Warwick Battery Days (WBD 2024)
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WBD 2024 – POSTER ABSTRACTS

Syed Abdul Ahad
University of Limerick

3D Nanowire architectures for dendrite-free Li Metal Batteries

"Lithium-ion batteries (LIBs) continue to dominate as the most widely used rechargeable battery technology in our time. However, they are currently encountering challenges in meeting the increasing demands for energy density, particularly in applications such as electric vehicles (EVs) [1,2]. Lithium metal is highly regarded as a promising battery material, primarily because of its impressive theoretical capacity (3860 mAh g-1) and low electrochemical potential (-3.07 V vs. standard hydrogen electrode (SHE)) [3,4]. Nevertheless, the commercialization of LMBs faces several obstacles, including the formation of an unstable solid electrolyte interface (SEI), excessive growth of Li dendrites, and the risk of hazardous fires during battery operation [5].

In this work, we introduced a hierarchical nanowire (NW) – carbon fiber (CF) host design aimed at facilitating dendrite-free cycling in LMBs. Synthesized on CF hosts using a vapor-liquid-solid (VLS) method, these lithiophilic NWs were subsequently infused with Li. Crucial in this design is the morphology of the NWs, which played a pivotal role in reducing the local current density on the NW-CF surface, thereby inhibiting dendrite formation. Extensive testing, including evaluations of symmetric cells and full cells against LiFePO4 (LFP) and sulfur cathodes, showcased the superior performance of Li-infiltrated NW-CF hosts over pristine Li metal anodes. Employing comprehensive material and electrochemical characterization, along with density functional theory (DFT) calculations, enabled us to delve into the role of various lithiated phases in dendrite suppression during electrochemical cycling. These findings pave the way for leveraging lithiophilic NWs to suppress Li dendrite formation, thus facilitating uniform Li deposition for high-energy-density LMBs.

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Carla Albenga
WMG, University of Warwick

Understanding degradation of Sn-based anodes for sodium-ion batteries

Alloying materials are a promising class of negative electrodes for Sodium-ion batteries (SIBs). Among them, tin (Sn) represents the most interesting candidate due to its high theoretical capacity, sustainability, and low cost. However, they also suffer from poor structural stability due to severe volume expansion upon (de-)sodiation. To alleviate the damages caused by the volume changes, nano-structuration and morphology optimization have been proposed, yet such approaches bring disadvantages in terms of toxicity and high synthesis costs as well as low density and large surface area which affects the electrochemical performance. Recently, micrometric Sn (μ-Sn) anodes showed unexpected stability after Na (de-)alloying in a particular class of electrolyte, paving the way for new considerations and approaches in investigating these materials. Herein, we present a comprehensive investigation of Sn-based electrodes by monitoring the effect of particle size and active material composition on morphology evolution and stability of the anode, to elucidate the degradation mechanisms occurring during the (de-)sodiation process. Through electrochemical analysis, X-ray diffraction (XRD), and ex-situ cross-sectional SEM studies, it is found that composite electrodes with high content of μ-Sn mixed with Hard Carbon (HC), exhibit good stability, high reversibility of the process and long cycle life as a result of the growth of a robust porous network of metallic Sn. The proposed Sn/HC composite electrodes have been investigated also in full sodium-ion cells, shedding light on the optimal loading required to achieve high energy-dense cells, while maintaining cycling stability. Differences observed in half and full cells highlight the importance of evaluating these systems under defined conditions, where sodium inventory loss and electrode/electrolyte interphases play a crucial role.

Brad Ayers

University Of Southampton

Modelling the Lithium Anode-Electrolyte Interface under Potentiostatic control

"The resurgence of the lithium anode in solid-state batteries has sparked significant interest, mainly owing to its exceptional qualities. Lithium metal anodes boast a high theoretical specific capacity of 3860 mAhg−1 and a low density of 0.53 gcm−3 at 25°C [1]. When paired with solid-state electrolytes, these characteristics hold the potential to revolutionise energy storage technology by enabling the development of compact, high-energy-density batteries capable of achieving output voltages up to 6V, while eliminating the need for hazardous and flammable organic solvents.

In this study, we undertake a computational analysis to explore the surface dynamics of the lithium anode, focusing on how its low-energy surfaces may adapt or reorganise when subjected to an applied voltage. By calculating the surface energies of lithium surfaces under such conditions, we can construct Wulff shapes—a technique that visually illustrates how the anode's exposed surfaces may evolve under bias. Alongside creating the Wulff shapes, we can also gather qualitative information such as electrolyte concentration profiles and total charge densities. Thereby allowing us to probe and observe the chemistry at these interfaces, such as double layers, and the homogeneity of charge distribution, etc. Such properties are particularly challenging to measure experimentally, necessitating computational investigation.

Our computational investigations are conducted under a consistent applied bias, employing the grand canonical approach [2] within ONETEP, a state-of-the-art, linear-scaling density functional theory programme[3].

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Meisam Babaie
University of Leeds

Integrated Powertrain Design and Battery Thermal Management System Analysis for Heavy-duty Electric Trucks

Transport is the largest emitting sector in the UK, accounting for 24% of the total 406 MtCO2e emissions. Among different modes of transport, Heavy Goods Vehicles (HGVs) stand as the second-largest contributors with a 19% share. Electrification emerges as a potential solution, and the phase-out deadline for non-zero (tailpipe) emission HGVs has already been set in the UK for 2040. However, the electrification of HGVs will be more challenging compared to passenger cars regarding significant battery range and size requirements in this sector. There is a lot of qualitative information for and against HGV electrification, but reliable quantitative data and numbers based on scientific powertrain design and analysis are very limited. Furthermore, battery thermal management system (BTMS) design and analysis are usually conducted separately from the actual power demand originating from accurate powertrain design. Therefore, this work presents a comprehensive methodology for integrated powertrain and BTMS design with three different HGV use cases. This approach requires powertrain design and extraction of power demand during standard driving cycles first, and then applies the extracted power loads to the battery for developing BTMS analysis. Advanced simulation methods for powertrain design are used in AVL Cruise M software, followed by both 1D and 3D thermal analysis using CFD simulations. The result of this work is expected to bring new insights for both electric powertrain and BTMS design, contributing towards a more realistic analysis of HGV electrification.

