makes them impractical. Nanosized Sn confined in porous carbons have been shown to compensate for the volume changes and allow excellent cycling. Such 'porous carbon-Sn' composites are impractical due to poor densities. Sn and Hardcarbon (Sn/HC) composites are presented as negatives for Na-ion batteries. Sn/HC leads to 30% more capacity after 10-15% Sn doping in Hardcarbons. Other Sn based negatives and effects of different electrolytes will also be presented.

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Batteries

Future Positive Electrode Materials for Potassium Ion Batteries (KIBs)

Xin Chen¹, Julia Payne¹

¹University of St Andrews

Abstract: In order to slow down the climate change caused by the excess CO₂ emission, electric vehicles are promoted to take place of traditional gas cars. Li-ion batteries are used extensively as power supplies of vehicles. However, the limited lithium reserves in the earth crust and the geographical distribution of Li-reserves make us have to consider alternatives to lithium. As the two alkali metal elements after lithium, sodium and potassium are expected to be possible alternatives to lithium and are both under investigation. We are currently investigating new positive electrode materials for potassium-ion batteries (KIBs).

There are several advantages of using potassium over sodium or lithium. Potassium exhibits a lower reduction potential than sodium, offering the prospect of developing batteries with a high operating voltage.[1] K-ions also have a smaller solvation shell in liquid electrolytes which enables the electrolytes to have a higher ionic conductivity.[2] In addition, dendrite formation is less likely in KIBs.[3] Although Na-ion batteries are currently receiving considerable interest, there are advantages of using potassium over sodium, particularly as unlike sodium, potassium can insert/de-insert into graphite, enabling graphite to be used as a negative electrode material.[4-6] In addition, in some non-aqueous electrolytes, potassium has a lower reduction potential than both sodium and lithium.[7] The large size of potassium can cause problems like excessive expansion and damage of electrodes, which greatly reduces the lifetime of the batteries. As a result, developing new positive electrode materials and understanding reversible K-insertion/extraction in these materials are of the most importance in improving the performance of KIBs.

One of the most studied positive electrode materials for KIBs are Prussian blue (PB) and its analogues. As reported in the recent study, PB $K_{0.22}Fe[Fe(CN)_6]_{0.805} \cdot 4.01H_2O$ can reach a reversible capacity of 73.2 mAhg⁻¹.[8] The open three-dimensional framework structure with large voids enables the insertion/deinsertion of potassium from the material. I am currently investigating double perovskites (KLaBB'O₆ where B and B' are transition metals, like Fe, Nb, Mn, and W) as the structure has some analogies to the PB due to K occupying the A-site of the perovskite, whilst also exhibiting considerable compositional flexibility.

Reference:

- [1] N. Xiao, W. D. McCulloch and Y. Y. Wu, *J. Am. Chem. Soc.*, 2017, **139**, 9475-9478.
- [2] X. Y. Wu, D. P. Leonard and X. L. Ji, *Chem. Mater.*, 2017, **29**, 5031-5042.
- [3] S.-Y. Lee, A. S. Lim, Y. M. Kwon, K. Y. Cho and S. Yoon, *Inorg. Chem. Front.*, 2020, **7**, 3176-3183.
- [4] J. Zhao, X. X. Zou, Y. J. Zhu, Y. H. Xu and C. S. Wang, *Adv. Funct. Mater.*, 2016, **26**, 8103-8110.
- [5] W. Luo, J. Y. Wan, B. Ozdemir, W. Z. Bao, Y. N. Chen, J. Q. Dai, H. Lin, Y. Xu, F. Gu, V. Barone and L. B. Hu, *Nano Lett.*, 2015, **15**, 7671-7677
- [6] S. Komaba, T. Hasegawa, M. Dahbi and K. Kubota, *Electrochem. Commun.*, 2015, **60**, 172-175
- [7] K. Kubota, M. Dahbi, T. Hosaka, S. Kumakura and S. Komaba, *Chem. Rec.* 2018, **18**, 459-479.
- [8] C. Zhang, Y. Xu, M. Zhou, L. Liang, H. Dong, M. Wu, Y. Yang and Y. Lei, *Adv. Funct. Mater.*, 2016, **27**, 1604307.

