



RSC INTEREST GROUP
SOLID STATE CHEMISTRY

Early Career Researcher Meeting

#2021ECRssc

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Virtual Meeting
16th - 17th

**September
2021**

Thursday 16th September 2021

	10:00 - 10:15	Welcome
	10:15 - 10:45	Invited Speaker: Dr Ivana Hasa Assistant professor, WMG, University of Warwick Sodium-ion batteries: from materials to cell development
Session 1 Chair: Wilgner Silva	10:45 - 11:05	Abby Haworth (Lancaster University) Understanding the Local Structure of Protective Alumina Coatings for Cathodes and the Coating-Cathode Interface
	11:05 - 11:25	Bo Dong (University of Birmingham) Garnet Solid State Electrolytes for Solid-State Batteries
	11:25 - 11:45	Evé Wheeler-Jones (University of Warwick) The influence of synthesis route on the crystallinity and rate capability of niobium pentoxide for energy storage
	11:45 - 13:00	Lunch
Session 2 Chair: Elizabeth Driscoll	13:00 - 13:30	Invited Speaker: Laura Woodward Career and Professional Development Advisor at the Royal Society of Chemistry
	13:30 - 14:00	Invited Speaker: Siddharth Patwardhan Professor, University of Sheffield, Sipat Consultancy and Training Plate Spinning: A Beginner's Guide to Surviving and Thriving as an Engineering/Science Academic
	14:00 - 14:30	Invited Speaker: Jamie Gallagher Freelance Communicator and Engagement Professional An Introduction to Outreach
	14:30 - 15:30	Poster Session (including break)
Session 3 Chair: Elanor Murray	15:30 - 16:00	Invited Speaker: Dr James Dawson NU Academic Track Fellow, Newcastle University Beyond the Bulk: Computational Approaches to Interfaces and Ion Transport in Energy Materials
	16:00 - 16:20	Seán Kavanagh (University College London) Rapid Recombination by Cadmium Vacancies in CdTe
	16:20 - 16:40	Struan Simpson (University of Aberdeen) Electronic phase segregation in the 6H-perovskite $\text{Ba}_3\text{SrMo}_2\text{O}_9$
	16:40 - 17:00	Khalid Naif Alharbi (Centre for Science at Extreme Conditions (CSEC) and University of Edinburgh) Synthesis of new cation-ordered perovskite oxides under high-pressure and investigation of their magnetic properties
	17:00 - 17:30	Social - breakout rooms

Poster Session 1

14:30 - 15:30

Poster No.	
1	Anna Peiro-Franch (University of Kent) Stabilisation of the perovskite phase of all-inorganic materials for photovoltaic applications
2	Celia Castillo-Blas (University of Cambridge) Metal-organic framework crystal- inorganic glass composites
3	Dashnor Beqiri (University of Warwick) Engineering soft modes in Layered Perovskites
4	Ethan Williams (University of Birmingham) Synthesis, Scale-up, and Optimisation of NMC-9.5.5
5	Georgina Robertson (University of Cambridge) Responses of metal-organic frameworks to various pressure states
6	Jaime-Marie Price (University of Birmingham) Optimising Synthesis of LiNiO_2 cathode material for Li-ion batteries
7	Lizzie Driscoll (University of Birmingham) Raman spectroscopy insights into the α - and δ -phases of formamidinium lead iodide (FAPbI_3)
8	Matthew James (University of Birmingham) Synthesis of Borate doped $\text{La}_{10-x}\text{Y}_x\text{GeO}_{27}$; Confirming the Presence of a Secondary Conducting Pathway

Friday 17th September 2021

	10:00 - 10:05	Welcome
	10:05 - 10:35	Invited Speaker: Dr Jason McNulty Associate Lecturer (Education focused) in Inorganic Chemistry, University of St. Andrews Research to Education: How I got here
Session 4 Chair: Dashnor Beqiri	10:35 - 10:55	Elizabeth Driscoll (University of Birmingham) The Building Blocks of Battery Technology: Inspiring the next generation of battery researchers
	10:55 - 11:15	Yao Yuan (University of Edinburgh) Ternary nitrides as rapid and durable electrocatalysts
	11:15 - 11:35	Mario Falsaperna (University of Kent) Exploring the magnetocaloric effect in the $\text{Ln}(\text{HCO}_2)(\text{C}_2\text{O}_4)$ family of Metal-Organic Frameworks
	11:35 - 12:05	Invited Speaker: Dr Andrew Cairns Research Fellow, Imperial College London 'Out' in Academia: Experiences of an LGBT+ Scientist
	12:05 - 13:00	Lunch
Session 5 Chair: Dr Nicolas Flores - Gonzales & Emily Hanover	13:00 - 14:00	Invited Speaker: Dr Akhil Kallepalli Dragonfly Mental Health Ambassador Mental Health Literacy
	14:00 - 14:30	Invited Speaker: Dr Lennie Foster Skills Manager for Energy Research Accelerator (ERA) and Centre for Post-doctoral Development in Infrastructure Cities and Energy (C-DICE) C-DICE and ERA: Creating a Pipeline Of World Class Talent to Meet Green Growth and Net Zero Challenges
	14:30 - 15:30	Poster Session (including break)
Session 6 Chair: Dr Alex Browne	15:30 - 16:00	Invited Speaker: Dr Alexandra Gibbs EPSRC Early Career Fellowship, St Andrews, ISIS Symboisis and serendipity in life and research at the physics/chemistry interface
	16:00 - 16:20	Ashutosh Kumar Singh (Jawaharlal Nehru Centre for Advanced Scientific Research, India) Electrical transport properties of half-Heusler ScPdBi single crystals under extreme conditions
	16:20 - 16:40	Charlotte Pughe (University of Sheffield) Site - Selective d^{10}/d^0 effect in a hexagonal perovskite: $\text{Ba}_2\text{CuTe}_{1-x}\text{W}_x\text{O}_6$
	16:40 - 17:00	Kunlang Ji (University of Edinburgh) Crystal and magnetic study on cation ordered $\text{A}_2\text{B}_2\text{O}_6$ phases
	17:00 - 17:15	Prize Winners Announced & Closing

Poster Session 2

14:30 - 15:30

Poster No.	
9	Rosie Madge (University of Birmingham) Organic acid leaching of LiMn_2O_4 from mixed cathode materials
10	Subhadip Mallick (University of Oxford) Influence of $6\text{S}^2 \text{Bi}^{3+}$ cation on the structures of $\text{A}'\text{BiNb}_2\text{O}_7$ ($\text{A}' = \text{Rb, Li, Na, K}$) layered perovskites
11	Thomas Hitchings (University of Kent) Re-examination of the polar transition in $(\text{N}_2\text{H}_5)\text{Mg}(\text{HCO}_2)_3$: Evidence of potential proton migration
12	Viktoria Falkowski (University of Oxford) Synthesis and topotactic manipulation of layered oxysulfide $\text{CaSrMnO}_2\text{Cu}_{4-\delta}\text{S}_3$
13	Xabier Martinez de Irujo Labalde (University of Oxford) $\text{LiFe}_{2-x}\text{In}_x\text{SbO}_6$ Oxides as Li-ion Electrode Materials
14	Yujiang Zhu (University College London) Temperature Dependence of the Physicochemical Characteristics and Glucose-sensing Behaviour of Copper Oxide Nanostructures Synthesised by Hydrothermal Method
15	Zheyang Xu (University of Oxford) Hole and electron doping of the Topochemically Reduced $n = 1$ Ruddlesden-Popper Rhodium-Containing Oxides

Organising Committee



Lizzie Driscoll
PhD
Slater Group
University of Birmingham



Struan Simpson
PhD
McLaughlin Group
University of Aberdeen



Dr Alex Browne
PDRF
Gibbs Group
University of St. Andrews



Wilgner Lima Da Silva
PhD
Walton/Kendrick Group
University of Warwick/
University of Birmingham



Jaime-Marie Price
PhD
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Anton Zorin
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Xin Chen
PhD
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Dr Nico Flores-González
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Elanor Murray
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Dashnor Beqiri
PhD
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Dr Javi Castells-Gil
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University of Birmingham



Zoë Wright
Undergraduate
Student
University of Birmingham



Dr Pooja Goddard
Senior Lecturer
University of Loughborough



Emily Hanover
Undergraduate
Student
University of Birmingham

Invited Speakers



Dr Ivana Hasa



Laura Woodward



Prof. Siddharth Patwardhan



Dr Jamie Gallagher



Dr James Dawson



Dr Jason McNulty



Dr Andrew Cairns



Dr Akhil Kallepalli



Dr Lennie Foster



Dr Alexandra Gibbs

Dr Ivana Hasa

Assistant Professor of Electrochemical Materials at WMG,
University of Warwick
Email: ivana.hasa@warwick.ac.uk



Ivana Hasa is currently Assistant Professor of Electrochemical Materials in WMG at the University of Warwick.

Ivana is a chemist by background and completed her PhD in 2015 on the design and characterization of sodium-ion battery materials at Sapienza University of Rome in Italy. During her PhD, Ivana has been visiting scientist at Massachusetts Institute of Technology (MIT, Cambridge, USA) and MEET Battery research center (Muenster, Germany). After her PhD, Ivana moved to the Helmholtz Institute Ulm (Ulm, Germany) for a postdoctoral position working on post-lithium chemistries in the group of Prof. Stefano Passerini. In 2016, she joined the Lawrence Berkeley National Laboratory (Berkeley, USA) to investigate the chemistry and evolution of the solid electrolyte interphase of silicon anodes in the group of Dr. Robert Kostecki. In 2019, she returned to the Helmholtz Institute Ulm as a Research Scientist responsible of the Sodium-ion battery group research activities within Prof. Passerini's group. Finally, in 2020 Ivana joined the Electrochemical Materials group in WMG at the University of Warwick. Her research activities are directed toward a fundamental understanding of the processes governing the chemistry of sodium-ion batteries. At the Energy Innovation Centre, she is also working toward the development and scale up of new battery chemistries from concept to full proven cell prototypes.

Sodium-ion batteries: from materials to cell development

I study and investigate the processes governing sodium-ion batteries (SIBs), which I consider one of the most promising next-generation energy storage technologies. My research focuses on the development of technically relevant battery materials, the characterization of their surface and bulk properties, and their implementation in electrochemical cells. My work is inherently interdisciplinary, tackling challenges at the interface of chemistry, materials science, electrochemistry and engineering. Great achievements in terms of materials development have been reported in the recent years in the SIBs scenario. However, further work is still needed to fully understand the structure-function correlation in several SIB materials.

This presentation gives an overview on the journey toward the development of SIBs linking chemistry and electrochemistry of the employed materials. A lab scale chemical approach for the development and understanding of SIB material will be presented with a case of study on transition metal layered oxides. Challenges on the transition from lab to scaled-up processes and the development of industrially relevant cell prototypes will also be discussed.

Laura Woodward

Career and Professional Development Adviser
Royal Society of Chemistry

Website: <http://my.rsc.org/careers>
Twitter: @lauracareers



Laura Woodward is a Career and Professional Development Adviser at the Royal Society of Chemistry. She has a background in recruitment and Human Resources and has been working with supporting members with their next career step for the last 10 years.

Laura's talk will provide you with an overview of things to consider when starting your career journey and long term career development alongside advice on how to be most effective in a job search. She'll also talk about the support that the RSC can provide as part of membership, including; mentoring, webinars and one to one careers advice.

Prof. Siddharth V. Patwardhan

Professor of Sustainable Chemical and Materials
Engineering, University of Sheffield
Website: www.svplab.com
Twitter: @GreenNanoRes



Siddharth V. Patwardhan, FRSC, is a Professor at the University of Sheffield and the Director of Sipat Consultancy and Training. He leads the Green Nanomaterials Research group focussing on developing sustainable, scalable and economical processes and products. Along with various funding awards, he received the Dedicated Outstanding Mentor award four-times in recognition of his mentoring skills that helped mentees "make a significant transition in knowledge, work, or thinking", two "SuperVisionary" awards in recognition of good all round supervision and Teaching Excellence Award twice.