Chantal Baer
University of Warwick

Simulating the microstructure and ionic conductivity of Li-metal/Li-argyrodite interfaces

"All solid-state batteries (ASSBs) have obtained increasing interest as next-generation battery technology due to their increased safety and the potential of enhanced energy density when combined with a Li-metal anode. However, mechanical failure arising at the interfaces can reduce ionic transport and thus limit the overall electrochemical performance of the battery. To develop a better understanding of the relationship between mechanical damage and ionic transport across various length scales, a multiscale modeling approach is required, linking first-principles calculations with the continuum framework via Bayesian inference.

The Li-metal/Li-argyrodite interface is well suited for this study due to the promising properties of Li-argyrodite (Li6PS5Cl) such as high ionic conductivity, and the increased performance the use of the Li-metal anode would offer. In this poster, I will detail the methodology used to create representative atomistic models for the Li-metal/Li-argyrodite interface based on the bulk structure and describe the challenges arising from size- and length-scale restrictions as well as a large configuration space at the atomistic scale. Using the resulting interface models, first principles and machine learning methods are used to simulate important parameters such as the chemical stability of the interface and the ionic conductivity within the bulk electrolyte and across the interface. The ionic conductivity is determined from the mean squared displacement of the ions, which can be extracted from a molecular dynamics (MD) trajectory. The longer MD trajectories that can be performed using machine-learned force fields allow for a more accurate description of the diffusion behavior and also enable us to study the early stages of solid electrolyte interface (SEI) formation which is crucial for the chemical stability of the solid-solid interface."

Arihant Bhandari
University of Southampton

Mechanisms of Li dendrite growth in Li-ion batteries

"Application of Li-ion batteries in electric vehicles requires improved safety, increased lifetime and high charging rates. One of the most commonly used intercalation anode material for Li-ion batteries, graphite, is vulnerable to Li nucleation, a side reaction which competes with the intercalation process and leads to loss of reversible capacity of the battery, ageing and short-circuits. In this study, we deploy a combined grand canonical large-scale electronic density-functional theory (DFT) and Poisson-Boltzmann electrolyte theory to study the nucleation and growth of Li clusters on the graphite anode in the presence of its surrounding electrolyte environment at different applied voltages with respect to the Li metal reference electrode. We find the voltage below which Li nucleation becoming energetically favourable (corresponding to the nucleation energy becomes negative), termed as the `potential of zero nucleation energy' (PZN). We observe a distinct minimum in the plots of PZN as a function of the size of nucleated clusters. When the applied voltage on the graphite electrode is below the minimum value of PZN, the nucleated clusters start growing unbounded on graphite electrode. We compare mechanisms of uniform surface coverage as well Li cluster growth. We observe that the potentials obtained with grand canonical ensemble DFT method in electrolyte are close to experimentally available data. The study has profound implications for the nucleation, growth and control of metal dendrites in a battery cell.

Bhandari et al. Li nucleation on the graphite anode under potential control in Li-ion batteries. J. Mater. Chem. A, 2022, 10, 11426"

Vidha Bhasin
Bhabhi Atomic Research Centre

Development of thin film electrodes for high performance lithium-ion micro-batteries

"As there is an increasing demand of microelectronic devices such as micro-batteries, the need of better performance within least possible space encourages comprehensive investigation on thin film electrodes for Li ion batteries (LIB). In this work we have prepared TiO2 thin film anodes for LIB on stainless steel (SS) substrates, wherein the top layer contributed as active material , and the bottom layer as current collector . This eventually boosted the energy as well as power density . We have obtained remarkable performance in LIB by utilizing the synergy between the structural stability of TiO2 and better diffusion kinetics of Fe2O3 layers present on the SS substrate [1,2].We could further improve the electrochemical performance of the LIB's at higher charge-discharge rate by doping TiO2 with transition metals (TM) [3]. Finally, we have obtained much superior performance in TiO2/ZnO thin film multilayer anode utilizing structural stability of TiO2 and high theoretical capacity as well as higher lithium diffusion properties of ZnO [4]. Additionally, we have optimised the fabrication of solid state electrolyte, lithium phosphorus oxynitride LIPON, and tested it with TiO2 and Li rich NMC 333 in half cell configuration. The cells have shown improved stability over the cycles. It has been observed that the LIB's fabricated with these easily scalable and highly reproducible magnetron sputter deposited thin film electrodes show very high capacity over large no.

of cycles in contrast with the conventional, more intricate, and multi-step chemical processes typically required for such electrode production.Hence, this study hold significant value for mass production of thin-film electrode-based LIB's, especially in the context of micro-battery applications when paired with solid-state electrolytes.

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Galen Brown
University of Oxford

Bilayering Enables Faster Charging and High Areal Capacity of Na-Ion Electrodes

"Sodium-ion batteries (NIBs) are a promising alternative to lithium-ion batteries (LIBs). Despite offering potential cost and safety advantages, NIBs still lag behind LIBs in capacity, power output and longevity. Considerable research effort is now being expended to develop more energy-dense electrodes in order for NIBs to become commercially viable.

A possible route to increasing the energy density of NIBs is to increase electrode thickness (and therefore areal capacity). However, achieving this in practice is limited by manufacturing and the rate performance. Slurry casting is the dominant manufacturing process for electrodes, where binder migration during the drying step typically constrains the maximum thickness to 50 - 90 μm. Furthermore, given the mobility of Na ions in the electrolyte in the torturous electrode pore network is normally restricted, thicker electrodes undergo greater polarisation and capacity loss as C-rate (current density) is increased.