**Study on Improving Resistance of Silicon Carbide Elements to Degradation
During Lithium Battery Materials Formation**

Shuoshuo Zhang¹, John TS Irvine¹

¹School of Chemistry, University of St Andrews, North Haugh, KY16 9ST Fife, Scotland, UK

Abstract: The reaction between SiC with a Li source will produce three silicates. Raman technique is very useful for the characterisation of these silicates. However, the characterisation through Raman is challenging when there is no standard reference to compare with. On top of this, the synthesis of stoichiometric composition of these silicates can be challenging mostly owing to the solubility difference of the Li precursor when considering the sol-gel method. Here we discuss various synthesis routes to get pure phases of these materials and the characterisation.

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Solid State Batteries

Li₇La₃Zr₂O₁₂ – electrolyte for solid state Li-ion battery

Mihkel Vestli¹ and John T.S. Irvine

¹ School of Chemistry, University of St. Andrews, St. Andrews, Fife KY16 9ST, UK

Abstract: Solid state batteries based on ceramic electrolyte and Li metal electrode represent promising energy storage devices because of their higher safety and energy density compared to current battery technology based on organic liquid electrolytes. Solid oxide electrolytes are attractive because of their chemical stability and convenient handling. Garnet-type oxide (Li₇La₃Zr₂O₁₂) is one candidate material for its reasonably high Li⁺-ion conductivity and (electro-)chemical stability. For high performance Li₇La₃Zr₂O₁₂ electrolyte must be fabricated as a thin layer with dense microstructure. In this study Li₇La₃Zr₂O₁₂ layers were produced by scalable tape-casting method and tested with Li electrode applied by using Ga-In

Optimising the interface of solid-state oxide batteries.

Cameron Bathgate, John TS Irvine

Abstract: Solid-state batteries are a promising technology to be one of the natural successors of Li-ion battery (LIB) technology. With the removal of organic liquid electrolytes and the ability to use metallic lithium as the positive electrode, solid-state oxide batteries will improve safety, energy, and power densities compared to conventional LIB. However, sizeable interfacial resistance is a major stumbling block for the technology¹. Observing the intrinsic wetting behaviour of lithium metal with both; the perovskite material Li_{0.5}La_{0.5}TiO₃ (LLTO) and the primitive body centred garnet Li₇La₃Zr₂O₁₂ (LLZO), it was found that the typical behaviour is poor wetting around 70° for electrolytes. Using Dupre-Young calculations, the work of adhesion (0.039 mJm⁻², 0.097 mJm⁻²) and the interface tension (-6.420 mJm⁻², -40.775 mJm⁻²) for the lowest contact angles (35°, 23°) for both electrolytes (LLTO, LLZO) points to the alloying condition of LLTO to lithium metal. Thus, to keep the work of adhesion low, impregnation techniques are being tested to impregnate sol-gel LLTO precursors into a porous LLZO scaffold. The static dropping of the precursors creates a partially covered nano-layer of LLTO bonded to LLZO with observed improvements in the lithium adhesion. These results point to a possible, industrially feasible method to improve the contact adhesion of metallic lithium with one of the most promising solid-oxide electrolytes to create a full battery to surpass LIB.

The study of Li_{7-x}La₃Ce_{2-x}Ta_xO₁₂ garnet solid-state electrolyte

Zipei Wan¹, John Irvine¹

¹School of Chemistry, University of St Andrews

Abstract: Li₅La₃Ta₂O₁₂ (LLTO) is a typical cubic garnet type material, but the conductivity is poor (10⁻⁵ S cm⁻¹ at 25 °C). In this work, Ce⁴⁺ (87 pm) is applied to dope Ta⁵⁺ (64 pm) site to obtain Li_{7-x}La₃Ce_{2-x}Ta_xO₁₂ (LLCTO x, x from 0 to 2.0) with better performance both than Li₇La₃Ce₂O₁₂ (LLCO) and LLTO. For LLCO, Ta⁵⁺ substituting Ce⁴⁺ position could realize a phase transition from tetragonal to cubic. Among all samples, LLCTO 0.75 shows the best conductivity (0.8 mS cm⁻¹ at 25 °C and 1.6 mS cm⁻¹ at 40 °C), with a low sintering temperature of 1150 °C.