Plate Spinning: A Beginner's Guide to Surviving and Thriving as an Engineering/ Science Academic

This short talk is intended as a quick overview for aspirant academic appointees in Science and Engineering. This presentation provides a gentle steer towards taking a strategic approach by adopting a new view: thinking as a CEO of a small enterprise while defining a vision and constructing a pathway to achieve that vision. It will be presented in the form of Top 10 tips I wish I was told when I started and points introduced include:

- the workings of modern universities and the role of teaching
- the academic transfer function for research success
- various career trajectories
- being sustainable and resilient

Dr Jamie Gallagher

Award-winning freelance communicator
and engagement professional
Website: www.jamiebgall.co.uk
Twitter: @jamiebgall



Jamie Gallagher is an award-winning freelance communicator and engagement professional with ten years' experience in the delivery and evaluation of quality engagement projects. Working across dozens of institutions and subject areas he has helped improve the reach, profile and impact of research engagement in almost every discipline. He has delivered training and events around the world, he has also written a pop science book and appeared on numerous TV and radio programs. When not talking about science Jamie works with universities, charities and museums helping them to demonstrate their impact and understand their audiences.

Jamie will be giving an introduction talk on outreach.

Dr Jason McNulty

Associate Lecturer (Education focused) in
Inorganic Chemistry, University of St. Andrews
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Jason completed his PhD under the supervision of Dr Finlay Morrison at the University of St Andrews in 2018. His thesis was on the structure-property relationships of tungsten bronze oxide materials. Following this, Jason took up a post-doctoral research position in the group of Prof Philip Lightfoot at the University of St Andrews, where he worked on the structure and synthesis of hybrid organic-inorganic halide perovskites. Jason joined the faculty of the UoStA earlier this year as an Associate Lecturer (Education Focused) in Inorganic Chemistry. Jason has been a member of the RSC Tayside Local Section committee since 2016, first as the Early Career Representative and since 2018 as Secretary.

Research to education: how I got here

If you'd asked me 10 or even 5 years ago where I'd be now, I wouldn't have been right. In this talk I'll share some of my experiences and how this led to my current position as an Education Focused Lecturer. This will include some of the opportunities I've had, some of my personal experiences in outreach and as someone who identifies as LGBT-QI+ in STEM and of course, some of my research looking at hybrid perovskites. I hope that from this you'll be able to get an idea of career routes that you can follow other than research and how the most important thing is to do what you enjoy!

Dr James Dawson

Academic Track Fellow at Newcastle University

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James is currently a Newcastle University Academic Track Fellow in the School of Natural and Environmental Sciences. His research utilises state-of-the-art computational techniques to investigate ion transport and interfaces in energy storage, generation and conversion materials to aid the transition to net zero. Before joining Newcastle University in 2020, James held postdoctoral positions at the Universities of Bath with Prof. Saiful Islam (2016–2019) and Cambridge with Prof. John Robertson FRS (2015–2016), as well as a prestigious JSPS Postdoctoral Fellowship at Kyoto University (2013–2015). He completed his PhD on the simulation of perovskite oxides for electronics applications at the University of Sheffield in 2013 under the supervision of Profs. John Harding and Derek Sinclair. James has received several early-career awards and was recently selected as one of three nominees from Newcastle University for the 2022 Blavatnik Awards in the UK.

Beyond the Bulk: Computational Approaches to Interfaces and Ion Transport in Energy Materials

Ion transport is pivotal to the performance of energy technologies and therefore the journey to net-zero emissions. The materials that exhibit ion conduction in these technologies present stunning heterogeneity and a plethora of complicated ion diffusion mechanisms from which they often derive their functionality. This situation is further complicated when we begin to consider the nanostructures, microstructures and interfaces of these materials. Nevertheless, it is imperative to understand these mechanisms and interfaces, and their influence on the performance of ion conductors, in order to design next-generation materials and devices, as well as improving existing technologies.

In this presentation, I will discuss how atomic-scale simulations can help us in the understanding, design and improvement of next-generation energy materials, as well as providing an overview of my career pathway thus far. I will present results from our recent work on solid electrolytes for solid-state batteries and solid oxide fuel cells. The importance of the synergy between experiment and modelling and its role throughout my career will also be explored.

Dr Andrew Cairns

Research Fellow
Faculty of Engineering, Department of Materials
Imperial College, London
Twitter: @abcairns



Andrew completed his doctoral studies at the University of Oxford in 2015 under the supervision of Prof. Andrew Goodwin. His thesis explored unusual mechanical properties and disordered structures that emerge in coordination frameworks, in particular metal-cyanide materials. During this time Andrew discovered what his favourite cyanide framework is, and was introduced to the world of high-pressure crystallography using both synchrotron X-rays and neutrons. This led to a postdoctoral position at the European Synchrotron Radiation Facility in Grenoble, France, where he worked on the high-pressure beamline ID27. In-between squeezing whatever samples came along, he improved his head for heights on hikes in the Alps and developed an appreciation for French bread. A return to more familiar shores called though, and in 2017 he took up a Departmental Research Fellowship and subsequently lectureship in the Department of Materials, Imperial College London. Andrew leads the FlexMat group that seeks to harness flexibility in materials for new multifunctional materials.

‘Out’ in Academia: Experiences of an LGBT+ Scientist

When reading a biography, like the one above, it can be easy to forget the huge impact that personal circumstances can have on a career. This can be even more true if that individual’s experience is underrepresented in a community, so that our differences become invisible. In this talk I will highlight the challenges of being an LGBT+ scientist from both a personal and wider perspective, and how this has impacted on my journey so far. More broadly, while a lot of progress has been made, there is still work to be done to improve research culture for everyone in science. I hope to show, by highlighting inspirational people and projects, the huge potential for our community of early career researchers to build a truly inclusive academia.

Dragonfly Mental Health

Talk Ambassador: Dr Akhil Kallepalli

Twitter: @DragonflyMH

Website: <https://dragonflymentalhealth.org/>



Intro to Mental Health Literacy

There are many misconceptions about psychiatric disease, what causes it, who is at risk, and how it manifests. Increasingly we are understanding how immense a problem this is in academia. “A Scientist’s Primer on Mental Health” is a 1-hour seminar and facilitated discussion which delivers the basics of mental health at a level that academics appreciate.

The talk includes:

- Prevalence of mental health illness in general and academic populations An overview of signs and symptoms highlighting those seen in academic settings
- The science underlying the causes and treatments of mental illnesses, with an
- emphasis on depression and anxiety (most common mental illness).

Dr Lennie Foster

ERA & C-DICE Skills Manager
Loughborough University

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Lennie is the Skills Manager for the ERA (Energy Research Accelerator) Skills Academy which draws on the expertise and world-class facilities of the Midlands Innovation group of universities – Aston, Birmingham, Cranfield, Keele, Leicester, Loughborough, Nottingham and Warwick, plus the British Geological Survey; and C-DICE (Centre for Postdoctoral Development in Infrastructure Cities and Energy), a world-class postdoctoral development programme which leverages the capability of 18 leading research-intensive UK universities. Lennie joined Loughborough University in 2017, first as part of the Research Quality and Visibility Team, and then as a Research Development Manager. Lennie gained a PhD in Systems Biology from the University of Warwick working with researchers in the Life Science and Computer Science departments. In her spare time, she enjoys gardening and playing DnD with her friends and family.

C-DICE and ERA: creating a pipeline of world-class talent to meet green growth and Net-Zero challenges

During her talk Lennie will outline the types of activities, events, and opportunities, available via ERA Skills Academy and C-DICE and explain how you can get involved with these programmes. ERA Skills Academy provides a holistic energy-related skills provision to develop high quality energy researchers; to create a diverse talent pipeline to secure the UK's position as a leader in energy research and innovation; and to facilitate knowledge transfer between researchers and industry to help accelerate the downstream impact of ERA-related research. We aim to develop, support, and maintain a dynamic multidisciplinary network of researchers supported by world class expertise and facilities to tackling huge societal challenges required to meet green growth and Net-Zero challenges. The Centre for postdoctoral development in infrastructure, cities, and energy (C-DICE) is an integral part of the ERA Skills Academy, with the majority of post-doctoral skills training being delivered via this programme. C-DICE leverages the capability of 18 leading research-intensive UK universities, bringing together the collective expertise of the UKCRIC universities with the partners of ERA.

Dr Alexandra Gibbs

EPSRC Early Career Fellowship, St Andrews, ISIS

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Alex completed her MPhys (arrived at via a transfer to a joint chemistry-physics degree from her original chemistry programme) at The University of St Andrews in 2008. She stayed there for her interdisciplinary PhD with Prof. P. Lightfoot and Prof. A.P. Mackenzie on emergent states in transition metal oxides. This involved mixed powder and single crystal synthesis, neutron diffraction and low-temperature measurements using bespoke apparatus. Following this she took up opportunities for interdisciplinary research in Japan (at the University of Tokyo and RIKEN) and Germany (Max Planck Institute for Solid State Research in Stuttgart) with Prof. Hidenori Takagi. She then moved to the ISIS Neutron and Muon Source in Oxfordshire to follow her continued interest in high resolution neutron diffraction. These research streams have now converged in her EPSRC Early Career Fellowship at St Andrews in association with the Crystallography Group at ISIS. Her research is at the chemistry-physics boundary, studying structure-property relationships in quantum and functional materials.

Symbiosis and serendipity in life and research at the physics/chemistry interface

My research group focuses on studying structure-property relationships at the chemistry-physics interface. This includes many classes of quantum and functional materials such as ferroelectrics, multiferroics, exotic magnets and superconductors. We often start from a chemically interesting problem only to discover that intriguing physics is found in the materials under study, and vice versa. The interplay of the differing approaches from each side of the problem can lead to some surprising and exciting results. I will give an introduction to some recent examples of this symbiosis and also some particularly serendipitous discoveries and connections. I'll also address the effect that these two principles have had on a more personal level throughout my career so far.

Joining Instructions

A joining link will be sent by the 15th September 2021 once registration closes on the 14th September.

Please do not share this link with others.

Our license has a limited capacity and we don't want those who have registered formally to miss out on the meeting.

The chat box will be in use for the meeting for chit-chat and the Q&A for questions you want to directly to the speaker.

During the talk, only the chair and speaker will be unmuted.

Please do not screenshot any of the speaker's slides without their permission!

Any issues, please do not hesitate to contact us:
ecrssc@gmail.com

Join in on Twitter

Share on Twitter about the meeting using the #2021ECRsscgc hashtag and tag the RSC Solid State Chem group account @SScgcR.



#2021ECRsscgc Feedback

After the meeting, we'd love for you to complete a quick survey on the meeting - what worked well, what didn't & what would you like to see more of.

Feedback survey will go live at the end of the meeting on Friday.

<https://2021ecrsscgc.wordpress.com/feedback>

Day 1

Thursday 16th September 2021
10:00 - 18:00 (BST)

Session 1

Oral Abstracts

10:15 - 11:45

Understanding the Local Structure of Protective Alumina Coatings for Cathodes and the Coating-Cathode Interface

Abby R Haworth,^{1,3} Beth I J Johnston,^{2,3} Samuel G Booth,^{2,3} Alisyn J Nedoma,^{2,3} and John M Griffin.^{1,3}

¹ Department of Chemistry, Lancaster University, Lancaster, LA1 4YB,

² Department of Chemical and Biological Engineering, University of Sheffield, Sheffield, S1 3JD,

³ The Faraday Institution, Quad One, Harwell Campus, OX11 0RA.

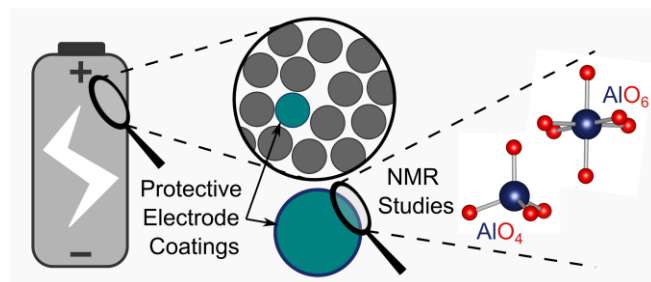


Figure 1: Schematic Representation of the Abstract

Batteries are becoming increasingly popular and are set to play an important role in the transition towards a net-zero carbon economy. In particular, lithium-ion batteries have gained considerable interest as a result of their use in portable electronic devices, as well as growing applications for electric and hybrid vehicles. However, they still face a number of challenges that need to be overcome. One such challenge is the capacity fade which arises over multiple charge-discharge cycles as a result of unwanted reactions at the electrode-electrolyte interface.