Here we present a novel bilayer architecture of Na-ion positive electrodes obtained through slurry casting two successive sub-layers of different active materials: sodium manganese oxide (Na0.7MnO2, NMO) and sodium vanadium phosphate (Na3V2(PO4)3, NVP). The bilayer electrodes are 100 μm thick with high areal loading of ≈17 mg/cm2. While there is no distinction at low current densities (< 1C ≡ 45 mA/gcm2), for higher C-rates the overall electrode capacity is sensitive to the relative position of NMO and NVP sub-layers. There is a significant increase in retained capacity when the NMO sub-layer is on the current collector. The sensitivity of sub-layer position is shown to relate to the large difference in voltage-capacity profiles of NMO and NVP. We also discuss how differences in charge-transfer resistance, electrical conductivity, and ionic mobility within the two materials have a role in how the critical Na-ion concentration profile evolves through the charge/discharge cycle."

David Burnett
University of Birmingham

Synthesis and optimisation of lithium and manganese-rich layered oxides for high energy density cells.

"Li-rich oxides are promising cathode materials for Li-ion batteries. While the drive towards increasingly nickel rich layered oxides has long led the push towards higher energy density materials. More recently with the increasing cost of nickel, manganese rich materials are becoming increasingly appealing. Herein Li1.2Mn0.54Ni0.13Co0.13O2 is investigated due to its high specific capacity of ≈300mAhg-1 resulting from a combination of both cation and anion redox.

This material suffers from an irreversible phase transition in the first cycle and relatively large: first cycle loss; hysteresis between charge and discharge and voltage fade upon extended cycling.

Tuning particle morphology and composition directly affect the electrochemical performance of the cathode materials and can mitigate some of the issues described above. Our cathode precursors were synthesised by both carbonate and hydroxide based coprecipitations, forming “spherical” secondary particles in the desired range 2-50 microns, with controllable primary particles shape.

Upon firing layered materials displaying Li2MnO3 type superstructure as produced, as demonstrated by the low angle XRD peaks. Depending on the synthesis route, the materials have tap densities between 0.9-1.8gcm-3 and reliably achieves reversible capacities of 240-280mAhg-1 in half cells when allowed to access oxygen anion redox (2.0-4.8V vs Li @ 10mAg-1), however when cycling at moderate rate of C/2 only 200-210 mAhg-1 is accessible, with only 5% capacity fade observed over the course of 50 cycles. Further electrolyte exploration was performed in full cells before production of single layer pouch cells."

Tom Chamberlain
University of Warwick

The Salamander Project: Smart Sensors and Self-Healing Functionalities for Increased Li-ion Battery Longevity

"With the announcement of the European Green Deal,1 an intensified effort is directed towards achieving a set of challenging targets to enable Europe to become the first climate-neutral continent by 2050. In this context, the European Commission has recognized batteries as one of the most important key enablers for the green energy transition.

The SALAMANDER project revolutionizes LIBs by integrating embedded sensors and self-healing functionalities to enhance their quality and lifespan, creating smart batteries that can autonomously detect and repair damage.2 Sensors will be embedded at key locations to allow the degradation mechanisms to be detected. A battery management system will then trigger the self-healing at predetermined critical points.

Here, we present a preliminary chemical and electrochemical compatibility study of a variety of Ag- and Ni-based sensor inks with standard Li-ion cell components. The sensor inks are printed directly onto the anode and separator materials where they can then be incorporated directly into cells for comparison with ink-free cells. In a chemical compatibility study, electrodes and separators with and without printed inks are exposed to an excess of electrolyte under inert conditions. The electrolyte is monitored by a combination of H, F and P NMR over 2-months and we show that no degradation of the electrolyte occurs after exposure to the inks. We then present a study of the inks in half cell and full cell formats to determine the stability of the ink materials at a range of potentials. The impact of the sensor inks on cell performance is reported and subsequent forensic studies detail the effect of cycling potentials on the inks and electrodes. Preliminary integration studies of sensing functionalities are also reported shedding light on the challenges and opportunities of sensors embedded in LIBs.

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Davide Clerici
Politecnico di Torino

Mechanics of Lithium-Ion Batteries: Degradation and States Estimation with a Modeling and Experimental Approach

"During operation, lithium-ion batteries (LIB) experience mechanical deformation due to the strain induced by the electrochemical processes, involving the interaction of lithium ions with the crystal structure of the active material of electrodes. Such deformation originating at atomic scale has two effects: firstly, it has an impact on the macroscopic deformation of the battery; secondly the lithiation-induced deformation of the electrode microstructure (active material particles) causes the so-called diffusion induced stress finally leading to fracture propagation in the electrode and battery performance decay.

An electro-mechanical-thermal battery model is defined to study the mechanical phenomena in LIB. Starting from the DFN electrochemical model, the inhomogeneous concentration distribution in the active material particles causes stress and thus stress intensity factor is computed to assess the level of fracture in the electrode. Concentration in active material particles causes the deformation of the electrode as well. Then, the macroscopic deformation of the battery is evaluated with a multi-scale mechanical model on the basis of the concentration level in the electrodes and the battery temperature. In a second stage, degradation mechanisms such as SEI growth and fracture propagation (computed on the basis of stress intensity factor) are embedded in the model, to compute how the battery performance and responses (voltage, temperature and deformation) change with aging.

Experimental measurements quantifying LCO-Gr battery deformation, as well as the voltage and temperature responses during operation, and their change with aging (more than 1000 cycles until SOH<70%) confirm the quality of the results of the model.

The model goals are: (a)To understand how different design solutions impact battery performances and responses, considering aging. (b)To provide the physics framework for algorithms estimating SOC and SOH from deformation measurements."