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Solid State Batteries

**Microscopical and spectroscopical investigation of the stability of garnet Ta/
Nb doped $\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta/Nb}_{0.6}\text{O}_{12}$ electrolyte**

Ioanna Maria Pateli¹, Mihkel Vestli¹, John TS Irvine¹

¹*School of Chemistry, University of St Andrews, North Haugh, Fife, UK, KY16 9ST*

Abstract: Ceramic garnet $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) solid state electrolyte (SSEs) have gained attention for use in lithium-ion batteries. They show high conductivity when in cubic phase ($\approx 1 \text{ mS cm}^{-1}$, 25 °C) and wide electrochemical window and higher stability in air than sulfide SSEs.¹

It is reported that LiOH and Li_2CO_3 are formed on the surface of LLZO after contact with air. Also, of lower conductivity tetragonal phase is formed at the interface with Li.² In this work, systematic microscopical and Raman investigation is conducted on LLZO materials to understand the air stability and stability after contact with Li, before and after electrochemical testing.

References:

1. Murugan, R.; Thangadurai, V.; Weppner, W., Fast lithium ion conduction in garnet-type $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$. *Angewandte Chemie International Edition* **2007**, *46* (41), 7778-7781.
2. Sharafi, A.; Yu, S.; Naguib, M.; Lee, M.; Ma, C.; Meyer, H. M.; Nanda, J.; Chi, M.; Siegel, D. J.; Sakamoto, J., Impact of air exposure and surface chemistry on Li-Li $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ interfacial resistance. *Journal of Materials Chemistry A* **2017**, *5* (26), 13475-13487.

Ca-doped LiYO_2 as a Solid State Electrolyte Candidate

Colm W. Boyle¹, Julia L. Payne¹

¹*School of Chemistry, University of St. Andrews, KY16 9ST, St. Andrews, UK*

Abstract: Doping materials can be an effective method of transforming a poor performing material into a potentially great one. LiYO_2 was reported by Biefeld *et al.* as a solid state electrolyte to have an ionic conductivity of 10^{-3} S/cm at 400 °C and not much work has been done to improve this. Zou *et al.* reported a Zr-doped LiYO_2 but found it was detrimental to the conductivity. Ca doping of LiYO_2 explores new chemical space with an attempt to improve the conductivity to competitive levels with other common solid state electrolytes

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Catalysis and Photocatalysis

**Turquoise Hydrogen – An Exploration
of Catalysts for Methane Pyrolysis**

Aida Fuente Cuesta¹, Cameron Findlay¹, Cristian Savaniu¹, John T.S. Irvine¹

¹ School of Chemistry, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9ST, United Kingdom

Abstract: The development of new and efficient processes for hydrogen production with minimal CO_x emissions is a critical challenge from an environmental point of view, in addition to overcoming the additional costs of purification associated to the current industrial processes used for its production. This study focusses on the synthesis of three different types of catalysts for the production of turquoise hydrogen by methane pyrolysis. Metal-supported (Fe-SiO₂), perovskite (La_{0.4}Ca_{0.4}Ti_{1-x}Fe_xO_{3-δ}) and mesoporous carbon catalysts were prepared by wet impregnation, sol-gel and carbonisation synthesis, respectively. A fixed-bed reactor was used to gauge their initial catalytic activity towards CH₄ conversion through GC analysis. The type of solid carbon by-product obtained was characterised by PXRD, SEM and Raman.