This project focuses on tailoring protective coatings to help improve cathode longevity and ultimately battery lifetime. Thin Al_2O_3 coatings have been demonstrated to extend the cycle life for various cathode materials, including LiCoO_2 (LCO) and $\text{LiNi}_x\text{Mn}_y\text{Co}_{1-x-y}\text{O}_2$ (NMC).^{1,2} Our studies, within the Faraday Institution-funded FutureCat project focus, on lithium nickel oxide (LiNiO_2 – LNO). This is a cobalt-free alternative to the commonly used cathode materials, LCO and NMC. Although it has the potential to be used as a cathode material in next-generation electric vehicles, it suffers from capacity fade over multiple cycles.³ Al_2O_3 coatings are being developed within the FutureCat consortium to mitigate side reactions causing capacity loss for LNO cathodes. However, the structure of Al_2O_3 within these coatings and how it interfaces with LNO are not well understood. In order to improve and tailor coatings for cathode materials, it is important to first fully understand the structure of the coating, any reactions occurring at the coating-cathode interface, and the ion dynamics at the coating-cathode interface.

To probe this further, Al_2O_3 coatings have been studied using solid-state NMR spectroscopy. The latest ^{27}Al MAS NMR data, which will be presented here, suggests that additional phases, e.g., LiAlO_2 , are present alongside the Al_2O_3 coating. These are believed to be the result of aluminium/lithium mixing occurring at the coating-cathode interface during the coating procedure. This is valuable insight into the structure of both these coatings and the coating-cathode interface. This additional structural insight, in conjunction with ab-initio computation studies ongoing within the FutureCat consortium, will enable the ion transport across the interface and through the coating to be understood in greater detail.

References

- ¹ S-T. Myung, *et al. Chem. Mater.* 2005, **17**, 3695-3704.
- ² A. M. Kannan, *et al. Electrochem. Solid-State Lett.* 2003, **6**, A16-A18.
- ³ M. Bianchini, *et al. Angew. Chem. Int. Ed.* 2019, **58**, 10434-10458.

Garnet Solid State Electrolytes for Solid-State Batteries

Bo Dong,¹ Mark P. Stockham¹, Stephen R. Yeandel², Abby R. Haworth³, Matthew S. James¹,
Pooja Goddard², Karen E. Johnston³, Peter R. Slater¹

¹ School of Chemistry, University of Birmingham, B15 2TT, UK

² Department of Chemistry, Loughborough University, Loughborough, LE11 3TU, UK

³ Department of Chemistry, Durham University, DH1 3LE, UK

Garnet solid-state electrolytes have attracted great interest due to their high Li ion conductivity and good electrochemical stability¹. To enable the production of All-Solid-State Batteries, several issues need to be addressed, such as to increase the Li⁺ ion ionic conductivity, lower the interfacial resistance between electrolyte and electrode materials and prevent the dendrite growth of Li metal through electrolyte materials.

There has been significant work investigating doping strategies to improve the conductivity of Li₅La₃(Nb/Ta)₂O₁₂ and Li₇La₃Zr₂O₁₂ systems^{2, 3}, with the key conclusions being that Li ion contents of the order of 6.4-6.6 are optimal. In this work, we illustrate a range of cations that can be successfully doped into the structure with extensive solid solutions, leading to improved conductivities and lower activation energies compared to the undoped samples⁴⁻⁶.

We have extended our doping studies to anion doping, which unlike cation doping, has had little research focused upon. We present the halogenation (F, Cl) of solid state electrolyte Li₇La₃Zr₂O₁₂ (LLZO) via a low temperature solid state synthetic route using PTFE and PVC polymers for the first time. The effects of surface fluorination were also investigated for Al-doped LLZO (Li_{6.4}Al_{0.2}La₃Zr₂O₁₂, LLAZO) which suggest this strategy has the ability to prevent full dendrite penetration at high current densities^{7, 8}.

References

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The influence of synthesis route on the crystallinity and rate capability of niobium pentoxide for energy storage

Evangeline C Wheeler-Jones,¹ Melanie J Loveridge¹ and Richard I Walton.²

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The complexity of the Nb₂O₅ system should not be underestimated, with a large variety of crystalline polymorphs, plus amorphous and semi-crystalline forms, that can all return a range of physical properties.¹ Not only are there various naming conventions to navigate, but synthesis procedures have been shown to further effect the materials properties within the same polymorph.² The orthorhombic phase (T-Nb₂O₅) is known as a high-rate anode for Li-ion batteries (LIBs) due to its ability to undergo pseudocapacitive intercalation.³ This process is heavily reliant on low tortuosity pathways for the ions to move through the structure. Due to this, the T- phase has been thoroughly explored, leaving other Nb₂O₅ polymorphs and non-crystalline forms lacking in comparison.⁴ This work presents an anisotropically crystalline 'as-synthesised' Nb₂O₅, produced via a simple hydrothermal route.⁵ The as-synthesised material is heat-treated to produce T-Nb₂O₅ at 600°C and monoclinic (H-) Nb₂O₅ at 1000°C. The electrochemical properties for all these materials were explored. Collectively we report rate sweeps and demonstrate high current stability (20 C-rate capability) and a long-life span, up to 200 cycles. Properties of the anisotropically crystalline Nb₂O₅ are reported for the first time, and we also propose the H-phase as a high-rate anode when synthesised in this manner. Such high-rate results are rare for Nb₂O₅ without integration with carbon materials, thus this work represents an important discovery in the development of very high-rate anode materials.

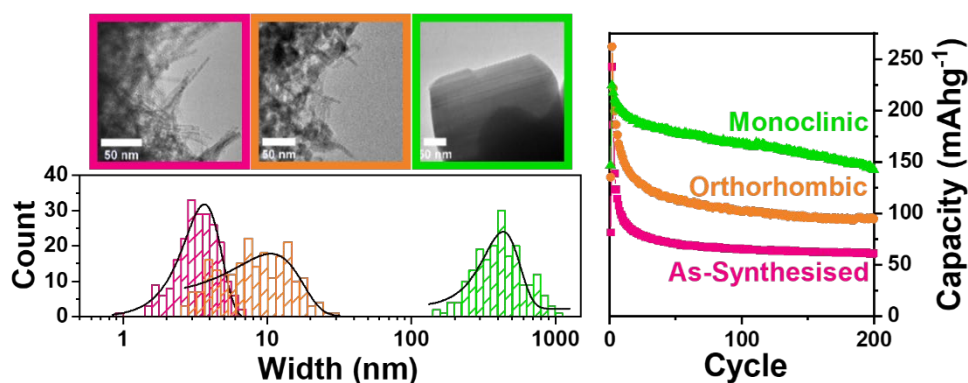


Figure 1 – Graphical abstract from Wheeler-Jones et al. showing the physical characteristics of the variety of Nb₂O₅ materials with corresponding electrochemical response.⁵

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Poster Session

1

14:30 - 15:30

Stabilisation of the perovskite phase of all-inorganic materials for photovoltaic applications

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Lead halide perovskites are promising materials in the field of optoelectronics, especially in photovoltaic applications. In 2009, hybrid organic-inorganic lead iodide solar cells became an area of focus, especially methylammonium lead iodide, MAPbI₃. A lot of progress has been made in the research of their photovoltaic applications, achieving efficiencies greater than 25%, which are competitive with commercial silicon devices. These materials have a high photovoltaic performance, but the presence of the volatile organic cation makes them unstable in air and high temperatures. The thermal instability of hybrid perovskites brought our attention to all-inorganic lead halide perovskites, APbX₃ (A= Cs, Rb; X= I, Br). In all-inorganic lead halide materials, the organic cation is replaced by a big inorganic cation (Cs or Rb). These all-inorganic materials do not contain the volatile moiety and therefore, have a higher thermal stability, as well as good optoelectronic properties. Nevertheless, the inorganic cations are smaller than the organic ones and their tolerance factor is lower. A low tolerance factor means that, at room temperature, these materials stabilise in a non-perovskite structure, that is also non-photoactive. In this study, we used different approaches to stabilise the perovskite phase of all-inorganic lead halides at room temperature (Figure 1). CsPbI₃ and RbPbBr₃ were synthesised in the non-perovskite phase using the self-flux method. The first approach used to stabilise the perovskite phase was doping. Doping increases the tolerance factor and therefore the stability of the perovskite phase at room temperature. CsPbI₃ was doped with Br and RbPbBr₃ was doped with Cs. We have also used quenching and annealing, two post synthetic treatments, to stabilise the perovskite phase at room temperature. The perovskite phase of CsPbI₃ was stabilised by quenching the non-perovskite sample. RbPbBr₃ was obtained in the perovskite phase by annealing the non-perovskite sample. The doped samples were also thermally treated, and the perovskite phase was obtained for all the intermediate compositions.

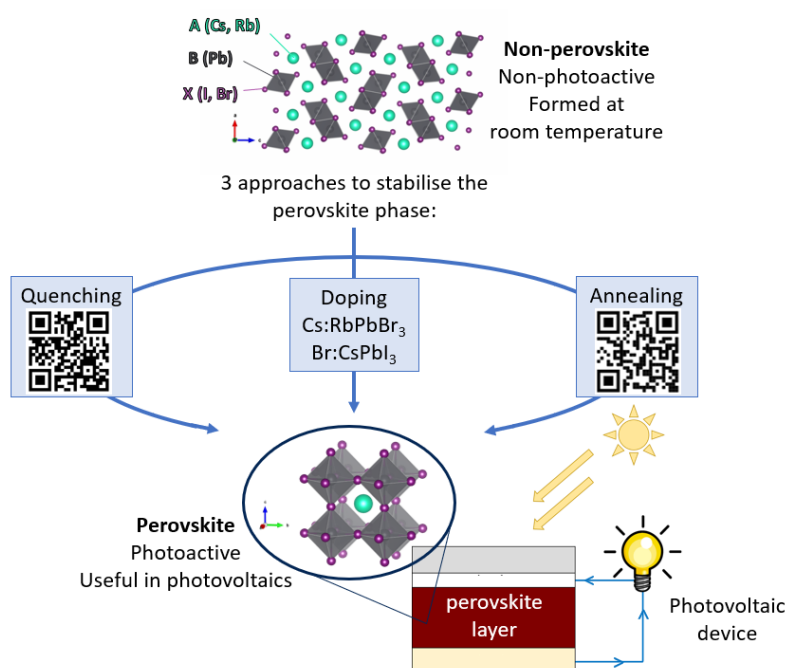


Figure 1: Stabilisation approaches of all-inorganic lead halide perovskites

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Metal-organic framework crystal- inorganic glass composites

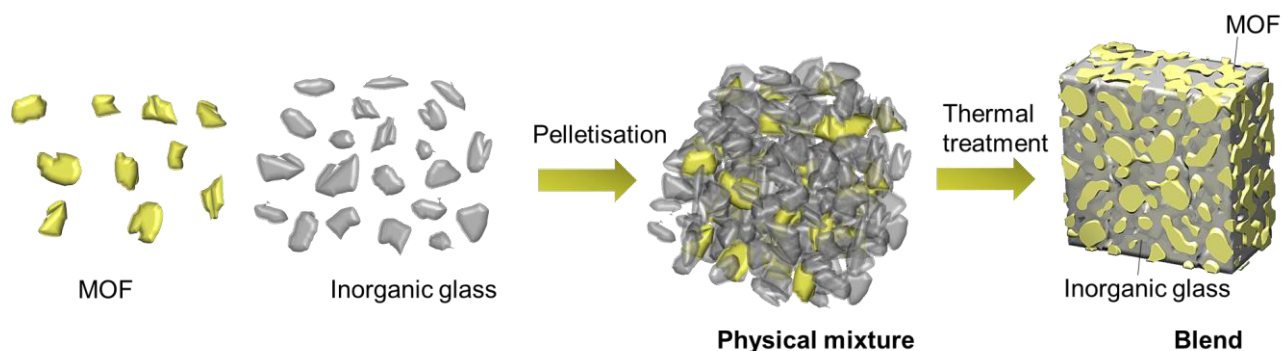
Celia Castillo-Blas,¹ Ashleigh M. Chester,¹ Bruno P. Rodrigues,² Lothar Wondraczek,² David A. Keen,³ Thomas D. Bennett¹

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Over the last two decades, metal-organic frameworks (MOFs) have been the focus of attention for material researchers on account of their intrinsically tuneable chemical structures, flexible architectures, high surface areas and multifunctional properties. However, MOFs are conventionally synthesised as microcrystalline powders, which creates practical and commercial barriers caused by their poor processability and weak mechanical performance. Thus, interest in combining MOFs with more processable materials to form new composites has expanded in recent years. Here we propose a new concept of combining a MOF and an inorganic glass matrix. Metal-organic framework crystal- inorganic glass composites (MOF-CiGCs) are synthesised via the dispersal of a crystalline MOF-808 within a phosphate-base glass matrix at a working temperature where the glass matrix can flow around the embedded MOF particles. A compositional series of this new material have been characterised by X-ray diffraction, differential scanning calorimetry, and SEM-EDS, among other techniques.