Jacob Compton
University of Warwick (WMG)

Prussian White/Hard Carbon Sodium-ion cells: From Lab to Upscaled Cell Prototypes

"Recently, a great interest has emerged in rechargeable batteries based on abundant and non-critical raw materials. Sodium-ion batteries (SIBs) have the potential to become the next generation, sustainable, low cost and efficient energy storage technology. This has been recently confirmed by the growing interest in this technology of several battery producers and the many successful companies working toward SIB commercialization. However, further work is still needed to fully understand the structure-function correlation in several SIB active materials and to successfully validate lab scale results in industrially relevant scales.

This work provides an overview on the journey toward the development of 1 Ah sodium-ion cell prototypes linking chemistry and electrochemistry of the employed materials. Challenges on the transition from lab to scaled-up processes and the development of industrially relevant cell prototypes are discussed with a case study reporting results obtained within Horizon 2020 funded SIMBA (Sodium-ion and sodium metal batteries) project. The combination of electrochemical and material characterization of the electrodes used gives key indications of their electrochemical, structural, and morphological properties.

Herein, the electrochemical behaviour of an aqueous-processed Fe-based Prussian white (PW) cathode material and bio-mass derived hard carbon anode material is presented. We demonstrate that through solid content, processing, and formulation optimization, it is possible to successfully transition from lab-scale to upscaled cell manufacturing.

1 Ah sodium-ion multilayer pouch cells have been manufactured with their electrochemical performance discussed. Different testing conditions, including high and low temperature cycling, different discharge rates as well as calendar aging enabled the benchmarking of the developed cells satisfying some of the key performance indicators requested for stationary storage application."

Nicola Courtier
University of Oxford

PyBOP: A Python Package for Battery Model Design Optimisation and Parameterisation

"Mathematical modelling allows us to understand, predict and compare battery performance. For accurate results, models need to be parameterised via a range of electrochemical and materials characterisation experiments. Fast and accurate parameterisation remains a significant challenge [1] due to the need for expert knowledge in experimental data acquisition, processing, system identification and numerical modelling.

We are developing a systematic software framework, PyBOP [2] to validate and establish novel parameterisation workflows for continuum battery models. This project aims to bridge the gap between experimental and modelling work by providing illustrative examples for battery researchers. We present benchmark results comparing different cost functions and optimisers using open-source datasets and models available in PyBaMM [3].

We also demonstrate PyBOP's capabilities in design optimisation. We maximise the gravimetric energy density within constraints on the geometric electrode parameters [4] using the single particle model with electrolyte (SPMe) and particle swarm optimisation (PSO). We show how PyBOP can be used to identify avenues for future improvement by unravelling how parameters affect performance.

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Ahmed Fares
EIC, WMG

Novel Smart modular battery system with Integrated Power Electronics

The talk will represented an invented smart modular battery system. The invented battery system aims to develop a new standard for battery system to be built based on a standardized smart module with integrated power flow control at the cell level, and this module acts as the battery system building block in a manner that is quite similar to the LEGO principle. i.e, the battery pack/system will be constructed faster and flexibly by simply hocking a number of these modules based on the required voltage and energy capacity, then configured to match the required application specifications accordingly. The proposed battery system is quite open to all applications that implements large battery packs like electric vehicles, electric air taxi (eVTOLs), ...etc that are extremely expanding nowadays for achieving plans toward NetZero emissions. As the proposed system provide significant improvements for the battery systems not only for the original applications that implements these battery systems, but also provide significant improvements for the utilization of these battery after retirement from these original applications by reducing the cost of utilization and operation be removing the need for the grouping/assessment process which increase the cost of the implementation of these batteries.

Peter Gillespie
CNR-NANO S3

Automating XANES Simulation of Battery Materials with AiiDA-QE

"X-Ray absorption spectra (XAS) has been an invaluable tool in the research of new battery materials[1] due to its capacity to probe the local chemical environments within a material and grant insight on the structural changes which occur during operation of the battery system. For Li-ion batteries (LIBs), such changes are notable in the cases of both layered lithium nickel oxide (LNO) and spinel lithium manganese oxide (LMO) cathode materials. Operando XAS studies of both systems[2,3] demonstrate a consistent shift of the Ni & Mn K-edge to higher energy as Li moves from the cathode, which has been attributed to a gradual shift of the average transition-metal oxidation state from Ni(III) to Ni(IV) in the case of LNO and Mn(III) to Mn(IV) in the case of LMO. In this work, we demonstrate at the atomistic level the effect of changes in the oxidation state and electronic structure of the transition metal ion on the K-edge of the material as a function of Li content. We demonstrate from this work the use of reliable and accurate automated workflows within the AiiDA automation platform[4] to compute K-edge XAS spectra at the density functional theory (DFT) level for LNO & LMO as a function of Li content. From this, we demonstrate both the site-specific contributions to the final K-edge spectrum and how this trend is reflected in the electronic structure of the transition metal ion.

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Priyanka Gupta
University of Warwick

Unraveling the Influence of Hetero Atom Doped Carbon Coating and Morphology Control on Electrochemical Behaviour of Na3V2(PO4)2F3 Cathode Material

"The rapid growth of the global battery demand has accelerated the search for efficient low-cost sustainable batteries. Among them, sodium-ion batteries (SIBs) represent one of the most promising electrochemical energy storage systems for stationary and light vehicle applications. To expedite SIB commercialization, research has been focused on the rational design of powerful cathode materials as they account for one-third of total battery expense. Polyanionic compound, Na3V2(PO4)2F3 (NVPF) has garnered widespread attention given its rich chemistry, ability to tolerate volumetric stress upon cycling, and high operating potential. Nevertheless, performance-limiting traits such as inferior electronic conductivity and the restricted reversible capacity obstruct the overall practical application for high energy density SIB.