**Integrating Photoelectrochemical Charging into Lithium Batteries for Use as a
Single Multifunctional Device**

Chayopas Tupberg¹, John T.S. Irvine¹

¹School of Chemistry, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9ST

Abstract: Solar energy is a promising renewable energy resource. The energy from the sun is typically converted by solar cells and collected into a battery in the form of chemicals. It requires at least two devices for energy conversion and storage. Lithium manganese oxide, particularly LiMn₂O₄, is commonly used as positive electrodes for lithium batteries. Due to its semi-conducting property, it is fascinating to integrate photoelectrochemical charging into lithium-ion batteries for use as a single multifunctional device. To allow the transmission of light to interact with LMO at the electrode-electrolyte interface, lithium manganese oxide was spin-coated on a transparent conducting oxide coated glass substrate. The 200 nm thick Li_{0.955}Mn_{1.910}O₄ film coated on FTO glass substrate possessed a band gap energy of 2.7 eV. Photoelectrochemical results reveal that the irradiation of light on the cell facilitated the generation of electrons and holes. The findings showed an increase in current and a decrease in potential with the irradiation of light. Photoelectrochemical responses of the Li_{0.955}Mn_{1.910}O₄ film at a potential of 2.6 V and 3.7 V (*vs Li/Li⁺*) corresponded to lithium insertion/extraction at octahedral and tetrahedral sites, respectively.

Reactor development for photocatalytic applications

Nikoletta Gkoulemani¹, John T.S. Irvine¹

¹School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, UK

Abstract: Photocatalysis is a continuously developing field, providing solutions to a variety of issues, while applying mild conditions to the processes. Treatment of wastes and toxic molecules in water, reforming of organic molecules to valuable chemicals and fuels, upgrade of biomass products, utilisation of CO₂ by reduction, and water splitting for hydrogen production are only some of the reactions carried out using heterogeneous photocatalysis.

Research has been focused on investigation and development of materials used as photocatalysts, in order to achieve better conversion, selectivity, yield in each process. Parameters as pressure, temperature, irradiation source, aerobic or anaerobic atmosphere, composition of solvents used, and many others are also under ongoing investigation. Targeting more efficient processes also includes the part of photoreactor design. Design and development of a photoreactor is a challenging process and many parameters on the efficiency of the reaction carried out should be investigated.

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Catalysis and Photocatalysis

**Doped strontium niobate titanates $\text{Sr}_m\text{Ti}_x\text{Nb}_{1-x}\text{Cr}_{1-x}\text{O}_{3-\delta}$ ($m \leq 1$)
for photocatalytic hydrogen production**

Yuan Liao¹

¹ School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, United Kingdom.

Abstract: In this work, the photocatalytic hydrogen production of doped strontium niobate titanates $\text{Sr}_m\text{Ti}_x\text{Nb}_{1-x}\text{Cr}_{1-x}\text{O}_{3-\delta}$ ($m \leq 1$) was explored through the gradual doping of B sites on the basis of SrTiO_3 perovskite materials. The band gap reduced after Nb doping and light absorption extended to visible light range when further Cr doping. Besides, $\text{SrTi}_x\text{Nb}_{1-x}\text{Cr}_{1-x}\text{O}_{3-\delta}$ series exhibit better photocatalytic hydrogen production than $\text{Sr}_{1-1/2x}\text{Ti}_x\text{Nb}_{1-x}\text{Cr}_{1-x}\text{O}_{3-\delta}$.

Research on bio-mass ashes collected from the Eden campus boiler

Mengyuan Guo¹, Xiangling Yue¹

¹ School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, UK

Abstract: Slagging and fouling are the main reasons for unscheduled plant shut-down due to the loss of efficiency in the heat transfer. Characterization results of the bio-mass ashes collected in the Eden campus boiler of different positions are evaluated. The fly ash shows higher pH values and is found stronger crystalline compared with the three types of ashes residue remaining in different positions in the combustion chamber (bottom ash). Besides, the high content of potassium-rich salts facilitated the adhesion of small particles to larger particles during the biomass gasification process. The characterization of ash deposits from the literature is summarized.