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Engineering soft modes in Layered Perovskites

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The tolerance factor, t , of the Ruddlesden-Popper (RP) phase Ca_2MnO_4 can be tuned through isovalent substitution on the B-site. Through this tuning, we can then control the magnitude of Uniaxial Negative Thermal Expansion (NTE) from a large negative to positive value. It has been found, through X-Ray diffraction, that the magnitude of NTE along the layering axis increases as t decreases through substitution on the B-site. At both low and high values of t , there is a transition between the NTE phase and a Positive Thermal Expansion phase.¹

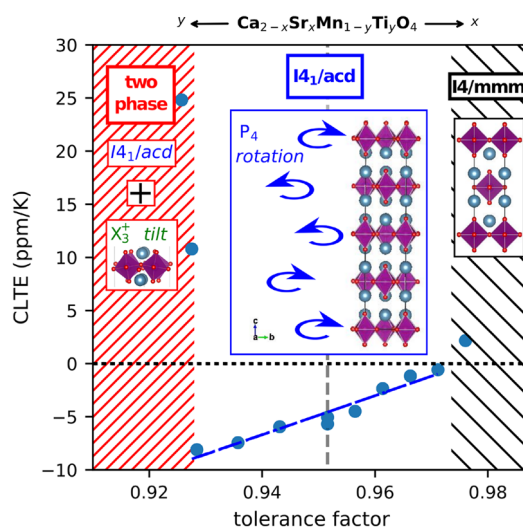


Figure 1: Plot showing the evolution of the Coefficient of Linear Thermal Expansion (CLTE) as the tolerance factor changes

Recent results based on first-principles calculations have shown that reducing the tolerance factor enhances the contribution of the lowest frequency lattice vibrations to thermal expansion.¹ These lattice vibrations are characteristic of octahedral tilts and have negative Grüneisen parameters along the NTE axis.

The aim of this project is to chemically optimise thermoelectric transport through the tuning of t by isovalent doping on the B-site with titanium, to further increase the magnitude of NTE, whilst attempting to synthesise the previously unreported Ca_2TiO_4 .

References

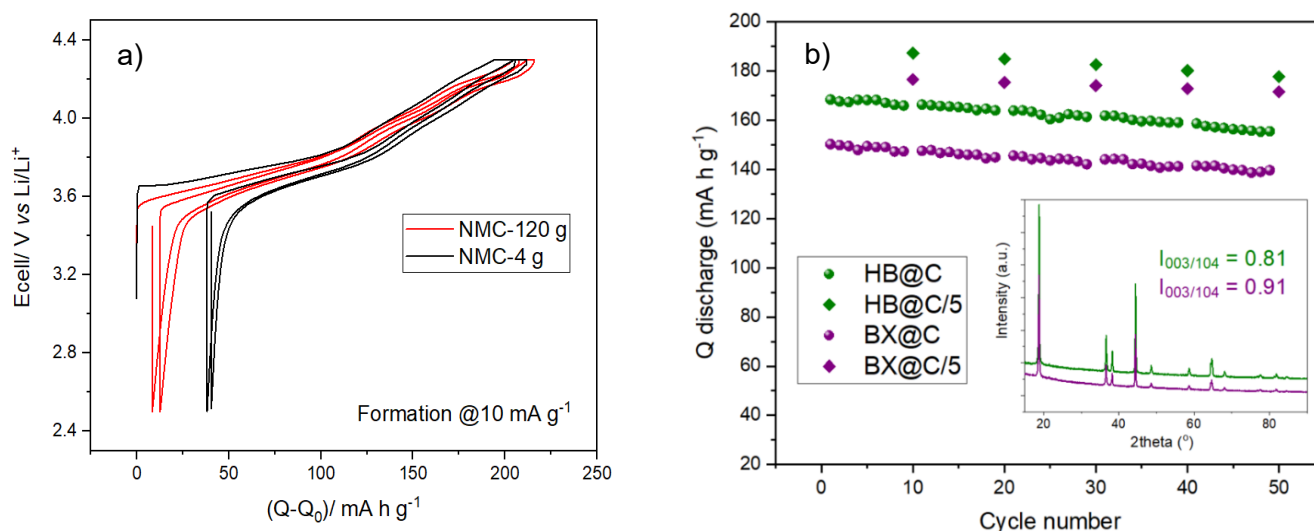
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Synthesis, Scale-up, and Optimisation of NMC-9.5.5

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Ni-rich Li-ion cathode materials like NMC-9.5.5 ($\text{LiNi}_{0.9}\text{Mn}_{0.05}\text{Co}_{0.05}\text{O}_2$) are of interest as they have a higher energy density and limit the cobalt content, aiding the transition away from questionably sourced raw materials, when compared to materials like NMC111 - 622. This has the advantage of reducing production costs while maintaining a high working voltage and capacity. However, the high nickel content of these materials can be detrimental due to disorder brought by $\text{Li}^+/\text{Ni}^{2+}$ cation mixing, lithium residuals, and irreversible phase changes during operation.¹ Similarly, the different synthesis methods and treatments drastically affect the morphological, structural, and electrochemical properties of these materials. We present the results of a study of the coprecipitation synthesis and scale-up of NMC-9.5.5 precursor prepared in a 5 L CSTR and the subsequent two-step firing method to obtain the active material. XRD characterisation of the NMC materials shows the cation mixing is stabilised with increasing firing loads of the precursor, which is reflected in the improved electrochemical performance of the assembled half-cell Li-ion batteries. The use of boron additives have been investigated as sintering aids to improve the morphology and structural stability of the active cathode material. It is observed that varying the boron sintering agent content in the calcination step is shown to impact the level of cation mixing in the cathode structure, with an excess of 0.5 mol% found to deliver the optimum electrochemical performance. Furthermore, the electrochemical properties (both capacity and cycle life) can be improved by reducing the furnace residency time as well as the temperature during the first firing step. Our results illustrate the utility of coprecipitation synthesis as a means for scale-up of next generation Li-ion cathodes and the ability to stabilise these materials by fine tuning the firing environment.



a) Initial charge-discharge profile of NMC-9.5.5 prepared at different firing loads at a rate of C/20. b) Cycle performance of NMC-9.5.5 prepared with boric acid (HB) and borax (BX) with the XRD profiles and the corresponding (003)/(104) Bragg peak ratios.

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Responses of metal-organic frameworks to various pressure states

Georgina Robertson¹ and Thomas Bennett.²

¹ University of Cambridge,

² University of Cambridge.

Metal-organic frameworks (MOFs) are highly porous crystalline materials composed of metal-based nodes connected into a framework by organic linkers. They have many potential applications in catalysis, gas storage and separation, biomedicine and sensing. This is primarily due to their large surface areas, with reported Brunauer-Emmett-Teller (BET) surface areas of up to 7000 m² g⁻¹, more than three times that of activated carbon.^{1,2} MOFs can also be designed with specific properties such as high selectivity for certain species, by altering the node or linker as needed.

However, MOFs demonstrate low mechanical stabilities, and tend to undergo pore collapse and amorphization when pressure is introduced. This has implications for their industrial utility, as shaping of the crystalline powders is often necessary for usage. Understanding the mechanisms of collapse will allow tailoring of MOFs to increase their mechanical stabilities and allow retention of high surface areas during processing.

This work examines the response of three zirconium-based MOFs (UiO-66, NU-1000 and MOF-808) to two processes used in industry that involve pressure: Pelletization and ball-milling. The crystalline structure of each was seen to collapse into an amorphous phase, with UiO-66 being the most stable. This is due to it having a more robust topology than the others (as predicted by Moghadam et al.³), shorter linkers and higher connectivity of the metallic node.

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Optimising Synthesis of LiNiO₂ cathode material for Li-ion batteries

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¹ School of Chemistry, University of Birmingham, Birmingham, B15 2TT

Battery technology currently is still not able to meet the ever-growing demands of the EV industry including high safety, lower cost and longer driving times between charges.¹ With the battery and particularly the cathode material being the most expensive component, researchers are focused on developing high-performance materials that can accommodate these requirements.

The layered oxide cathode material LiCoO₂ has been shown to be a successful commercial material. However, it also has severe drawbacks including only reaching approximately half of its theoretical capacity. Furthermore cobalt is expensive, unevenly distributed globally with serious ethical concerns, and current reserves are running low.^{2,3} With the desire to drive down costs and eliminate the use of cobalt, LiNiO₂ has been explored as a potential cathode material since the 1990s. In February 2021 the price of Co was 5 times that of Ni, with Ni also being more abundant.⁴ Although LiNiO₂ has a promising theoretical capacity of 274 mAh g⁻¹ and a higher experimental capacity than LiCoO₂, the material suffers its own drawbacks which limits its application as a commercial material. This includes LiNiO₂ currently suffering fast capacity fade and being very difficult to synthesise with the correct stoichiometry due to cation mixing, with the easy reduction of Ni³⁺ to Ni²⁺.⁵ The presence of Ni²⁺ ions results in Ni accommodating some of the Li⁺ sites within the Li layers and vice versa, leading to antisite defects and structural disorder.^{6,7}

This work therefore focusses on optimising synthesis of stoichiometric LiNiO₂, through systematic study of different synthesis routes, with variations in synthesis time, temperature, atmosphere, lithium source and lithium excess.

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Raman spectroscopy insights into the α - and δ -phases of formamidinium lead iodide (FAPbI₃)

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Solar perovskites have received phenomenal attention and success over the past decade, due to their high power conversion efficiencies (PCE), ease of fabrication and low cost which has enabled the prospect of them being a real commercial contender to the traditional silicon technology. In one of the several developments on the archetypal MAPbI₃ perovskite absorber layer, FAPbI₃ was found to obtain a higher PCE, likely due to its more optimum band gap, with doping strategies focusing on the inclusion of MA⁺/Cs⁺ cations to avoid the unfavourable phase transformation to a photo inactive phase. To better understand the phase change from the photoactive cubic (Pm-3m) black (α) phase to the unwanted photoinactive (P6₃mc) yellow (δ) phase, we make use of variable temperature Raman spectroscopy to probe the molecular species and its relationship to the inorganic framework. We show there to be no Raman active modes for the α phase up to 4000 cm⁻¹, which can be correlated to the Pm-3m cubic symmetry of that phase. Our results suggest that previous reports of the observation of Raman peaks for this phase are likely associated with degradation reactions from the localised laser exposure and the formation of Raman active lead oxide. In addition, we have identified water as a contributing factor to the transformation, and observed a corresponding signal in the Raman spectra, although confirmation of its exact role remains inconclusive.

