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**FC02. 能源材料与交叉学科材料国际前沿论坛**

分会主席：潘复生、邹志刚、麦立强、Patrick Maestro、胡国华、Sanjay Mathur

**FC02-01****Multifunctional materials for emerging technologies**

Federico Rosei

University of Trieste

This presentation focuses on structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of various emerging technologies. In particular, nanostructured materials synthesized via the bottom-up approach present an opportunity for future generation low cost manufacturing of devices. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, including third generation photovoltaics, solar hydrogen production, luminescent solar concentrators and other optoelectronic devices.<sup>[1-18]</sup>

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**FC02-02****Materials for Eco-Design Strategies**

Rodrigo Martins、Suman Nandy、Pedro Barquinha、Lu í Pereira、Elvira Fortunato

Nova School of Science and Technology | NOVA FCT - CENIMAT|i3N

With the growing smartness in electronic manufacturing worldwide, printed electronics technologies draw tremendous attention because of their ability to overcome the limitation of traditional high-cost manufacturing approach which is mostly based on rigid silicon substrate. In these issues, printing technology can be used to fabricate devices on various kind of flexible substrate such as paper, textile, bendable polymers even on human skin. On the other side, printed electronics has a great potential to offer biodegradable and recyclable solutions, by choosing low-cost substrate for printing devices, that may be recycled and/or naturally degraded in nature. This is a way forward to minimize the electronic waste (e-waste) caused by the ever-increasing number of disposable electronic devices. Relevantly, “printing electronics on paper” technology is rapidly developing in both research and electronic industry fields during the last decade.<sup>[1]</sup> Generally, printing processes involve a sequence of tasks, starting with the selection of functional materials along with the envisioned functionality, moving to the formulation of inks, and then the selection of a suitable substrate. Printing technique depending on the ink’s properties and intended features for the printed film. There are several printing technologies, that are being used in research and industrial sectors from lab-scale to large-scale application, such as screen printing, flexographic (or flexo-) printing, gravure printing, gravure-offset printing, and roll-to-roll (R2R) printing. A long list of functional materials, from conductive polymers, ionic liquids, and carbon nanostructures to metallic nanoparticles, and metal oxide nanostructures with conductive, semiconducting, or dielectric properties, can be used to formulate these

inks.<sup>[2-4]</sup> The development of stable, cost-effective, non-toxic, and eco-friendly printable inks with desired printability is crucial to deposit and pattern these materials onto a substrate to enable the production of a new class of devices for electronics and energy purposes that are extremely lightweight, affordable, readily customizable, thin, flexible, and recyclable.

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## FC02-03

### **Advances in Photon-harvesting Technologies for Perovskite Absorbers and Water Splitting Reactions**

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Hybrid halide perovskites have made significant progress in power conversion efficiencies (> 25 %) and high stability achieved through chemical engineering of the AMX<sub>3</sub> composition. Compositional engineering of perovskite precursor inks minimizes batch-to-batch variations and fluctuation in PCE values, however the understanding of perovskite inks and solution behavior remains a key step towards the exploitation of solution-processed perovskite devices. Herein, a comprehensive <sup>207</sup>Pb nuclear magnetic resonance spectroscopy (NMR) study performed on various lead perovskite precursor inks will be presented. The NMR data provide fresh insights in identifying molecular species that are invariably and predominantly formed in precursor mixtures to coexist with larger networks and colloids. The solution chemistry of PbI<sub>2</sub>+I is dominated by the type of connectivity as edge- face- and corner-sharing (PbI<sub>6</sub>)-octahedra and their dimensionality. The trends in the <sup>207</sup>Pb chemical shifts revealed dynamic equilibria in the inks that can be controlled by stoichiometry, nature of the solvents and temperature. Furthermore, perovskite precursor ink development can be applied to fabricate devices beyond the planar device structures, such as direct electrospinning of the three major perovskite solar cell components, namely, photo absorber, hole, and electron transport materials, as continuous single triaxial fibers of μm radial dimensions. These perovskite fibers lay the foundation of materials engineering for fabricating tiny solar cells, which can either be woven into fabrics or incorporated as single fibers to power wearables and a variety of devices or sensors, forming the internet of things. They are also suited for tandem PV-PEC set-up for solar-assisted photoelectrochemical production of hydrogen by water-splitting reactions.