7th Meeting of the Energy Materials Discovery Characterisation and Application
Group: Ben Wyvis Strathmore Hotel, Strathpeffer
5th May 2022

Solid Oxide Cells

Direct Ammonia Protonic Solid Oxide Fuel Cell

Kamil Nowicki, George Carins, John Bayne, Chayopas. Tupberg, Gavin Irvine, John T. S.

Irvine

School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, UK

Abstract: Here we seek to demonstrate a low-carbon electrical power generation system based on Protonic Solid Oxide Fuel Cells (P-SOFC) fuelled by ammonia for port and maritime applications.

The performance of a tubular cell with proton conductive $\text{BaCe}_{0.5}\text{Zr}_{0.3}\text{Y}_{0.16}\text{Zn}_{0.04}\text{O}_{3-\delta}$ (BCZYZ) electrolyte, composite Ni/ $\text{BaCe}_{0.5}\text{Zr}_{0.3}\text{Y}_{0.16}\text{Zn}_{0.04}\text{O}_{3-\delta}$ (Ni/BCZYZ) fuel electrode and $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.5}\text{Fe}_{0.5}\text{O}_{3-\delta}$ / $\text{BaCe}_{0.5}\text{Zr}_{0.3}\text{Y}_{0.16}\text{Zn}_{0.04}\text{O}_{3-\delta}$ (LSCF/BCZYZ) air electrode has been investigated using pure ammonia fuel.

The tested cell generated up to 8.5 W with a maximum power density of 0.236 W/cm^2 at 750°C . The cell was operated for over 360h in pure NH_3 , repeatedly characterised using I-V and EIS techniques, and tested under load to generate current for more than 200h at 750°C .

**An electrochemical membrane reactor for reaction-separation
coupling: to produce pure hydrogen**

Xuefa Xia¹

¹*University of St Andrews*

Abstract: An electrochemical hydrogen pump with proton conductor has the ability to extract hydrogen from dilute hydrogen. So, an innovative route can be developed by coupling reaction and H_2 removal in an electrochemical membrane reactor to coproduce valuable chemicals and pure hydrogen on opposite sides of the membrane. Here, H_2 is in-situ extracted by the membrane reactor that only allows the permeation of H_2 as protons through the electrolyte with infinite selectivity. With $\text{BaCe}_{0.7}\text{Zr}_{0.1}\text{Y}_{0.16}\text{Zn}_{0.04}\text{O}_3$ as the electrolyte, the hydrogen pump was demonstrated with high performance for H_2 separation, which is an excellent candidate for electrochemical membrane reactor.

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Solid Oxide Cells

Investigation of microstructure impact on SOFC using CFD simulation

Xiaoqiang Zhang^{1,2}, Martin Andersson¹

¹ Department of Energy Sciences, Faculty of Engineering, Lund University, P.O. Box 118, SE-221 00, Lund, Sweden

² School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST UK

Abstract: Solid oxide fuel cell (SOFC) comprises the porous electrodes that sandwich the dense electrolyte. An optimized microstructure of porous electrodes can improve the transport and catalyzing properties. A microstructure CFD simulation of electrode material for a SOFC 3D model is constructed focused on optimizing the tortuosity and solid phase volume fraction. Governing equations coupled between electrochemical reaction, heat transfer, transport of charges, species, and momentum are solved based on the finite element method (FEM) using commercial software COMSOL Multiphysics. The impact of decreased ionic, electronic, and pore phase tortuosity, and the volume fraction of the electronic phase are investigated.