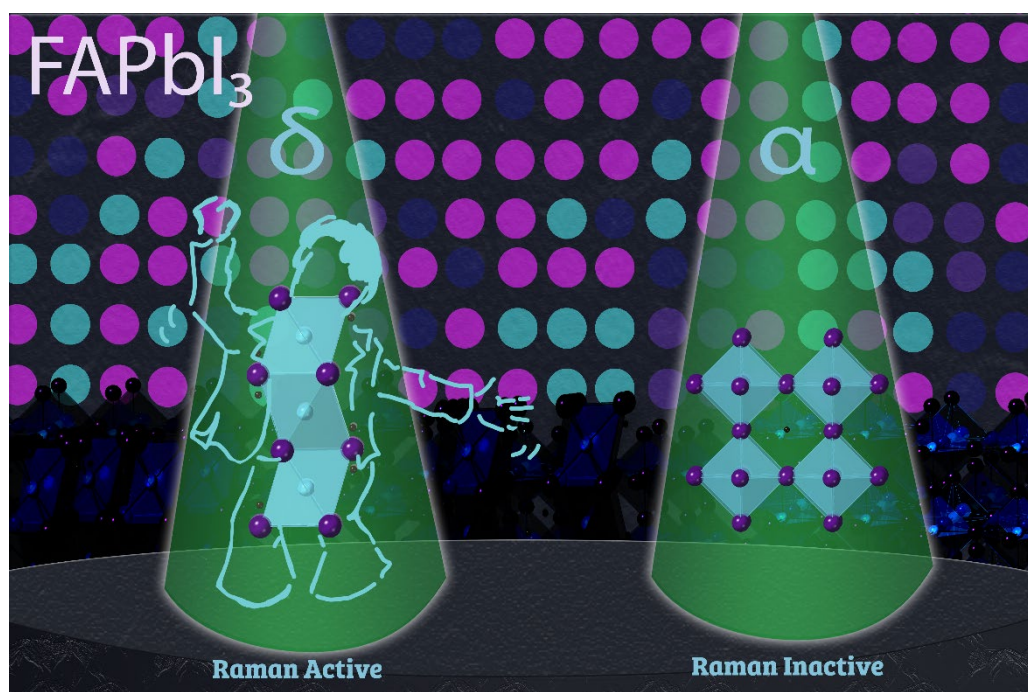


Figure 1: Graphical abstract depicting the δ -FAPbI₃ phase to be Raman active, while the α -phase remains inactive.

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Synthesis of Borate doped $\text{La}_{10-x}\text{Y}_x\text{GeO}_6\text{O}_{27}$: Confirming the Presence of a Secondary Conducting Pathway

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Lanthanum silicate/germanate apatite materials have attracted significant interest as Solid Oxide Fuel Cell electrolytes due to their high oxide ionic conductivity at lower temperatures (500-800 °C). In these structures, oxide ion conduction is due to interstitial pathways associated with the high oxygen excess within the structures. Therefore, cation doped $\text{La}_{8+x}\text{A}_{2-x}(\text{M}_{6-x}\text{B}_x\text{O}_4)\text{O}_{2+x/2}$ (A = Ca, Sr, Ba; M = Si and Ge; B = Mg, Ga, Al, Zn, B) have been reported to increase oxide ion conductivity via the introduction of excess oxide ions.^[1-3]

Whilst apatite silicate has higher conductivities at lower temperatures due to lower activation energies, apatite germanates can achieve higher oxygen excess and therefore higher conductivities at elevated temperatures. However, in increasing oxygen content there is a change in symmetry from hexagonal to triclinic leading to a subsequent reduction in conductivity.^[4] Previous studies have shown the issue may be overcome by the incorporation of Y doping e.g $\text{La}_8\text{Y}_2\text{GeO}_6\text{O}_{27}$ which leads to stabilisation of the higher conducting hexagonal phase.^[5]

Herein, we demonstrate the successful incorporation of borate into $\text{La}_{10-x}\text{Y}_x\text{GeO}_6\text{O}_{27}$ and show that it also stabilises the higher conducting hexagonal form. We show that B can be doped into both the Ge site and the oxide ion channels. Interestingly, the conductivity of samples with borate in the channels (which would be expected to block channel oxide ion conductivity along the *c* direction) is still reasonably high, which supports suggestions that there is significant conduction perpendicular to the channels in these apatite germanates.

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Session 2

Oral Abstracts

15:30 - 17:00

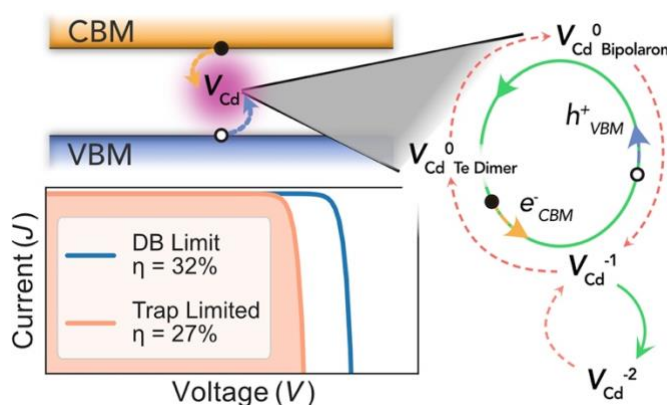
Rapid Recombination by Cadmium Vacancies in CdTe

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The ability to accurately model, understand and predict the behaviour of crystalline defects would constitute a significant step towards improving photovoltaic device efficiencies and semiconductor doping control, accelerating materials discovery and design.¹ In this work, we apply hybrid Density Functional Theory (DFT) including spin-orbit coupling to accurately model the atomistic behaviour of the cadmium vacancy (V_{Cd}) in cadmium telluride (CdTe).¹ In doing so, we resolve several longstanding discrepancies in the extensive literature on this species.

CdTe is a champion thin-film absorber for which defects, through facilitation of non-radiative recombination, significantly impact photovoltaic (PV) performance, contributing to a reduction in efficiency from an ideal detailed-balance limit of 32% to a current record of 22.1%. Despite over 70 years of experimental and theoretical research, many of the relevant defects in CdTe are still not well understood, with the definitive identification of the atomistic origins of experimentally observed defect levels remaining elusive.^{2–4}

In this work, through identification of a tellurium dimer ground-state structure for the neutral Cd vacancy, we obtain a single negative-U defect level for V_{Cd} at 0.35 eV above the VBM, finally reconciling theoretical predictions with experimental observations. Moreover, we reproduce the polaronic, optical and magnetic behaviour of V_{Cd} ¹ in excellent agreement with previous Electron Paramagnetic Resonance (EPR) characterisation.^{5,6} We find the cadmium vacancy facilitates rapid charge-carrier recombination, reducing maximum power-conversion efficiency by over 5% for *untreated* CdTe—a consequence of tellurium dimerisation, metastable structural arrangements, and anharmonic potential energy surfaces for carrier capture.



The origins of previous discrepancies between theory and experiment, namely incomplete mapping of the defect potential energy surface (PES) and approximation models, are highlighted and discussed. Importantly, these results demonstrate the necessity to include the effects of both metastability and anharmonicity for the accurate calculation of both charge-carrier recombination rates in emerging photovoltaic materials and the efficiency limits imposed by both native and extrinsic defect species.

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Electronic phase segregation in the 6H-perovskite $\text{Ba}_3\text{SrMo}_2\text{O}_9$ S. Simpson¹, S. Fop¹, H. A. Hopper¹, G. B. G. Stenning², C. Ritter³, and A. C. Mclaughlin¹¹ University of Aberdeen, Meston Walk, Aberdeen, AB24 3UE, U.K.² ISIS Experimental Operations Division, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, OX11 0QX, U.K.³ Institut Laue Langevin, 71 Avenue des Martyrs, BP 156, F-38042 Grenoble Cedex 9, France.

Strongly correlated transition metal oxides are renowned for their ability to segregate into multiple competing phases with distinct electronic properties. Prominent examples include colossal magnetoresistant (CMR) manganites, where chemical disorder mediates segregation into ferromagnetic metallic and antiferromagnetic charge/orbital-ordered states¹. This phenomenon has drawn considerable attention in oxides containing 3d transition metals, yet reports are comparatively scarce for their 4d/5d counterparts.

In recent years, 6H-perovskites of the form $\text{Ba}_3B'M_2\text{O}_9$ (B' = rare earth, M = 4d/5d transition metal) have been investigated for their potential to exhibit spin-liquid ground states². This structure type is distinguished by bioctahedral $M_2\text{O}_9$ dimers; short distances between the M cations, combined with spatially diffuse 4d/5d orbitals, can facilitate the formation of quasi-molecular $M_2\text{O}_9$ clusters with spin-gapped excitations³. However, most $\text{Ba}_3B'M_2\text{O}_9$ compositions feature magnetic moments localised on the M cations so that the formation of quasi-molecular clusters is suppressed.

We have observed an unprecedented electronic phase segregation (EPS) in the new 6H-perovskite $\text{Ba}_3\text{SrMo}_2\text{O}_9$. Below 230 K, $\text{Ba}_3\text{SrMo}_2\text{O}_9$ segregates into two electronically distinct phases: a hexagonal $P6_3/m$ phase consisting of $\text{Mo}^{5+}_2\text{O}_9$ spin dimers, and a monoclinic $P2_1/m$ phase containing stripe-ordered quasi-molecular $\text{Mo}^{5+}_2\text{O}_9$ clusters and localised Mo^{5+} spins (**Figure 1**). We propose this segregation has a unusual origin related to competition between direct Mo–Mo bonding and Mo–O–Mo superexchange. In contrast to established electronic materials like CMR manganites, EPS appears to manifest without the aid of charge order or chemical disorder. Accordingly, $\text{Ba}_3\text{SrMo}_2\text{O}_9$ comprises a seemingly unique electronic material.

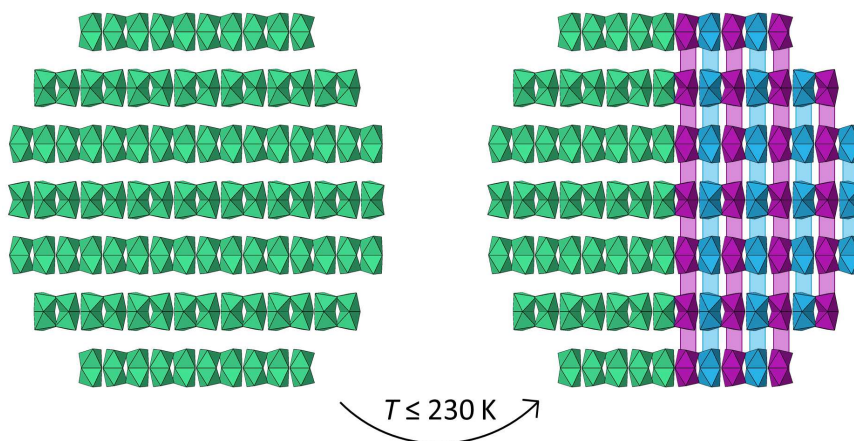


Figure 1. Electronic phase segregation in $\text{Ba}_3\text{SrMo}_2\text{O}_9$.

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Synthesis of new cation-ordered perovskite oxides under high-pressure and investigation of their magnetic properties

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² Univ. Lille, CNRS Centrale Lille, Univ. Artois, UMR 8181, UCCS Unit de Catalyse et Chimie du Solide, F-59000 Lille (France).

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Perovskites, with general formula ABO_3 , and related structures have been extensively studied due to their large variety of interesting physical properties. The use of A and B site cations with different sizes and charges induce cation order giving rise to $AA'B_2O_6$ and $A_2BB'O_6$ double perovskites (DPv).^{1,2} Furthermore, both sites can become ordered giving rise to double double perovskites (DDPv) $AA'BB'O_6$. The A site is usually occupied by a large cation with 12-fold coordination, but it can host smaller cations comparable in size to the B-site cations. The smaller the ionic radius of A, the higher the distortion and higher pressures are required to stabilise the perovskite structure.^{3,4} Two new materials synthesised under high-pressure are reported here.

$CaMnCrSbO_6$ adopts the DDPv structure with space group $P4_2/n$, combining columnar order over the A-sites, while B-sites ordered in rock-salt arrangement.⁵ $CaMnCrSbO_6$ shows collinear ferrimagnetism below $T_C = 49$ K, where Mn^{2+} and Cr^{3+} spins order into antiparallel ferromagnetic sublattices. $CaMnMnWO_6$ shows a complete structural phase transition from DDPv to $(Ca_{0.5}Mn_{0.5})_2MnWO_6$ (DPv), which has been driven by temperature at 10 GPa. Structural transition here also dramatically switches the magnetic properties as DDPv phase shows a ferrimagnetic spin ordering below 45 K. A-site and B-site spins are coupled antiferromagnetically with all pointed along the z-axis. While with disordered A-site cations in DPv- $CaMnMnWO_6$, a much lower spin freezing temperature $T_m = 8$ K was observed and was confirmed to have a spin glass feature.⁶

References

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Cheese & Wine Social

17:00 - 18:00

The organisers will set up breakout rooms if you wish to socialise.