To address the listed challenges, we have examined the synergistic role of structural and surface modification strategies through the synthesis of boron-doped carbon-coated hollow microsphere NVPF materials deploying solvothermal, chemical vapor deposition with a subsequent solution-mixing technique. The prepared materials were analyzed via physical-chemical characterizations and the electrochemical activity was demonstrated in half-cell configuration using rate capability and galvanostatic charge-discharge (GCD) cycling.

In this work, we discuss the comparison among pristine NVPF (S1), 10 wt% boron-doped carbon-coated NVPF (S2), and 20 wt% boron-doped carbon-coated NVPF (S3) materials. It is found that the optimal conditions for improved rate performance and cyclability are identified for S2 material with capacity retention of 97% after 300 cycles when compared to S1 and S3 which displayed capacity holding of 64% and 94% respectively. Further, an in-depth analysis through impedance spectroscopy and post-mortem characterization has been carried out to shed light on the effect of the boron-doped carbon coating on interfacial and structural stability."

Sam Hare
University of Birmingham

Using Positron Emission Particle Tracking to study the mixing dynamics of a lithium-ion battery slurry in an Eirich mixer.

"The mixing of lithium-ion electrode slurries is a key processing step during manufacture of batteries, and poor mixing can have a dramatic effect on final cell electrochemical performance as well as introduce significant problems in manufacturing. The slurries are multi-component, high solids fraction with a complex, evolving non-Newtonian rheology. In this study, Positron Emission Particle Tracking (PEPT) is used to determine the fluid dynamics and dispersion of a model graphite-based anode slurry in a scaleable mixer design (1-12,000 L). The Eirich EL1 mixer features a rotating outer pan, scraper and internal rotor.

Different rotor tip speeds (2 – 10 m/s) yield different levels of tracer velocity and dispersion but does not impact tracer occupancy. At the low mixing speed (2 m/s) a complex shear region arises from the interplay between the flows generated by the rotating pan and internal rotor. Mixer Effectiveness (average mixer dispersion) increases with rotor tip speed due to a combination of more active mixing volume from 2 – 6 m/s, and then an increase in dispersion intensity from 6 – 10 m/s.

Circulation time of the tracer can be calculated and by splitting the mixer into different regions, it is possible to build a network-of-zones model by comparing movement of the tracer in and out of each region, with the regions being selected around notable features of the mixer such as the wall-scraper, rotor and pan wall.

CMC is a common water-based binder with complex rheology properties, with high concentrations of CMC dramatically increasing viscosity. Comparing 3 different (1.5, 2 and 3 %) CMC concentrations, mixing dynamics are highly dependent on viscosity and Mixer Effectiveness is supressed 3 %. Also, at high concentrations, mixing is further supressed at 10 m/s due to the visco-elastic behaviour of the CMC."

Zeeshan Hassan
University of Derby

Advancing Structural Design and Manufacturing Routes for Sodium-Ion Battery Composites

The development of green and sustainable future is a global aim; however, the increase in carbon emissions poses a significant threat, particularly from the aviation and automotive sectors. To minimize carbon emissions, the electrification of transportation presents a potential solution. Structural battery composites, capable of both storing charge and enduring mechanical loads, offer a compelling solution by reducing vehicle weight and optimizing energy utilization. Most of the research on structural energy storage focuses on either embedding lithium-ion batteries in load-bearing structures or integrating lithium salts into the matrix of fibre composites. However, lithium-ion chemistries, while exhibiting high energy density are not favourable in terms of moisture sensitivity and thermal characteristics for structural battery design. As an alternative, sodium-ion batteries have emerged as a promising option to replace lithium-ion batteries. In this research work, a novel configurations of structural electrodes have been utilized and developed the first generation of sodium ion structural battery composites. Cycling performance of the battery composites have been investigated at various c-rates to investigate the formation phase. The manufactured battery composites demonstrated an energy density of 28 Wh kg-1 and exhibited high cycling stability. The bending properties exhibited high flexural strength, and the composite maintained electrochemical stability even after undergoing the bending test. Hence, the encouraging electrochemical, mechanical, and multifunctional attributes of sodium ion structural battery composites advocate for their integration in micro mobility vehicles and the advancement of sustainable infrastructure.

Sandra Huster
Karlsruhe Institute of Technology

Estimating Demand and Supply of Reconditioned Electric Vehicle Batteries Under Consideration of Stakeholder Preferences

"The growth in electric vehicle (EV) sales is anticipated to result in a substantial quantity of end-of-life (EoL) batteries in the future. As landfilling of batteries is prohibited in numerous countries, recycling serves as the final treatment option for these EoL batteries. However, prior to this final recovery stage, reconditioning of EoL EV batteries for use as spare parts in older vehicles, or repurposing them for other applications, might be economically and environmentally feasible options. While recycling and repurposing primarily involve business entities, such as original equipment manufacturers (OEMs), recyclers, and energy providers, reconditioning also involves private car owners as potential customers, who may have a more personal connection to the product. Due to the numerous stakeholders involved, predicting market trends in the reconditioning sector can be particularly challenging.

A simulation model is presented that estimates the demand and supply of reconditioned EV batteries up to the year 2050, taking into account the economic considerations of OEMs and recyclers, as well as the legal limitations imposed by mandatory minimum recycled content rates. Additionally, the model incorporates consumer preferences regarding battery replacement, which were gathered from an online discrete choice experiment conducted among 1152 participants, with 837 providing sufficient data for analysis. The simulation model integrates the methodologies of discrete event and agent-based simulation, and is implemented using the simulation software AnyLogic.

The simulation model allows for the assessment of potential future scenarios with respect to elements that stakeholders can affect and those that are outside of their influence. As a result, it may be used for robust strategic and tactical planning, such as determining whether to undertake reconditioning initiatives and establishing factory capacity levels."