## FC02-04

### **Various functional oxide films with high performances deposited by reactive sputtering**

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Reactive sputtering with alloy targets to deposit oxide or nitride films indeed presents a promising avenue for achieving high deposition rates in industrial applications. The higher sputtering yield of metallic surfaces

compared to oxide surfaces, coupled with the ability to apply higher sputtering power densities due to higher thermal conductivity, makes this technique attractive for various applications. However, the reactive sputtering process is sensitive to the oxygen flow ratio, leading to hysteresis in the deposition rate concerning the  $O_2$  flow rate. This behavior stems from the oxidation state of the target surface, causing a noticeable decrease in deposition rate with increasing  $O_2$  flow. To address this challenge and ensure high-quality transparent conductive oxide (TCO) films with both high deposition rates and reproducibility, precise control over the sputtering conditions is crucial. In response, specially designed feedback systems incorporating discharge impedance or plasma emission intensity, combined with mid-frequency pulsing, have been adopted. These systems enable precise control over the deposition process, ensuring high-quality films with desired properties. The presentation will delve into the details of achieving very high-rate deposition of various TCOs, including Al-doped ZnO (AZO), Sn-doped  $In_2O_3$  (ITO), Nb-doped  $TiO_2$  (NTO), or Sb(Ta)-doped  $SnO_2$  (ATO, TTO) films, through reactive sputtering using Zn-Al, In-Sn, Ti-Nb, or Sn-Sb(Ta) alloy targets, respectively. Additionally, it will cover depositions of  $TiO_2$  or  $WO_3$  photocatalysts and various optical films, showcasing the versatility and potential of reactive sputtering in diverse applications.

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## FC02-05

### Flexible Thermoelectric Devices and Application Scenarios

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In recent decade, organic or organic/inorganic thermoelectric (TE) composites, flexible devices and diverse applications have attracted much of current interest. Herein, we would introduce some recent results in our research group.<sup>[1-4]</sup>

1) A three-dimensional flexible TE device with spring-like architecture was fabricated. The special struture exhibited excellent flexibility and compressibility, which enabled it harvesting heat under vertical temperature gradient.<sup>[1]</sup>

2) A flexible film of PEDOT/Te/single-walled carbon nanotube (PEDOT /Te/SWCNT) ternary TE composite was prepared. Then, the device was assembled with a spiral 3D architecture with flexibility, stretchability and compressibility. Moreover, the TEGs could harvest human body heat by mounting on wrist to generate electricity.<sup>[2]</sup>

3)The intercalated composites of reduced graphene oxide/reduced PEDOT:PSS we synthesized. Then, a self-powered TE wearable glove sensor was assembled, exhibiting outstanding sensing performance in precision motion monitoring. The hand motions include “Point”, “Pinch” and “Grip” patterns.<sup>[3]</sup>

4) An intelligent sensing system for human IoT fire warning was developed, using the composite with light/heat dual-parameter responsive composite of SWCNT/poly(3-hexylthiophene-2,5-diyl) (P3HT). The intelligent sensing system could effectively identify and alarm for fire sources.<sup>[4]</sup>

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#### FC02-06

##### Topological catalysis: from charge to spin

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Exotic electronic states are realized in various topological phases, from topological insulators to recently reported Weyl/Dirac semimetals, nodal line semimetals, and magnetic semimetals. They strongly influence the surface electronic structures of the investigated materials and could serve as a good platform to gain insight into the catalytic mechanism of surface reactions. Topological non-trivial surface states are observed at the crystal surfaces, which are located near the Fermi level. These topological surface states can act as both electron acceptors or donors for molecular adsorption, thus tailoring the adsorption energy and Gibbs free energy in the electrochemical catalytic reactions including water splitting and fuel cell reactions. We also investigated the spin polarization at the transition metal sites in the topological materials, where we found the vital role of spin-polarized electrons for catalytic efficiency optimization. More importantly, the exploration of electron spin as a novel parameter in catalyst design offers a wealth of opportunities for the development of new chemical reactions, ranging from the recognition of enantiomorphs to the exploration of the origins of life.

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## FC02-07

### **X850: The development of a toughened material for use as primary structures on the C919**

Kingsley Ho\*

Syensqo

The commercial air travel domestically within China as well as within the APAC region has always been a key market for OEMs. According to Boeing, there is a demand for 8,560 airplanes in the next 20 years just China alone [[1]]. In the meantime at Airbus for example, it has delivered over 2,100 aircrafts to Chinese airlines which represents more than 50% of the market [[2]]. The trend of reducing carbon emissions for air travel is a fundamental objective and according to the chief designer of COMAC (Commercial Aircraft Corporation of China). New aircrafts are designed to reduce carbon emissions by up to 60% compared to older models and one of the approaches is to design more energy fuel efficient engines as well as reduce weight on structures of aircrafts which in return would lower the overall carbon footprint of jet travel.

Syensqo, as a solution provider, has been focusing on developing toughening systems for such applications. For time to go back to the 1st-gen of un-toughened carbon fibre (CF) reinforced epoxy systems to the 2nd-gen of continuous toughened carbon fibre reinforced epoxy systems (e.g. Cycom® 977) and nowadays with the latest 3rd-gen of particles toughened carbon fibre reinforced epoxy systems (e.g. Cycom® X850), one can see how through the evolution of product development has led to the opening up of various new applications.