Have some snacks and a drink ready (doesn't have to be alcoholic, we highly rate tea!).

Day 2

Friday 17th September 2021
10:00 - 17:00 (BST)

Session 3

Oral Abstracts

10:05 - 11:35

The Building Blocks of Battery Technology:

Inspiring the next generation of battery researchers

Elizabeth H. Driscoll¹, Ruth Patchett², Emily Hayward¹, Paul. A. Anderson¹,

Emma Kendrick³ and Peter R. Slater¹

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Since the turn of the century, secondary batteries have become big business. The portable electronics industry in the 1990's was driven by the design of the Li-ion battery, and in more recent times, these batteries are underpinning the drive for electrification of vehicles to mitigate the increasingly apparent effects of climate change; thus Li-ion batteries can be described as being everywhere in everyday life.

With our reliance on portable electronics, and the growth of the electric vehicle market, it is important to not only inspire the younger generation to think of their future career in the sciences, but also allow for important concepts which relate to policy to be accessible and understandable to the wider public.

Common current outreach demonstrations for battery work make use of potato-/lemon-electrolyte batteries with a copper coin and zinc nail. Although a great demo to introduce the concept of electrochemical potentials between the metals and circuits, students often struggle to differentiate between the two types of batteries – primary (non-rechargeable) and secondary (rechargeable) and often mistakenly assume the voltage generated to originate from the potato/lemon itself.

With this in mind, we have set out to create demonstrations, which can complement primary battery demos, while showcasing operation of rechargeable batteries using the LiCoO_2 – graphite as a basis of the set-up. The talk will highlight our work from the past year through a variety of demonstrations, including our battery jenga¹ set-up and the Royal Society of Chemistry IYPT2019 funded Lithium Shuffle Project battery operation videos². The talk will also highlight more recent resources and advances during COVID19.



Figure 1: Left - Jenga adapted to mimic the electrode set-up of LiCoO_2 – graphite cell, tactile textures to be accessible for blind and partially sighted students. Right - The Royal Society of Chemistry IYPT2019 funded Lithium Shuffle Project – human sized battery demonstration videos showing charging and discharging processes, suitable for 12+.

1 E. H. Driscoll, E. C. Hayward, R. Patchett, P. A. Anderson and P. R. Slater, *J. Chem. Educ.*, 2020, **97**, 2231–2237.

2 Lithium Shuffle. <https://www.rsc.org/news-events/community/2020/mar/lithium-shuffle/> (accessed January 2021)

Ternary nitrides as rapid and durable electrocatalysts

Yao Yuan,^{1,2} Samira Adimi,² Peilin Liao,³ Ye Zhu,⁴ Jiacheng Wang,⁵ Minghui Yang² and J. Paul Attifield¹

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² Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201, China

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Efficient catalysts are required for both oxidative and reductive reactions of hydrogen and oxygen in sustainable energy storage and conversion technologies, which has become a key requirement to satisfy rising global energy demand.¹ In a number of cases, the catalytic performance of nitrides is analogous with that of noble metals,² due to their very similar Fermi energy and electronic structure to that of group VIII noble metals,³ but their activity mechanisms are unclear.

Urea-glass route is employed to synthesize a ternary nitride $\text{Ni}_2\text{Mo}_3\text{N}$ ⁴ which is found to be an outstanding oxygen evolution reaction (OER) catalyst that outperforms the benchmark material RuO_2 . $\text{Ni}_2\text{Mo}_3\text{N}$ exhibits a current density of 10 mA cm^{-2} at a nominal overpotential of 270 mV in 0.1 M KOH with outstanding catalytic cyclability and durability. Structural characterization and computational studies reveal that the excellent activity stems from the surface electronic structure of active Ni-sites and Mo electron pumps in the discovered surface oxide-rich activation layer. Similarly, porous $\text{Co}_3\text{Mo}_3\text{N}$ ⁵ prepared via a facile method is found to be an efficient and reliable multifunctional electrocatalyst for three essential energy conversion reactions; OER, oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER) in alkaline solutions. In practical demonstrations, $\text{Co}_3\text{Mo}_3\text{N}$ gives high specific capacity ($850 \text{ mA h g}_{\text{Zn}}^{-1}$ at 10 mA cm^{-2}) as the cathode in a zinc-air battery, and a low potential (1.63 V at 10 mA cm^{-2}) using in a water-splitting electrolyzer. Availability of Co and Mo d-states appear to result in high ORR and HER performance, while the OER properties result from a cobalt oxide-rich activation surface layer.

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Exploring the magnetocaloric effect in the $Ln(\text{HCO}_2)(\text{C}_2\text{O}_4)$ family of Metal-Organic FrameworksMario Falsaperna¹, Paul J. Saines¹, Gavin G.B. Stenning², Ivan da Silva²¹School of Physical Sciences, University of Kent, Canterbury, UK,²ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, UK.

Low-temperature cooling is a necessary requirement in many areas of fundamental research and applied technologies. Many applications, including quantum computing¹, spintronics² and medical imaging, rely on liquid helium to operate at temperatures below 20 K. In particular, liquid helium ^4He is used for $T > 2$ K and a mixture of the two isotopes ^3He and ^4He is commonly employed for cooling below this. Liquid helium is costly, expensive and prone to disruptions in supply, so it is necessary to explore efficient and cost-effective alternatives. Paramagnetic magnetocalorics³ are great He-free candidates for low-temperature cooling, with much higher thermodynamic efficiencies below 20 K than cryocoolers, although most magnetocalorics are tailored for use below 1 K and very high applied fields.

Recent work on coordination frameworks have shown compound such as $\text{Gd}(\text{HCO}_2)_3$ and GdOHCO_3 , having comparable or greater MCEs than $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ (GGG), the benchmark magnetocaloric for cooling below 10 K, with the incorporation of other lanthanides leading to excellent performance above 4 K in low applied fields.^{4,5,6} Inspired by these results we have synthesised members of the $Ln(\text{HCO}_2)(\text{C}_2\text{O}_4)$ family ($Ln = \text{Gd}^{3+}$, Tb^{3+} , Dy^{3+} , Ho^{3+}) that crystallise in the orthorhombic $Pnma$ space group and feature low-dimensional chains arranged on a distorted triangular lattice. We have studied the magnetic properties and MCE of these materials.

We have found $\text{Gd}(\text{HCO}_2)(\text{C}_2\text{O}_4)$ to be an excellent candidate for applications at around 2 K with one of the highest magnetocaloric entropy changes amongst coordination frameworks. Generally, the incorporation of Ising-like cations was previously shown to lead to improved performance at higher temperatures under low applied fields that can be generated more easily using permanent magnets. We have observed this only for $\text{Dy}(\text{HCO}_2)(\text{C}_2\text{O}_4)$, in contrast with results found for the $Ln(\text{HCO}_2)_3$ and $Ln\text{OHCO}_3$ families of compounds. Indeed, characterisation using neutron diffraction indicates these compounds might lack the strong local magnetic correlations found in the related analogues, indicating this likely negatively affects the optimisation of the MCE performance for these compounds.

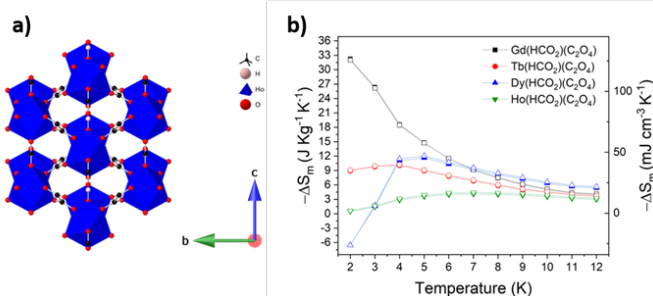


Fig. 1: a) Crystal structure of $\text{Ho}(\text{HCO}_2)(\text{C}_2\text{O}_4)$ with infinite 1-D chains arranged in a triangular lattice on the bc -plane. b) Maximum entropy change $-\Delta S_m^{\max}$ for a magnetic field change of 0-2 T for members of the $Ln(\text{HCO}_2)(\text{C}_2\text{O}_4)$ family with filled and hollow symbols representing gravimetric and volumetric $-\Delta S_m^{\max}$, respectively.

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Poster Session

2

14:30 - 15:30

Organic acid leaching of LiMn_2O_4 from mixed cathode materials

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¹ School of Chemistry, University of Birmingham, B15 2TT, UK.

As the number of electric vehicles increases there is a consequent increase in the number of spent lithium ion batteries that need to be recycled. Recycling processes often focus on the cathode as it accounts for around a third of the cost of the battery.¹ The cathode is normally made from a mixture of different transition metal oxides as this allows the advantageous properties of the different materials to be combined. For example, LiMn_2O_4 (LMO) is often combined with $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ (NCA) to provide good thermal stability along with high capacity and long lifetime.^{2,3} However, this increases the complexity of recycling as there are more components within the cathode that must be considered during recycling processes.

This poster reports that a weak organic acid can selectively leach LMO from the cathode into solution while leaving the remaining NCA as a solid. 1 M acid at 50 °C was found to completely leach 30 g/L of cathode material in 20 minutes. The leaching process also acts as a delamination step to remove the remaining NCA from the aluminium current collector. This LMO can then be recovered or upcycled to form new cathode materials while the leftover cathode materials can then be regenerated before being reused in new lithium ion batteries.

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Influence of $6S^2$ Bi^{3+} cation on the structures of $\text{A}'\text{BiNb}_2\text{O}_7$ ($\text{A}' = \text{Rb}, \text{Li}, \text{Na}, \text{K}$) layered perovskites

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Solids with non-centrosymmetric (NCS) crystal structures are extremely rare as centrosymmetric packing configurations are inherently more stable than asymmetric analogues. The most common approach to synthesize NCS materials is to utilize a Second Order Jahn-Teller (SOJT)¹ effect. An alternative non-conventional approach is to use “octahedral rotations and tilting” in perovskite lattices to engineer non-centrosymmetric structures. Recent theoretical² and experimental³ studies have demonstrated the possibility of breaking the inversion symmetry in layered perovskites using a mechanism known as the “hybrid improper mechanism.”

We have reinvestigated the $n = 2$ Dion-Jacobson phase $\text{RbBiNb}_2\text{O}_7$ and carried out monovalent cation exchange reactions to synthesize $\text{LiBiNb}_2\text{O}_7$, $\text{NaBiNb}_2\text{O}_7$ and KBiNb_2O_7 layered perovskites. Second harmonic generation, synchrotron X-ray diffraction and neutron powder diffraction data were used to determine the structure of these phases, and understand the effect of interlayer cation size and asymmetric coordination geometry of Bi^{3+} ion on octahedral tilting and structural distortions.