Martin Hutereau
University of Namur

High throughput screening of boron electrolytes

Commonly used salts for the electrolyte component of lithium-ion batteries (LIB) suffer from a number of drawbacks. Key among these is a tendency for poor water stability, which leads to electrolyte degradation and the formation of toxic byproducts, both compromising battery health and hindering recyclability. This additionally entails that the synthesis proceed via a non-aqueous solvent, compounding the environmental cost of LIBs. To resolve this challenge, we aim to identify new water-stable lithium salts (LinX) for use as electrolytes, limiting ourselves to boron-containing counteranions given the outstanding properties of lithium bis(oxalate)borate and its derivatives. This will proceed through a high-throughput workflow: materials databases (the Cambridge Structural Database and Novel Materials Discovery, NOMAD) have already been screened for organic complexes containing both lithium cations and boron anions, yielding 250 candidate systems. The energies of different ions (Xn-, X(n+1)-, and X(n-1)-) will be calculated with density functional theory (DFT) in order to estimate for each electrolyte its electrochemical stability window. A second batch of calculations with a combination of force field and DFT methods will be carried out on the LinX complexes to evaluate dissociation energies as a proxy for ion mobility. The most promising candidates will be selected for more detailed analysis including static and dynamic DFT in order to ascertain water stability.

Masoud Jabbari
School of Mechanical Engineering, University of Leeds

Numerical modelling of battery electrode drying using coupled free-flow-porous-medium approach

The drying process and its influencing parameters during electrode manufacturing has a crucial impact on the distribution of materials within the coating, and the structure of the porous coatings, which directly affects the performance of battery cells. More importantly, since drying is inherently slow, expensive, and energy intensive, understanding and controlling the dynamics of drying will help improving the processing speed and energy demand. This study presents evaporation of solvent (in this study water) from a thin battery electrode to simulate drying. A continuum-based model is developed on a Representative Elementary Volume (REV) scale where non-isothermal multi-phase compositional porous-media flow and single-phase compositional laminar free-flow are coupled. The developed model is used to analyse the influence of ventilation speed magnitude, vmax, the equivalent diameter of particles of the porous medium, dp, the porosity of the porous medium, ϕ, the initial temperature in the free-flow region, Tff , and the initial temperature in the porous-medium region, Tpm, on the characteristic drying curves. The effects of varying each of the parameters are shown with particular attention to the maximal drying rate as well as the final time for the drying process, which are both key factors of initiating cracks in ceramic drying.

Faduma Maddar
WMG, University of Warwick

Investigating the Impact of 0 V Storage on Prussian White Cathode-Based Sodium-ion Battery Cells

"Sodium-ion batteries (SIBs) represent the next generation of sustainable and low-cost energy storage systems. Although their energy density with respect to lithium-ion batteries (LIBs) is generally lower, they have a great potential in applications, such as stationary large-scale storage and light electric vehicles due to their lower costs and higher sustainability. An important additional characteristic presented by SIBs is their ability to be stored at zero-volt (0 V), which is a substantial advantage in terms of cost and safety during storage and transportation not presented by LIBs. Indeed, when a lithium-ion cell is discharged to 0 V, the Cu current collector at the anode reaches a high potential that eventually leads to irreversible oxidation and Cu-dissolution that can trigger the growth of Cu dendrites and internal short. In contrast, SIBs utilize an Al current collector, given the inability of Na to form alloys with Al, which is strongly resistant against oxidation, enabling their 0 V stability. Mariyappan et al. have comprehensively examined the impact of 0 V storage on SIBs, emphasizing the crucial role of the cathode chemistry and electrolyte composition in attaining stability at such low voltage levels.1

Herein, we specifically focus on iron-based sodium-rich Prussian White (PW) of composition Na1.80(5)Fe[Fe(CN)6]·1.84(3) H2O. We investigate the 0 V storage behaviour of full cells consisting of an aqueous-processed PW paired with a hard carbon anode and assess the performance of two different electrolytes composed of NaPF6 in carbonate and diglyme-based solutions. Through the complementary use of EIS and XPS, we shed light into cell cycling stability and the dynamics of the solid electrolyte interface. This investigation spans across different durations and temperatures, providing a comprehensive exploration of these critical aspects in cell battery performance and behaviour.

References:

1. P. Desai et al., J. Power Sources, 2022, 551, 232177."

Alexis Manche
University of St-Andrews

The Challenge of Polyanion Redox Process in Oxalates

"Lately, polyanionic compounds have received great interest as alternative cathode materials to conventional oxides due to their different advantages in cost, safety, structural stability, as well as being environmentally friendly. However, the vast majority of polyanionic cathodes reported so far rely primarily upon the redox reaction of the transition metal for lithium/sodium transfer.

The development of multielectron redox-active cathode materials is a top priority for achieving high energy density with long cycle life in the next-generation secondary battery applications. Triggering anion redox activity is considered to be a promising strategy to successfully enhance the energy density of polyanionic cathodes for Li/Na-ion batteries. In addition to transition metal redox activity, the oxalate group itself also shows redox behaviour enabling reversible charge/discharge and high capacity without gas evolution.

Recently, our group reported dual ion redox in the lithium iron oxalate, in the potassium iron oxalate and in the sodium lithium iron oxalate, Li2Fe(C2O4)2, K2Fe(C2O4)2 & NaLiFe(C2O4)2 in which both the iron and the oxalate group appear to exhibit reversible redox activity. We also found this phenomenon present in the lithium-rich KLi3Fe(C2O4)3.

Different characterisation techniques such as Raman spectroscopy or Synchrotron HAXPES and XAS analyses make it possible to show this phenomenon experimentally. First-principles calculations also help to understand the interactions between the transition metal and the oxalate group as the main factor that modulates the cationic and polyanionic redox couples in these materials.

In our work, we demonstrate that oxalate has a role as a family of cathode materials and suggests a direction for the identification and design of electrode materials with polyanionic frameworks."