The C919 program was launched back in 2008 and made its first maiden flight back in 2017. The aircraft was officially certified by CAAC in Sept 2022 with composite materials made up to 12% of the total weight of the aircraft. Some of the key applications can be found in the radome, wing leading and trailing edges, movable airfoil, wingtip winglets, wing fairing, rear fuselage, vertical and horizontal stabilizers as well as the rudder. In this paper, the evolution of Cycom X850 as a chosen material for use on the Chinese developed C919 single aisle aircraft will be presented. The fact that the C919 currently has over 1000+ orders and deployed Syensqo's material(s) which exhibits superior compression strength after impact (CSAI) properties and resistance to microcracking represent a huge milestone for Syensqo (previously known as Cytec Engineered Materials and Solvay).

[[1]]

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## FC02-08

### **Electrochemical Investigation of Key Reactions for Sustainable Energy**

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The electrode/electrocatalyst/electrolyte interface is extremely complex because the interactions between the phases are both chemical (short-range) and electrostatic (long-range), and the analysis of the properties of this

interface remains challenging. Particularly, it is the case of the electrocatalytic processes such oxygen evolution reaction (OER), oxygen reduction reaction (ORR), and hydrogen evolution reaction (HER) which involve many electrochemical and chemical steps. During these steps, there are not only heterogeneous electron transfers but also adsorption of the intermediates and ions transfer. Herein, we analyze the electrochemical impedance spectroscopy (EIS) responses of modified electrode based on nanoparticles during the electrocatalytic water oxidation [1,2], oxygen reduction [3], and hydrogen evolution processes [4]. One observe that the determination of the transfer coefficient plays a crucial rule for analyzing the mechanism. A key challenge in heterogeneous electrocatalysis is to ensure that electrochemical responses truly represent intrinsic activity of the catalyst.

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## FC02-09

### 2D Materials for Micro-electrochemical Energy Storage Devices

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Micro-supercapacitors (MSCs) and micro-batteries (MBs) with in-plane geometry are a new class of micro-electrochemical energy storage devices for various microelectronics circuits. Two dimensional (2D) materials with the advanced merits of ultrathin flat structure, high specific surface area, and excellent mechanical characteristics, are one of the perfect candidates for planar MSCs and MBs. In this talk, our recent progress on 2D materials-based planar MSCs and MBs will be reported. This involves the strategies for preparing high capacitance 2D materials such as electrochemically exfoliated doped graphene, MXene, metal oxides and mesoporous polymers via techniques like electrochemical exfoliation, liquid exfoliation, graphene template, and supramolecular self-assembly methods. The inherent advantages of these materials are leveraged and translated into high-performance MSCs and MBs for integrated micro-systems through state-of-the art techniques like inkjet-printing, screen-printing, 3D printing and photolithography. The all-solid-state planar integrated MSCs can achieve ultrahigh output current/voltage through series or parallel connection. Taking a step towards achieving practical internet of things, integrated microscale energy storage systems with different application scenarios are exploited, like high-performance planar integrated system of MSCs and gas sensors, wearable pressure sensor system, and all-flexible self-powered integrated systems. Such self-powered integrated microsystem combines energy generation/harvesting, storage, and consumption in one system, catering to a wide variety of demands.

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## FC02-10

### 硫电化学与硫基电池储能

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可充电电池是支持清洁能源高效利用及交通电气化的重要一环，这于碳中和目标至关重要。硫是一种地壳储量极为丰富的元素，廉价且能提供较高的氧化还原容量，因此是极具前景的电池电极材料。本次报告将总结我们在两个方面的研究（1）锂硫电池的高性能电解液设计，（2）低成本、高安全铝硫电池的构筑。本报告将重点介绍高性能硫基电池的底层化学设计原则，调节硫电化学反应路径的策略以及实现该策略的材料设计准则，并将举例说明最终如何实现高性能硫基电池。

## FC02-11

### Studies on high-performance inverted perovskite solar cells towards industrial applications

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After reporting the first world efficiency record of inverted perovskite solar cells on *Science* in 2015, Wei Chen led a research group focusing on resolving the key bottlenecks preventing this new photovoltaic technology towards industrialization, especially focusing on breaking the efficiency limits, large-area controllable fabrication and intrinsic instability. By studying the highly photothermal stable FACsPbI<sub>3</sub> perovskite crystal growth and defect passivation mechanism, large area perovskite film's controllable formation mechanism, the development of new molecular interface materials, an unique Bi-based inert metal electrode system, and the construction of a limited reaction system based on multiple barriers, the basic certification efficiency and stability of inverted perovskite solar cells have been effectively improved. Up to now, we have obtained a small area PSC certification efficiency of 26.5% through a credible certification center, and a mini module certification efficiency of 23.1% (area 11.1cm<sup>2</sup>), both of which exceed the current efficiency records and are competitive to be written into the international solar cell efficiency tables. The certified efficiency of all-perovskite tandem solar cell has reached 29.8%, also largely surpassing the current world record of 29.1%. In addition, we have also obtained a third-party certification report on the stability of inverted perovskite solar modules issued by VDE, Germany. In this conference, we will report all of the above mentioned progresses in our research lab and our recent progress on industrial scale-up production of inverted PSCs in our newly launched innovation company, i.e., Wuhan 91PVKsolar, Ltd., Co.