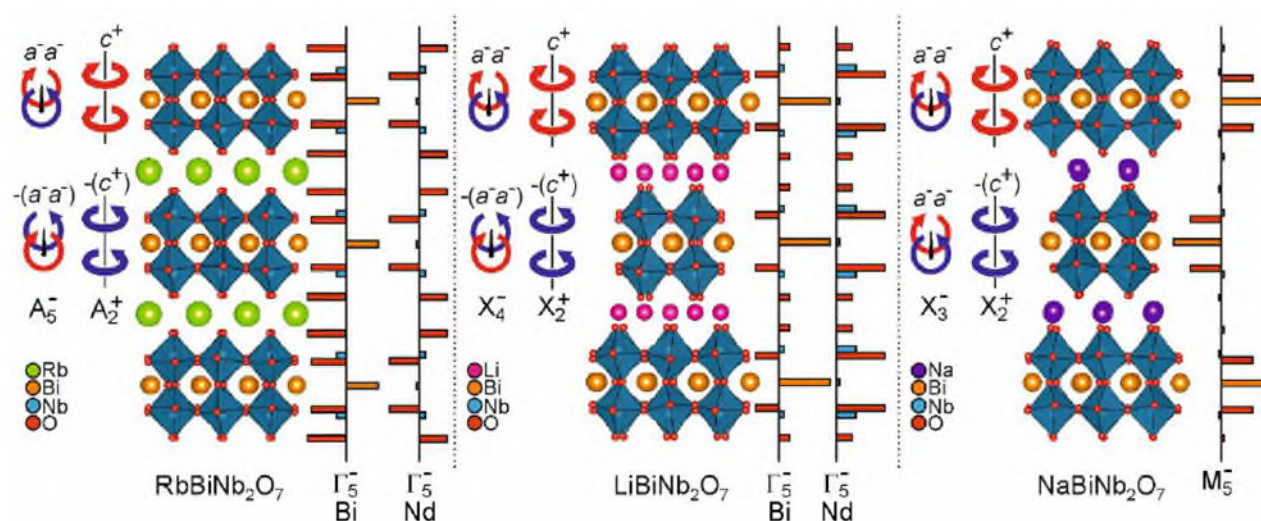


Figure 1. The structural distortions of $\text{A}'\text{BiNb}_2\text{O}_7$ ($\text{A}' = \text{Rb}, \text{Li}, \text{Na}$) phases. The distortion modes relate to the experimental structures to the $P4/mmm$ or $I4/mmm$ aristotype structures.

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- (2) Benedek, N. A. Origin of Ferroelectricity in a Family of Polar Oxides: The Dion-Jacobson Phases. *Inorg. Chem.* 2014, **53**, 7, 3769-3777.
- (3) Zhu, T.; Cohen, T.; Gibbs, A. S.; Zhang, W.; Halasyamani, P. S.; Hayward, M. A.; Benedek, N. A. Theory and Neutrons Combine To Reveal a Family of Layered Perovskites without Inversion Symmetry. *Chem. Mater.* 2017, **29**, 21, 9489-9497.

Re-examination of the polar transition in $(\text{N}_2\text{H}_5)\text{Mg}(\text{HCO}_2)_3$: Evidence of potential proton migration

Thomas Hitchings,¹ Helen Wickins,² Ross Piltz,³ Anthony Phillips,⁴ Paul Hodgkinson,² and Paul Saines.¹

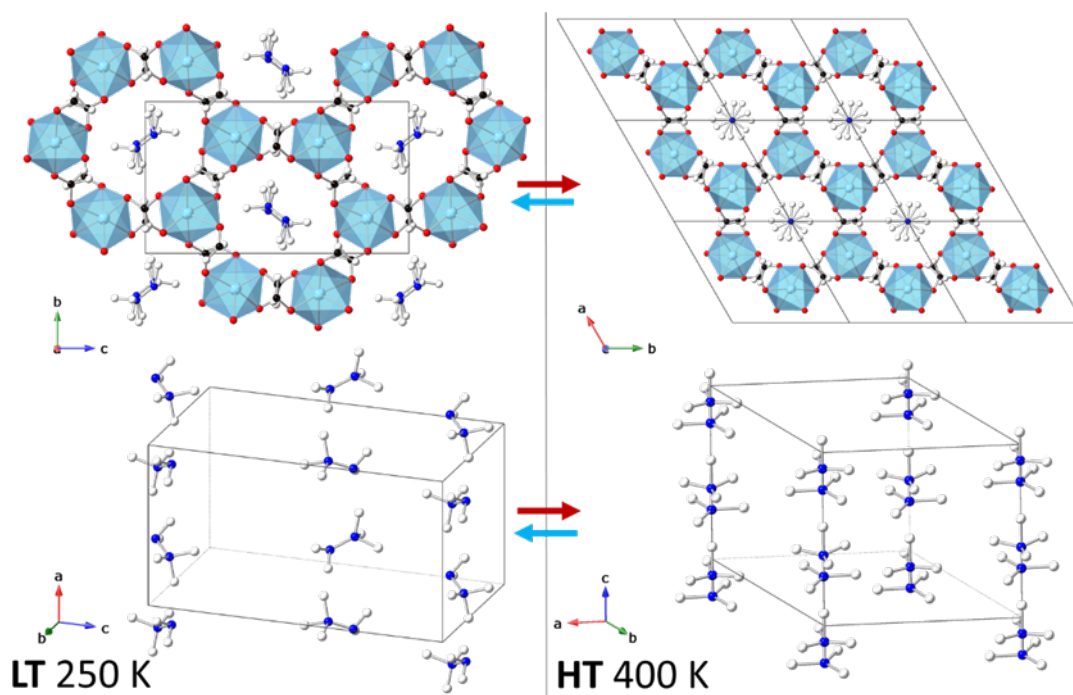
¹ School of Physical Sciences, Ingram Building, University of Kent, Canterbury, Kent, CT2 7NH,

² Department of Chemistry, Durham University, DH1 3LE, Durham, UK.

³ Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia,

⁴ School of Physics and Astronomy, Queen Mary University of London, London, E1 4NS,

Dense frameworks are extended solid-state materials with limited or occupied porosity. These materials can exhibit many properties, including the expression of electrical, magnetic, and conductive phenomena. $\text{AB}(\text{HCO}_2)_3$ frameworks have been widely studied for their potential ferroelectric properties, which arise from ordering of amine-based molecular A-site cations in the cavities of the framework as a result of strong H-bonding interactions between the cations and the formate ligands. Among these, $(\text{N}_2\text{H}_5)\text{Mg}(\text{HCO}_2)_3$ is particularly interesting, undergoing an order-disorder transition above ambient temperature with frequency dependant dielectric spectroscopy consistent with relaxor-like behaviour. Furthermore, the material transitions from a centrosymmetric $P2_12_12_1$ phase at low temperature (LT) to a polar $P6_3$ phase on heating (HT).¹ The origin and dynamics of these unusual ferroelectric properties are unclear; therefore, we have re-examined the phase transition in this material using a combination of single crystal neutron diffraction, quasielastic neutron scattering, and solid-state NMR. These studies indicate the transition is associated with the reorientation of the NH_3NH_2 cations within the pores, with the alignment of the molecular cations along the channel direction, allowing the hopping of protons between neighbouring molecules. This provides new insights into the origins of the promising ferroelectric properties of this material.



References

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Synthesis and topotactic manipulation of layered oxysulfide $\text{CaSrMnO}_2\text{Cu}_{4-\delta}\text{S}_3$

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The utilization of transition-metal based layered compounds is already established in industrial applications. Considering a combination with mixed-anion systems creates an extended pool of materials that can be screened for superior functionality. The option for post-synthetic alterations to the system offers further possibilities to control properties and gives access to kinetically stable products.

Previous works explored the possibility to influence magnetic properties and reversibly insert lithium in the oxysulfides $\text{Sr}_2\text{MnO}_2\text{Cu}_{2m-\delta}\text{S}_{m+1}$ ($\delta \approx 0.5$).¹⁻³ While trying to minimize the weight of these materials we obtained the compound $\text{Ca}_x\text{Sr}_{2-x}\text{MnO}_2\text{Cu}_{4-\delta}\text{S}_3$ with $x = 1$ and $\delta \approx 0.5$ by ceramic synthesis. The compound consists of antifluorite-type copper sulfide double layers exhibiting a copper deficiency and square planar MnO_2 sheets separated by the alkaline-earth cations. The copper ions in this material exhibit high mobility enabling topotactic cation exchange and deintercalation reactions enabling access to kinetically stable products. We show how oxidative copper deintercalation provides control over the oxidation state of Mn, thus altering the magnetic properties, and how replacing Cu^+ by Li^+ under reductive ion exchange conditions also makes the material interesting for lithium ion battery applications.

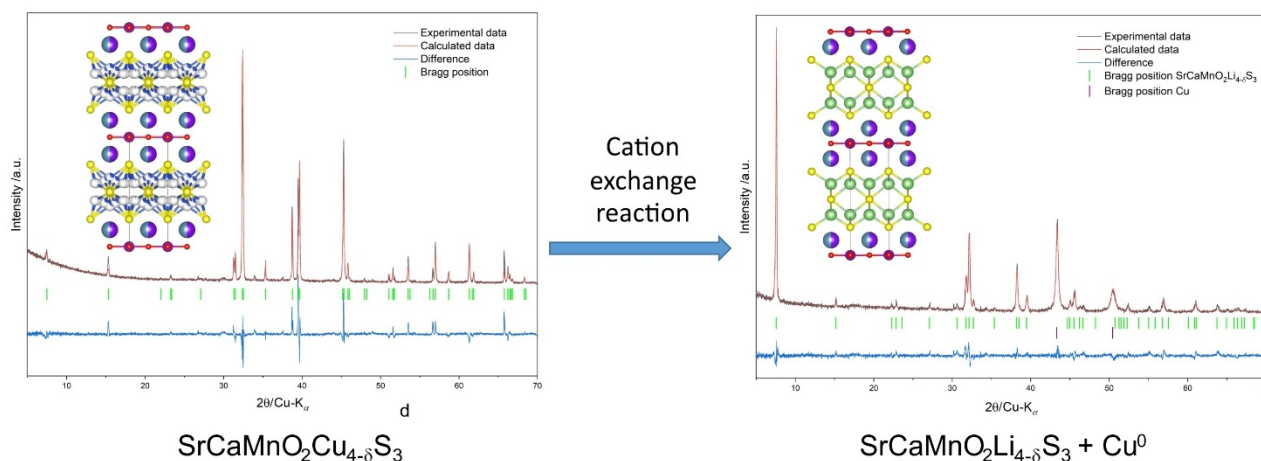


Figure 1: The compound $\text{SrCaMnO}_2\text{Cu}_{4-\delta}\text{S}_3$ can be topochemically modified by reductive cation exchange to form $\text{SrCaMnO}_2\text{Li}_{4-\delta}\text{S}_3$.

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LiFe_{2-x}In_xSbO₆ Oxides as Li-ion Electrode Materials

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Li-ion batteries have transformed daily life by acting as energy dense, rechargeable power sources for a wide range of electronic devices. As part of the UK Faraday Institute FutureCat project¹ we are investigating a range of new lithium-ion battery cathode materials for application in all-electric vehicles. In addition to the normal requirements of maximizing energy density and power output, as part of this project we are also trying to move away from cobalt-based materials due to their poor environmental impacts; we have focused on materials containing earth-abundant elements, with a particular emphasis on iron-based materials. Most of the iron, in particular, Fe³⁺ materials, that have been investigated to-date suffer from a capacity loss after long term cycling, although a good performance can be achieved for the first cycle². This capacity loss is generally attributed to the easy migration of Fe³⁺ between different coordination sites. To get more insight into these issues, we are currently investigating a novel Fe-based system, LiFe_{2-x}In_xSbO₆.

In the present work, we have performed a detailed structural characterization of the different members of the solid solution, as well as their electrochemical properties. Based on these results, we will discuss the implications of partial substitution of Fe by In over the electrochemical performance of these Fe-based materials.

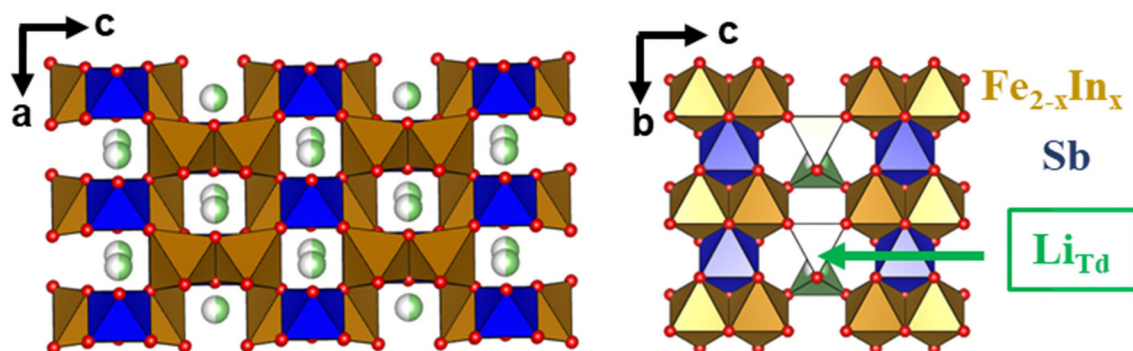


Figure. Crystal structure of LiFe_{2-x}In_xSbO₆.