Kirstie McCombie
WMG /University of Warwick

Direct Recycling of Li-ion Battery Cathode Active Materials from Production Scraps

"Production of lithium-ion batteries within Europe and worldwide is set to vastly increase in the next several years to meet consumer demand for EVs, resulting in a significant increase in production scrap. Efficient, cost-effective, and flexible recycling processes are thus needed to recover materials to be reutilised in new batteries. Recycling the cathode active material is of particular importance as this accounts for ~ 50 % of the total Li-ion cell cost and contains critical transition metals. [1]

Direct recycling routes to recover cathode materials offer several advantages over indirect recycling routes, which involve the breakdown of the materials into the precursor metal salts to synthesise pristine cathode materials. Direct recycling methods represent a more environmentally friendly and efficient recovery method, preserving the original cathode structure.

In this study, we investigate pre-treated black masses which have been recovered and then purified to remove residual impurities (Al, Fe, and Cu). Our main goal is to identify scalable regeneration procedures to remove remaining impurities and restore the required morphology or structure observed in the pristine cathode material, including by re-lithiation of the materials and hydrothermal treatments to re-incorporate any leached metals. In-depth characterization of both the pristine cathode material and the recovered black mass has allowed us to establish targets for the recycled material and has informed the next steps in the process.

Herein, we investigate and compare the structural properties, morphology, chemical composition and electrochemical performance of the purified black mass from production scraps to that of the pristine materials used in the production process. Our scope of work covers both LFP and the nickel-rich NMC material LiNi0.9Mn0.05Co0.05O2, in order to demonstrate direct recycling processes which are flexible.

[1] https://www.mining.com/web/breaking-down-the-cost-of-an-ev-battery"

Ashok Menon
WMG, University of Warwick

Neutron diffraction studies of unmodified and undeuterated pilot-line electrochemical cells

Neutron diffraction studies although ideal for probing structural changes in Li-ion battery electrodes, is often performed using modified electrochemical cells with (expensive) deuterated electrolytes and 7Li-enriched cathodes. This restricts their applicability and renders routine studies difficult. Here, we demonstrate how excellent ex situ and operando diffraction data can be collected on multiple neutron instruments using both single- and multi-layer electrochemical cells built on the industrial pilot line at WMG (Uni. of Warwick). These cells are unmodified in any manner to aid neutron transmission, and hence offer possibilities of operando investigation of electrochemical systems in conditions very close to their real-world operation. The utility of these cells on different instruments that are designed to probe different reciprocal space length scales offer unparalleled insights into the structural changes of the battery electrodes, which are not decipherable using X-rays. This is illustrated using the LiNi0.8Mn0.1Co0.1O2-Graphite cells as a model.

Puritut Nakhanivej
University of Warwick

Biomass/Silicon Composite Anodes for Lithium-Ion Batteries

Silicon (Si) is a promising anode material for lithium-ion batteries (LIBs) with high theoretical specific capacity of 3579 mAh/g, low working voltage and is earth-abundant. However, the low conductivity and huge volume change during charge/discharge process causes the growth of solid electrolyte interphase (SEI), granular material pulverization. All of this results in deteriorated electrochemical performance and has impeded the large-scale commercialization of Si-dominant anodes. Silicon-carbon composite anodes have emerged as a groundbreaking contender, combining the benefits of both silicon and carbon to mitigate the limitations of pure silicon anodes. A sustainable, cost-effective way to produce C/Si is to use biomass derived materials obtained via low-cost chemical process in the anode. Biomass includes agricultural residues and wood waste. Silicon is the second richest element after oxygen on the earth. Barley is the 4th largest cereal crop worldwide. In this study, C/Si composite anode was derived from barley husks (BHs), which currently offer little to no economic benefit as a byproduct from brewery industry. With a series of physical and chemical treatments, the barley husks were transformed into C/Si anode materials. Pure nano-silicon was mixed with the biomass C/Si with different formulation to increase specific capacity of the anode, thereby improving energy density of lithium-ion batteries. This innovative approach not only addresses the challenges of Si anodes but also taps into sustainable resources, paving the way for a more efficient and eco-friendly energy future.

Johannes Nokelainen
LUT University

Determining the effects of Tungsten Doping on Lithium Nickel Oxide via Compton Scattering

Nickel (Ni)-based cathodes have emerged as crucial components in lithium-ion batteries (LIBs), offering high energy density and storage capacity at a reduced cost. Among these, LiNiO2 (LNO) stands out due to its excellent performance despite structural and thermal stability challenges. Recent studies have focused on tungsten (W) doping in nickel-rich cathodes to enhance battery performance and safety. In this study, we employ high-energy X-ray Compton scattering experiments alongside first principles modeling to investigate the quantum mechanical aspects of W doping in LNO. Through detailed analysis, we explain how W influences the electronic structure of the LNO cathode, providing insights into the doping effects for advancing the efficiency of LIBs. Synthesis of W-doped LNO involved coprecipitation of Ni(OH)2 followed by lithiation, with the resultant samples analyzed via experimental Compton profiles. Our results indicate that

W doping stabilizes the crystal structure, improves electron transport, and enhances oxygen redox reactions, thereby increasing battery longevity and safety. Furthermore, our calculations reveal an increase in the magnetic moment per Ni ion upon W doping, with significant magnetization observed on oxygen ions neighboring W impurities. Overall, this study contributes to a deeper understanding of doping effects in LIBs and emphasizes the potential of W-doped LNO cathodes for next-generation battery technologies.

Andrey Poletayev
Materials, Univ. of Oxford

Fingerprinting Nickel L-edge probes of disproportionating LiNiO2

"Lithium nickel oxide LiNiO2 (LNO) is a model for industry-leading lithium-ion battery cathodes, Li(NiMnCo)O2. Its properties are responsible for the high-voltage degradation of such cathodes. However, the correlated electron physics of this material complicates its characterization in the battery context. As such, a comprehensive model for LNO does not yet exist. Here we characterize the nickel speciation in LNO using three soft x-ray spectroscopies, with its sodium analog NaNiO2 (NNO) as a control. Unlike in NNO, in LNO three nickel environments, distinguished by spins S = 1, ½, and 0, and reminiscent of formal charge states of +2, +3, and +4, interconvert dynamically.