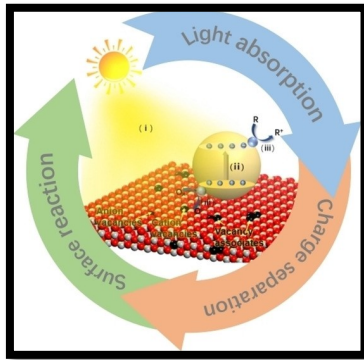
Waste to energy direct carbon fuel cell development with lanthanum strontium calcium titanate based anode

Xinyu Liu¹, John T.S. Irvine¹

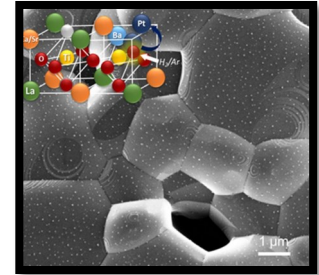
¹ School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, UK

Abstract: With the growth of global population, the command for energy continues to grow. At the same time, the increasing production of waste has brought challenges as well. Utilising solid oxide fuel cell technology, it is possible to convert chemical energy in the waste to electricity.

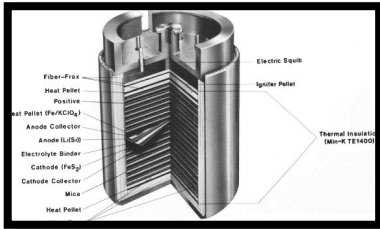
Solid oxide direct carbon fuel cell has been developed for use with waste derived materials. In this presentation, solution-based synthesis of $\text{La}_{0.2}\text{Sr}_{0.25}\text{Ca}_{0.45}\text{M}_x\text{Ti}_{1-x}\text{O}_{3-\delta}$ (M=Ni, Fe, or Co) will be introduced. Performance of solid oxide fuel cells made with $\text{La}_{0.2}\text{Sr}_{0.25}\text{Ca}_{0.45}\text{M}_x\text{Ti}_{1-x}\text{O}_{3-\delta}$ anode, YSZ electrolyte, and LSM cathode will be demonstrated both with hydrogen as the fuel and solid carbon as fuel. The potential of $\text{La}_{0.2}\text{Sr}_{0.25}\text{Ca}_{0.45}\text{M}_x\text{Ti}_{1-x}\text{O}_{3-\delta}$ anode as direct carbon fuel cell will be discussed in the presentation by comparison with state-of-art Ni/YSZ anode.



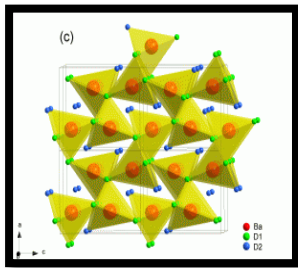
Photocatalysis



Exsolution

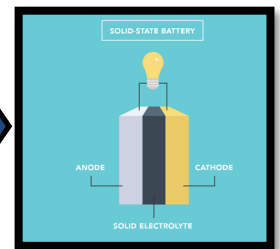


Thermal Batteries

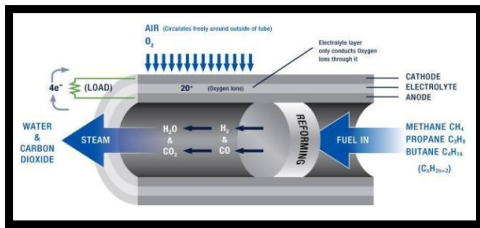


Hydrides & Hydrogen Storage

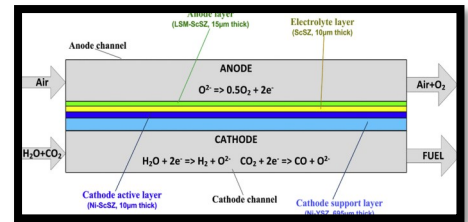
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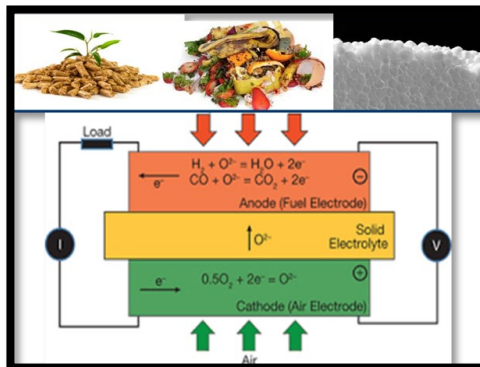
Solid-state Batteries



Fuell Cells



Electrolysis



Waste to Energy