References

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Temperature Dependence of the Physicochemical Characteristics and Glucose-sensing Behaviour of Copper Oxide Nanostructures Synthesised by Hydrothermal Method

Yujiang Zhu,¹ and Anna Regoutz.¹

¹ Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, UK.

Non-enzymatic glucose sensors are gradually replacing their enzymatic counterparts due to their advantages in stability and efficiency in glucose detection.¹ Copper oxide, especially in nanostructural form, is a promising candidate to fabricate non-enzymatic glucose sensors, due to its tuneable size and shape-dependent behaviour as well as electrochemical properties.² However, extensive previous work shows that even if the synthesis is performed under nominally similar conditions, entirely different product nanostructures are obtained, resulting in different physical and chemical properties of the final product, thereby leading to different performance in glucose detection.³⁻⁴ A critical synthesis parameter for common hydrothermal synthesis routes is the temperature, where even minute variations can lead to dramatically different outcomes.

In this work, copper oxide (CuO) nanostructures are synthesised using a hydrothermal method, where the synthesis temperature is varied between 45 and 85°C. The physicochemical characteristics of the nanostructural samples are characterised extensively by SEM, TEM, XPS, Raman spectroscopy, and UV-Vis spectroscopy. Through this combination of techniques, the morphology, structure, surface chemistry and electronic structure of the nanostructures can be explored. Clear differences are observed following the change in synthesis parameters, including a change in morphology from nanoneedles to nanoparticles across the explored temperature range. Electrochemical tests to study the glucose sensing capability of the synthesised nanostructures show a high level of selectivity for all samples, and differences in behaviour are correlated with the results from physicochemical characterisation.

This work provides clear evidence of the strong influence the synthesis temperature has on the resulting nanostructures and ultimately on their performance in glucose sensors. It confirms the importance of the control of temperature and showcases how controlling it can enable targeting of specific nanostructures and sensing behaviour and performance.

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Hole and electron doping of the Topochemically Reduced $n = 1$

Ruddlesden-Popper Rhodium-Containing Oxides

Zheyang Xu¹, Robert G. Palgrave² and Michael A. Hayward¹

¹Inorganic Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford OX1 3QR, United Kingdom

² Department of Chemistry, University College London, London WC1H 0AJ, United Kingdom

Complex transition metal oxides exhibit a wide range of useful chemical and physical properties which can, in general, be rationally tuned and optimized by modifying the chemical composition and/or crystal structure of the system.

Anion vacancies can be introduced via topochemical reduction to modify the structure of complex transition metal oxides. Using this approach, a number of phases containing square planar transition metal centres can be made, such as Ni^{2+}O_4 square-planar centres in $\text{La}_2\text{Ni}_2\text{O}_5$, Fe^{2+}O_4 in SrFeO_2 , Ru^{2+}O_4 in LaSrNiRuO_4 [1].

Topochemical reduction of the $n = 1$ $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_4$ ($M = \text{Co}, \text{Ni}$) Ruddlesden – Popper phases with Zr yields $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_{3.25}$ [2], as shown in Fig.1. Magnetization and XPS data reveal that while the rhodium centres in the $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_{3.25}$ phases have an average oxidation state of Rh^{2+} , they are actually mixed valence $\text{Rh}(\text{I},\text{III})$ compounds, with the disproportionation of Rh^{2+} driven by the favorability of locating $d^8 \text{Rh}^{1+}$ and $d^6 \text{Rh}^{3+}$ cations within square-planar and square-based pyramidal coordination sites, respectively.

Inspired by the insulator-to-metal transition found in superconducting cuprates as a result of A-site doping [3], manipulations of the La:Sr ratio in $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_4$ were carried out to form phases of composition $\text{La}_x\text{Sr}_{2-x}\text{M}_{0.5}\text{Rh}_{0.5}\text{O}_4$ ($0.85 \leq x \leq 1.15$) which were subsequently reduced with Zr. Thermogravimetric data and synchrotron diffraction data have confirmed the number of oxygen vacancies in the structure. Magnetization data reveals the disproportionation of Rh centres and the oxidation/reduction scheme of B sites upon hole/electron doping. The detailed analysis is further discussed in the poster.

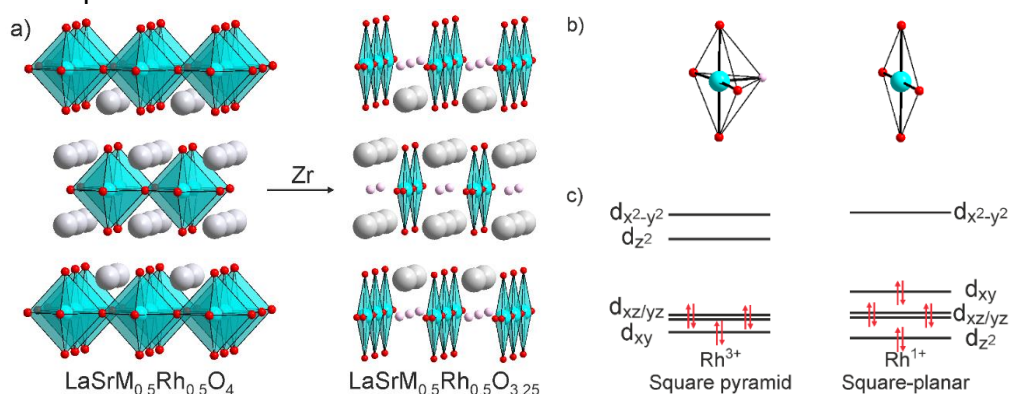


Fig.1 (a) Schematic of the conversion of $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_4$ to $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_{3.25}$. Grey, blue, red, and pink spheres represent La/Sr, M/Rh, O, and partially occupied O positions respectively. (b) Square-based pyramidal and square-planar transition metal coordination sites in $\text{LaSrM}_{0.5}\text{Rh}_{0.5}\text{O}_{3.25}$. (c) Local electronic configurations of $d^6 \text{Rh}^{3+}$ and $d^8 \text{Rh}^{1+}$ in square pyramidal and square-planar coordination, respectively.

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Session 4
Oral Abstracts
15:30- 17:00

Electrical transport properties of half-heusler ScPdBi single crystals under extreme conditions

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We synthesize single-crystals of ScPdBi, a Half-Heusler compound by self-flux growth technique and report its physical properties such as magneto-transport and specific heat down to 2 K. Resistivity measurements were performed on these single-crystals at ambient and high-pressure conditions. Temperature-dependent resistivity measurements reveal that ScPdBi has the metallic character at ambient pressure and without applied magnetic field. The metallic character of ScPdBi was un-altered even in extreme conditions such as high pressure (up to 19 GPa) and magnetic field (up to 9 T). We observe an upturn in the resistivity which persists even at high pressure. We rule-out the presence of the Kondo effect by performing the specific heat measurements down to 2 K which resulted in a low Sommerfeld coefficient ($\gamma = 2.6 \pm 0.9 \text{ mJ mol}^{-1} \text{ K}^{-2}$). This anomaly in resistivity below 30 K could be attributed to an electron-hole scattering process or a carrier imbalance effect¹.

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Recently, non-magnetic $B'' d^{10}$ and d^0 cations have been employed in $A_2B'B''O_6$ perovskites to tune the magnetic interactions between magnetic B' cations.¹ The differences in orbital hybridization can direct the interactions towards different types of magnetic ordering.^{2,3} Furthermore, introducing mixtures of d^{10} and d^0 cations introduces frustration that can stabilise novel quantum ground states. For example, introducing a 50:50 mixture of Te^{6+} (d^{10}) and W^{6+} (d^0) to the $Sr_2CuTe_{1-x}W_xO_6$ double perovskite creates a spin-liquid like state that evades magnetic ordering even at zero Kelvin.⁴

So far studies have focused on double perovskites, therefore we have investigated whether the d^{10}/d^0 effect can be extended to more complex perovskite structures. To do this we doped the hexagonal perovskite Ba_2CuTeO_6 with W^{6+} creating a $Ba_2CuTe_{1-x}W_xO_6$ ($0 \leq x \leq 0.3$) solution. The structural analysis we present shows W^{6+} strongly prefers to occupy the corner-sharing site in the hexagonal structure. This leads to site-specific tuning of the intra-ladder interactions in the Cu^{2+} spin-ladder structure.⁵ Our magnetic data suggests introducing W^{6+} d^0 leads to the formation of a quantum disordered ground state, similar to $Sr_2CuTe_{1-x}W_xO_6$. This further demonstrates the d^{10}/d^0 effect can be utilized in a of range perovskite structures to tune the material towards unusual quantum ground states, that are often difficult to realize experimentally.

KEYWORDS: Hexagonal perovskites, site-selective, spin ladder, quantum-disorder, synchrotron X-rays, neutron diffraction, EXAFS.

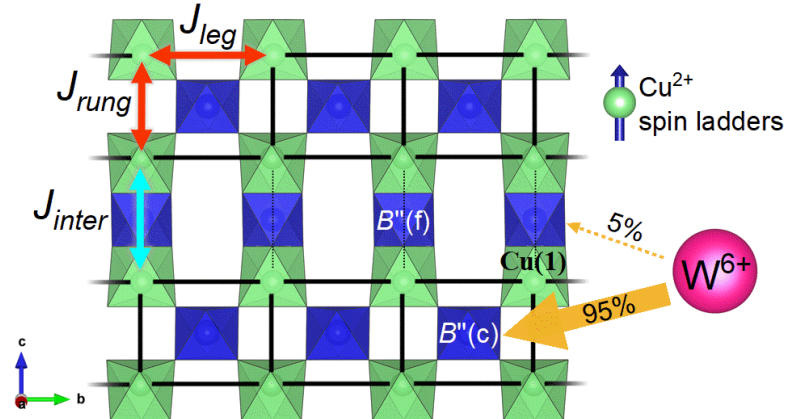


Fig. 1. The Cu^{2+} spin-ladder structure of $Ba_2CuTe_{1-x}W_xO_6$ wherein W^{6+} strongly prefers the corner-sharing $B''(c)$ site vs the face-sharing $B''(f)$ site. Hence, the d^{10}/d^0 effect site-selectively tunes the intra-ladder J_{leg} and J_{rung} interactions.

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Crystal and magnetic study on cation ordered $A_2B_2O_6$ phases.Kunlang Ji ¹ and J. Paul Attfield ¹¹ CSEC and school of Chemistry, University of Edinburgh, Peter Guthrie Tait Road, Edinburgh, UK

ABO₃ oxides have proven to accommodate a wide variety of chemical compositions, to crystallise with several structures in competition and to develop diverse physical properties. Hence, they are intensively studied in the search for new functional materials.¹ High pressure technique helps to stabilize structure with smaller cations that results in useful properties.² Here we present the cation ordered $A_2B_2O_6$ phases with interesting magnetic properties.

The $A_2B_2O_6$ double corundum phase Co_2ScSbO_6 adopt the polar Ni_3TeO_6 -type structure and order magnetically below 60 K.³ A complex incommensurate $[0\ 0\ k_z]$ spin structures coexist with a ferrimagnetic $[0\ 0\ 0]$ phase was discovered. Metamagnetic transition was observed in solid solution $Ni_{2-x}Co_xScSbO_6$ ($x < 0.5$) and the field neutron diffraction data confirms the presence of intermediated magnetic phases. The presence of electrical polarisation and spontaneous magnetisations offers possibilities for multiferroic properties.

The $A_2B_2O_6$ double double perovskite adopt the $P4_2/n$ tetragonal structure. Many of them has been synthesised since the first $RMnMnSbO_6$.⁴ Recently, a series of $RMnMnTaO_6$ perovskites were successfully prepared using the full range of rare earth cation group.⁵ The observed A-site order-disorder transition induces different magnetic behaviours. $CaMnFeB'O_6$ ($B' = Ta, Nb$) double double perovskite, on the other hand, exhibits anti-site cation disorder at all transition-metal sites, leading to the unusual cluster spin glass ground state.⁶

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Prizes & Closing

17:00