## FC02-12

### Ru/Si 2D nano-heterostructure for alkaline hydrogen evolution reaction

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Two-dimensional (2D) heterostructures represent one of the pinnacle achievements in the field of artificial nanomaterials. They possess not only the properties of the component materials but also unique reconstructed interfaces, and therefore have attracted a surge of interests in the areas of electronics, spintronics, photonics, energy storage and catalysis. However, fabrication of 2D superlattices is technically highly challenging, and materials with such structures are extremely scarce.



In this presentation, we will report the discovery of a highly ordered self-assembled 2D Ru/Si superlattices (RSHS) readily prepared by employing a selective chemical etching method, similar to the preparation of the 2D MXenes from MAX phases. Specifically, we employed the quasi-2D structural features of the intermetallic electride LaRuSi, and selectively removed the chemical active La-e-La layer by an acid etching. The Ru-Si residues then formed RSHS via a self-assembly process. The current method is significantly more efficient than traditional approaches for rapidly producing a large quantity of heterostructure materials. Possessing periodic alternating Ru/Si layers and gradually varied Ru and Si concentrations across the interface, RSHS would be an excellent catalyst for various reactions. We tentatively employed RSHS for alkaline hydrogen evolution reaction (HER), and found that the overpotential was only 14 mV at 10 mA/cm<sup>2</sup> and the Tafel slope was as low as 33 mV/dec, demonstrating it as one of the best HER catalysts. This presentation will emphasize on the design and preparation strategy of RSHS and its catalytic application potentials.

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#### FC02-13

##### **Ion-sieving accelerating channels constructed by the layer-by-layer self-assembly of polyelectrolytes for highly stable Zn-ion battery**

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Aqueous zinc-ion batteries (AZIBs) are increasingly recognized as a sustainable alternative to lithium-ion batteries (LIBs) due to their abundance, safety, and lower environmental impact. However, the hydrogen evolution reaction (HER) and uncontrolled diffusion of Zn<sup>2+</sup> and SO<sub>4</sub><sup>2-</sup> ions lead to the dendrite formation and side reactions, which hinder their practical application by forming a non-conductive layer on the Zn anode. This layer impedes the ion transport and electron flow, reducing the Coulombic efficiency (CE) for the Zn nucleation. Here, to simultaneously regulate the diffusion of H<sup>+</sup>, Zn<sup>2+</sup>, and SO<sub>4</sub><sup>2-</sup> in the electrolyte, an ion-sieving accelerating channel was constructed to unify the Zn deposition by introducing an eco-friendly layer-by-layer self-assembly of a flocculant poly(allylamine hydrochloride) (PAH) and its tautomer poly(acrylic acid) (PAA). The dual-ion channels, created by strong electrostatic interactions between carboxylate anions (COO<sup>-</sup>) and ammonia cations (NH<sub>3</sub><sup>+</sup>), promote the uniform Zn deposition along the (002) plane, exhibiting a CE of 99.8% after 1600 cycles in the Zn||Cu asymmetric cell. With the facile fabrication of the layer-by-layer self-assembled Zn anode, an Ah-level pouch cell (17.36 Ah) with a high mass loading (> 8 mg cm<sup>-2</sup>) demonstrated exceptional performance, retaining a capacity of 93.6% for at least 250 cycles at 1.7 C. This research offers a universal strategy for optimizing

electrode mechanisms and advancing the manufacturing process of eco-friendly, high-performance aqueous batteries.

#### FC02-14

##### **Microwave-assisted Synthesis of In<sub>2.77</sub>S<sub>4</sub>/Exfoliated Graphene/Multiwall-Carbon-Nanotubes Ternary Nanocomposite and Its Application as An Active Material in A Supercapacitor**

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Nanoscale indium sulfide was successfully deposited on a mixture of exfoliated graphene (EG) and multiwall carbon nanotube (MWCNT) to produce a ternary nanocomposite of the formula In<sub>2.77</sub>S<sub>4</sub>/EG/MWCNT. This synthesis was completed in 5 minutes and made possible via a rapid microwave-assisted thermal decomposition of indium acetate/thiosulfate mixture in a uniform dispersion of EG and MWCNT at 200 °C. The ternary nanocomposite was characterized using a combination of PXRD, FESEM, HRTEM, BET, UV-VIS-DRS, FTIR and Zeta Potential measurement. The ternary nanocomposite was electrochemically characterized via cyclic voltammetry and galvanic charge-discharge and found to exhibit a Csp of 150 Fg<sup>-1</sup> in a simple two electrode supercapacitor set-up. Experimental results showed that the ternary design outperforms binary and single material electrode based on indium sulfide and carbon electrode controls. Interestingly three dimensional indium sulfide nanoflower with a surface area of 60 m<sup>2</sup>/g was produced in the absence of EG and MWCNT and the nanoflower exhibited a Csp of 500 Fg<sup>-1</sup> in a three-electrode system. The performance of the nanoflower as an anode material for lithium and sodium battery in a coin-cell assembly would be discussed.