The nickel L-edge shows qualitative differences between LNO and NNO. LNO exhibits two additional peaks relative to NNO, and a temperature variation of their intensities. We model the Ni L-edge spectra with a charge-transfer multiplet model consistent with density-functional theory simulations. First, we distinguish surface reduction from bulk speciation by comparing surface-sensitive electron yield and bulk-sensitive inverse partial fluorescence yield spectra. Second, we use x-ray magnetic circular dichroism (XMCD) to probe the unpaired electron densities on the nickels. The differences between XMCD signatures of LNO and NNO reflect the presence of high-spin (S = 1) nickel species, consistent with a formal 2+ state, in bulk LNO. Third, nickel resonant inelastic x-ray scattering (RIXS) contains a distinct signature of a spin-zero state in LNO, which is consistent with a formal 4+ oxidation state in the same calculations.

Combining three spectroscopies, we fingerprint the three nickel species in LNO at all states of charge. The three-state structure of LNO explains its unusual physical properties, including (1) gradual lattice distortions absent phase transitions upon cooling, (2) heat-activated electronic conductivity, and (3) magnetic moments too high for a 3+ formal oxidation state."

YING TIAN
University of Birmingham

Mg/Na Hybrid Battery: a Hidden Gem that Awaits Polishing

"Mg-Na hybrid battery (MNHB), using earth abundant Na and Mg elements, bears huge commercial potential for its sustainability, low cost, and enhanced safety as well as prolonged cycle life. It’s characterized by fast kinetic of Na+ intercalation at cathode and dendrite free and fast Mg plating/stripping at anode, with Mg/Na mixed electrolyte of a wide electrochemical window and ideal ionic conductivity. Thus, it solves dendrite formation issue in sodium ion batteries (SIBs) while utilizing well designed cathode material that selectively, reversibly, and easily intercalate Na ions without suffering from drastic volume expansion or structural instability during repeated charging/discharging, to overcome sluggish intercalation of Mg2+ into cathode, the main bottleneck in Mg ion batteries (MIBs).

Given the largely different charge and ionic size, the co-intercalation of Mg2+ and Na+ in cathode material has been proved to be unlikely, with only Na+ selectively intercalated in NASICON-type, PBAs, FeS2, NaCrO2, TiS2(with negligible Mg2+ co-intercalation). Likewise, only Mg2+ have been detected at Mg anode after cycling, indicating that Na+ do not participate in anode reaction. Thus, MNHB can be defined as Daniel type hybrid battery with a simple mechanism, thus allowing for precisely controlling the cathode reactions.

However, due to the limited options of electrolytes, MNHBs suffer from low energy density. Thus, future work can focus on seeking suitable mixed electrolyte with higher concentrations (for sufficient ion supplies) and wider electrochemical window (for higher energy density) while expanding available cathode options. Initial thoughts are to combine novel Mg electrolytes reported compatible with Mg anode in MIBs with emerging Na cathode materials in SIBs, then pair them with various combination of Mg/Na dual cation electrolytes, to construct MNHB with higher energy density while preserving its high stability, and fast kinetics."

Michael Wharmby
Bruker AXS GmbH

D6 PHASER: Battery Research and Pair Distribution Functions on the Benchtop

"Powder diffraction is a key tool for understanding the behaviour of materials in battery cells before assembly, during use and in postmortem analysis. The technique is widely applied in research, development and production environments; in all these settings power and cooling as well as device footprint can be serious considerations for which instrument to choose.

The D6 PHASER is a new benchtop powder diffractometer with a small footprint and air cooling, which can be powered from a wall socket. With a 1200 W generator, it offers a high photon flux making it ideally suited for time dependent and flux-hungry measurements, such as operando studies or total-scattering measurements, for Pair Distribution Function (PDF) analysis. The BioLogic SP-50, which was successfully integrated in the D8 family of diffractometers, has now been integrated in the D6, and sample stages are available for research and development operando studies of coin or pouch cells.

When equipped with an Mo tube and a capillary stage, the instrument is a good platform for PDF studies, with total-scattering data collected to a maximum of Q~17Å-1. PDF data can be obtained simply through a new interactive processing routine in DIFFRAC.EVA.

This presentation will showcase the most relevant features of this new and highly capable instrument for battery research, and also touch on its wider capabilities in powder diffraction as well as materials research."

Dongrui Xie
University of Birmingham

Effect of surface modifiers on the performance of O3-type NaNi1/3Fe1/3Mn1/3O2 cathode material for Na-ion batteries

Na-ion batteries as alternative for Li-ion batteries have been widely investigated due to their lower cost and higher safety especially for large-scale energy storage applications. The main challenge of Na-ion batteries is to overcome relatively low energy density. Thus, O3-type NaNi1/3Fe1/3Mn1/3O2 (NFM111) as a novel cathode material with high theoretical energy density has been attracting significant attentions. However, due to the high surface reactivity of NFM111, the cycle life and storage stability of NFM111 need to be improved. Using surface modifiers is a promised way to overcome these challenges. To investigate the effect of different surface modifiers, the surface charge of NFM111 particles was analysed by Zeta potential measurement, the stability of cathode slurry was investigated by measuring the changes in viscous flow and viscoelastic properties using steady shear and oscillatory response respectively, the cycle life of NFM111 coating with different surface modifiers was analysed by battery cycling using coin cells (half-cell). The results showed addition of oxalic acid can improve capacity retention to 73% after 120 cycles whilst remain the initial capacity of 131 mAh·g-1.