#### FC02-15

##### **Structurally Integrated 3D Carbon Tube Grid Electrodes for Miniaturized Line-filtering Capacitors**

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Filter capacitors play a critical role in ensuring the quality and reliability of electrical and electronic equipment. Aluminum electrolytic capacitors are the most commonly used but are the largest filtering components, limiting device miniaturization. The high specific capacitance of electric double-layer capacitors (EDLCs) should make them ideal miniaturized filter capacitors, but they are hindered by their slow frequency responses. We report the development of interconnected and structurally integrated carbon tube grid-based EDLCs with high areal capacitance and rapid frequency response. These capacitors exhibit excellent line filtering of 120-hertz voltage signal and volumetric advantages under low-voltage operations for digital circuits, portable electronics, and electrical appliances. The outstanding performance of the capacitors is attributed to the high density, high orientation, and high integrality of carbon tube arrays that facilitate and accelerate ion distribution onto the electrode surface. These findings provide a sound technological basis for developing EDLCs for miniaturizing filter and power devices.

#### FC02-16

##### **多尺度电化学储能材料研究**

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电化学功能材料的多尺度物理化学本质是制约其储能活性和器件储能稳定性的核心问题，这也激发了材料科学家们探索多种物理化学方法来提升材料的电化学储能性质。在材料的形成过程中，组成元素经历了从原子/离子/分子到胶体、纳米晶/微米晶、粉末/薄膜或块状单晶的系列跨尺度相变过程。这些相变过程极大地限制了材料的结构、尺寸、形态和特性及其器件功能。本报告从理论研究和实验观察相结合的角度，从多尺度结晶本质揭示了材料的形成与性质变化规律。从多尺度结晶视角审视，材料的成核和晶体生长过程分别控制了具有多尺度特征的团簇/材料之间的跨尺度相变，热力学和动力学之间的耦合控制着材料形成过程中跨尺度模式。以一些典型材料为例，我们发现了结晶过程中多种尺寸的可变材料状态在储能和可持续能源的实际应用中发挥的主导作用。从多尺度结晶的角度揭示材料的物理和化学特性，利于我们加深对微米/介尺度尺寸范围内材料形成的理解，并促进其功能提升。

## FC02-17

## 高性能钾离子电池研究进展

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由于锂、镍、钴、铜等核心元素对外依存度高，我国锂离子电池的发展面临较大的原料供应风险，难以保障未来大规模批量使用的需求。与锂离子电池相比，钾离子电池具有钾元素储量丰富、与商业化石墨负极兼容、溶剂化钾离子半径小且去溶剂化容易、不含以上低储量元素等优点。因此，钾离子电池有望作为锂离子电池的补充，支持我国电化学储能技术的发展。虽然上述优点使得钾离子电池具有吸引力，但钾离子电池的发展主要依赖于其低成本，这就要求除了组成钾离子电池的原材料必须使用储量丰富的廉价元素外，更重要的是钾离子电池需要达到与目前锂离子电池和钠离子电池相当（甚至更长）的循环寿命，从而降低其生命周期成本（cost over cycle life, \$ kWh<sup>-1</sup> year<sup>-1</sup>）。钾离子电池的循环寿命主要取决于其电极材料的充放电稳定性，本次报告将汇报课题组近年来在高性能、低成本钾离子电池方面的一些研究成果，并对钾离子电池未来的发展进行展望。

## FC02-18

## 水系金属空气电池界面研究

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水系金属（锌镁铝）空气电池具有安全、高比能、低成本的特点，但仍需解决化学稳定性、金属利用率、和电化学可逆性等问题，其中电解液设计和电解液/电极界面是关键。本报告主要介绍了水系金属空气电池电解液设计和固液气三相界面研究进展：(1) 锌空气二次电池，采用中性电解液大幅提升了锌空气电池的化学稳定性和电化学可逆性，并解析了锌盐阴离子对空气正极反应机制的影响规律，提出了“疏水阴离子(OTf<sup>-</sup>)-两电子氧还原(2eORR)-过氧化锌(ZnO<sub>2</sub>)”和“亲水阴离子(SO<sub>4</sub><sup>2-</sup>)-四电子氧还原(4eORR)-碱式水合物(ZHS)”两类锌空气电池反应新机制；(2) 镁、铝空气一次电池，设计复合电解液体系，通过电解液阳离子和阴离子组分调控，平衡金属阳极固液界面腐蚀和钝化副反应，大幅提升镁、铝空气电池的化学稳定性和阳极利用率；(3) 发展了针对金属空气电池固液气三相界面研究的原位 XRD、FTIR、pH、气体压强、DEMS、含氧量测试等多表征联用技术。

## FC02-19

## 高性能聚合物基固态电解质的设计及固态电池界面性能调控

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追求高比能量，高安全性是锂离子电池开发的主要技术趋势。使用新型固态聚合物电解质代替传统的有机电解液可进一步提高电池的能量密度和安全性<sup>1-3</sup>。然而，聚合物固态电解质存在离子电导率低、界面性能差、生产成本高等问题，限制了其商业化应用。为了进一步提升锂电池的性能，我们利用原位聚合，填料掺杂改性等方法，设计制备了一系列新型的具有高离子电导率，高界面适配性的聚合物固态电解质，并匹配一系列高压正极材料(NCM811, NCM622, LiCoO<sub>2</sub> 等)，实现了全固态聚合物锂电池优越的电化学性能的显著提升<sup>4-9</sup>。

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## FC02-20

### Optimizing interface charge transport of electrode materials for advanced aqueous batteries

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Nowadays, secondary electrochemical energy storage systems have entered every aspect of our lives, e.g., from bulky mobile phones to current lightweight smart wearables, electric vehicles, drones, etc. However, with the improvement of human production, living styles and technological level, there are higher requirements for the electrochemical performance and resource sustainability of batteries, such as the national "double carbon" strategy and energy transformation strategy. In this context, high-performance aqueous batteries for large-scale energy storage stations have become more prominent. Thus, our group takes interface charge transport of electrode materials as the breakthrough point to accelerate the development of advanced aqueous batteries. 1) According to the energy storage principle of electrochemical reaction processes, the transport behavior of ions/electrons in electrode materials is closely related to electrochemical polarization. Therefore, by applying interface engineering to materials design, charge transport behavior can be promoted. For example, in  $\alpha$ -MoO<sub>3</sub> nanosheets, the abundant oxygen vacancies impede the insertion of Al<sup>3+</sup> ions due to their strong adsorption, while permitting the insertion and diffusion of H<sub>3</sub>O<sup>+</sup> ions via the Grotthuss proton conduction mechanism, resulting in 73.6% capacity retention ratio after 1000 cycles. This finding offers novel insights into the selective intercalation chemistry of H<sub>3</sub>O<sup>+</sup> ions for enhancing the transport of high-efficiency reaction ions. 2) Utilizing a BiOI layer accelerates the transport of Ni<sup>2+</sup> and Co<sup>2+</sup> during the electrodeposition of NiCo hydroxide precursors. The heterostructure of metallic Bi and nickel-cobalt phosphide possesses a built-in electric field, enabling charge transport at the interface of the heterogeneous structure, thereby facilitating the adsorption and diffusion of OH<sup>-</sup> ions on/in the electrode. 3) By utilizing the characteristics of rapid interaction between transition metal ions and cyanide iron ([Fe(CN)<sub>6</sub>]<sup>3-</sup>) ions, a SEI-like layer is formed at electrode/electrolyte interface, optimizing interface charge transfer and successfully

suppressing the dissolution of copper and iron ions, ultimately achieved a 99.8% capacity retention after 40,000 cycles, and this is suitable for a variety of ions ( $\text{NH}_4^+$ ,  $\text{Li}^+$ ,  $\text{Mg}^{2+}$ .....) in aqueous batteries.4) Using FEC to regulate the structure of the CEI (cathode electrolyte interphase) on the graphite surface to facilitate the easy passage of TFSI- ions through the CEI for electrochemical reactions with the graphite cathode. By optimizing the ion transport in this interphase, the discharge specific capacity of the graphite cathode is increased from 22 to 47  $\text{mAh g}^{-1}$ . 5) In summary, the charge transport behavior in electrode interface can be optimized by surface/interface modifications of electrode materials, thereby obtaining high-power of electrode materials. Thus, the applications of large-scale energy stations can be broadly realized.

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## FC02-21

### High-performance and Stable Flexible Perovskite Solar Cells

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Flexible perovskite solar cells (FPSCs) with light-weight and flexibility have attracted considerable attention as a promising technology for next-generation photovoltaic applications, e.g., portable chargers, intelligent vehicles, and building-integrated photovoltaics. However, due to the uncontrollable growth of perovskites on flexible substrates, the power conversion efficiencies still significantly lag behind that of the rigid counterparts. In addition, the polycrystalline perovskite films with high Young's modulus always produces numerous cracks in the FPSCs during bending and stretching test, which significantly reduce the efficiency of devices, thus limiting their commercial development. Therefore, we have devoted our research on the basic scientific issues of FPSCs as follows: 1) we explored an in-situ crosslinking bis((3-methyloxetan-3-yl) methyl) thiophene-2,5-dicarboxylate (OETC) along with perovskite growth, and its carefully designed coordination ability and crosslinking temperature enabled to finely regulate the quality of perovskite in real-time, thus effectively weakening the substrate-matrix dependence; 2) we firstly revealed that the delayed heat-transfer effect resulting from the low thermal conductivity of the plastic substrate will lead to spatial crystallization inhomogeneity. To solve the problem, we designed a functional monomer MZ with carboxyl, imidazole, and oxetane groups to enable organic cations to rapidly downward diffuse into the  $\text{PbI}_2$  layer for sufficient reaction, thus alleviating the spatial

compositional variation and releasing residual strain; 3) A cross-linkable monomer TA-NI with dynamic covalent disulfide bonds, H-bonds, and ammonium is carefully developed, and acts as “ligaments” attached on the perovskite grain boundaries to enhance moisture resistance, release the residual tensile strain and mechanical stress in perovskite films. Finally, the efficiency of a  $5 \times 5 \text{ cm}^2$  FPSCs module reached 20.5%, and maintained approximately 92% of their initial efficiencies after 20000 bending cycles with a radius of 5 mm, promoting the industrialization of flexible photovoltaic devices.

## FC02-22

### 硅基固态电池性能提升策略与机理解析

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发展高能量密度、高功率密度和长循环寿命二次电池是当前国内外前沿研究热点，也是能源电化学材料研究的核心。先进电极材料开发是实现高比能二次电池的关键前提，这迫切需要对现有电极材料进行优化并探索新型高性能电极材料，同时借助清晰、精确的先进实验表征手段对新机理、新材料和新设计进行深入探讨，以形成系统的科学认识。

本报告将围绕高比容量硅基负极材料在固态电池中的结构设计及性能提升的机理解析而展开，以先进显微和谱学表征为研究手段，深入解析其微观结构与宏观电化学性能间的构效关系，以期为解决目前硅基负极应用于固态锂离子电池存在的瓶颈问题提供新的研究思路。

## FC02-23

### Lithium penetration and void growth in solid-state Li metal batteries investigated by in-situ transmission electron microscopy

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Solid-state batteries (SSBs) with lithium metal anodes have shown great promise for achieving high energy density and excellent safety. However, the development of SSBs are still severely hindered by the interface issues between Li and solid electrolytes (SEs), such as Li filament growth and void formation. These two major problems occurs at the Li/SE interface during Li deposition and dissolution, respectively. SEs that form no or passivating interphases with Li are often vulnerable to Li penetration, leading to a short circuit and even safety hazard. The formation of voids is actually more prevalent for SEs, and the resulting contact loss can not only cause impedance increase but also increase the risk of triggering Li metal penetration. Addressing these issues requires the operando observation of these interfacial processes with high spatio-temporal resolution and their direct linkage to electrochemistry. Herein, we present the first attempt by visualizing the stripping and plating interfaces of a microscale SSB cycled in galvanostatic mode in a transmission electron microscope. These results not only offers valuable insights for understanding the rate-dependent stresses and the resultant SE failure, but also solid evidence for linking voids to battery deterioration. Moreover, this work gives a stress-release-oriented guideline that enables fast charging of SSBs, as well as new insight for void suppression to stabilize the Li/SE interfaces in SSBs.

**keyword:** solid-state battery; lithium filament; LLZO; in-situ TEM; void growth

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**FC02-24****锂离子溶剂化结构调控及新型电解液**

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锂离子的溶剂化结构与电池的安全性、循环稳定性和界面电化学过程有着密切的联系。因此，对锂离子溶剂化结构的调控一直都是新型多功能电解液开发的研究重点。然而，在过去几十年的研究中，研究者们对溶剂的溶剂化能力仍没有一个明确一致的概念和认识。本报告将对溶剂的溶剂化能力和溶剂化过程的本质进行重点阐述，并提出调控溶剂化结构的方法和策略。基于此，介绍了一类新型的超低温功能性电解液，以及阐述基于  $\text{LiNO}_3$  单一锂盐的电解液的形成机制和稳定性原理。

**FC02-25****Multicomponent ruthenium-based oxides electrocatalytic materials**

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Developing efficient electrocatalytic materials for water splitting is of great significance for the green hydrogen production. Given by this, the reporter mainly focuses on constructing high-performance and cost-efficient ruthenium-based oxides electrocatalytic materials for hydrogen and oxygen evolution. The research works have been carried out on the synthesis control, structural stabilization, and electrocatalytic performance regulation of multicomponent ruthenium-based oxides, which devotes to deal with the synthesis problems, fine structure construction, and further improving catalytic performance. These works aim to establish a comprehensive understanding of the synthesis-structure-property-performance relationship based on multicomponent ruthenium oxides to promote the commercial application of ruthenium-based electrocatalytic materials.

**FC02-26****Encapsulation of Metals as High Temperature PCMs with Controllable Shell Structure and Super Thermal Properties**

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Thermal energy storage (TES) has been developed in recent years to reduce the  $\text{CO}_2$  emission. High temperature phase change materials are extensively studied to increase the thermal efficiency of TES using their latent heat with relative steady phase change temperatures. Metals and their alloys show great potential due to their high latent heat storages and thermal conductivities. Encapsulation of metals is the effective technique to solve high temperature leakage and corrosion. Commercial micro powders of Al-Si alloys and Al-Si-Fe alloys were encapsulated with ceramic shells. Different shell structures including  $\text{Al}_2\text{O}_3$  shell with controllable shell thickness, double-layer ceramic shells with sponge effect, AlN fibers network structure embedded with  $\alpha\text{-Al}_2\text{O}_3/\text{AlN}$  shell were obtained. Thermal stability was evaluated by thermal cycle test. The microcapsules treated at  $1000^\circ\text{C}$

achieved zero heat loss after 5000 thermal cycles, whose latent heat absorption/ release were 448.3 J g<sup>-1</sup>/ 456.8 J g<sup>-1</sup>. the microcapsules possessed a giant heat storage density of 938.8 J g<sup>-1</sup> within 300-700 °C, and the figure of merit was  $6336.9 \times 10^6 \text{ J}^2 \text{ K}^{-1} \cdot \text{s}^{-1} \cdot \text{m}^{-4}$ , about 15 times higher than that of commercial solar salt. This work solves the defects of Al-Si alloy as phase change material and ensures its high-performance and service life.

## FC02-27

### 基于仿生微纳孔材料的离子能量体系

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在自然界中，细胞膜上离子通道和离子泵中的精妙智能传输过程与信号传递，电位调控，能量转换与存储等多种生命活动息息相关。相关仿生体系的研究不仅对于我们理解生命体传质过程，而且对解决盐差能转换等相关应用领域中的关键瓶颈都有着重要意义。受生命体离子通道的结构与功能启发，我们构筑了基于仿生微纳孔材料的纳流离子传输膜，总结出了利用结构、电荷、以及界面浸润性协同作用调控离子传输进而实现功能性增强的新策略，并进一步将生命体以蛋白质离子通道为核心的能量机制引入到人工微纳米通道，构筑了多种高性能离子能量体系。

## FC02-28

### 二维储锂材料

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近年来，二维材料如石墨烯、类石墨烯等表现出许多独特的物理化学性质，在能量储存与转化甚至电子等领域具有广阔的应用前景。超薄二维材料通常可以通过自上而下（Top-down）和自下而上（Bottom-up）法制备，但其单层率（<1 wt.%）/产率（微克级）低，严重限制超薄二维材料在新能源材料中的应用。近期，杨树斌课题组提出拓扑转化新方法，通过将非范德华固体如 MAX 相等逐步转化为二维范德华材料，突破了上述方法的限制，并阐明了该方法热动力学控制的非范德华固体-范德华二维拓扑转化机制，宏量制备出一系列具有超高单层率（91%）和高稳定结构的范德华二维材料，为超薄二维材料在柔性电子、能源储存与转化领域的实际应用奠定了基础。同时，杨树斌课题组基于超薄二维材料的不同特性如二维特性、柔软、可调官能团等，设计制备出系列超薄二维复合材料，并应用于电化学储能器件如金属锂电池等。

## FC02-29

### 三维复合锂负极的研究及应用

陈立宝

中南大学

锂金属具有极高的理论比容量（3860mAh/g）和最低的电极电势，是极具潜力的下一代高能量密度电池负极材料。然而循环过程中不可控的锂枝晶生长和体积波动，引发死锂累积和电解液消耗，进而使得锂金属负极库伦效率低、循环性能差，甚至引发安全隐患，这严重阻碍了锂金属负极的实际应用。为锂金属引入三维骨架，是解决锂金属负极实际应用时力学强度不足、体积变化大等问题最有效的措施。锂硼复合负极一种内部具有天然纤维状 LiB 化合物骨架的复合材料，通过硼含量调控、合金元素添加、多骨架结构设计等策略，提升了锂硼纤维的结构稳定性，有效抑制了锂负极的体积变化。在复合锂负极轧制加工过程中，基于机械力化学反应，原位形成高强、高导锂人工 SEI 膜，解决了枝晶生长的问题。研究为构筑高效能实用化复合锂负极的提供了新思路。

## FC02-30



### 钠离子电池磷酸盐正极材料

吴兴隆\*

东北师范大学

在基于“摇椅式”储能机理的碱金属离子电池中，电极材料（尤其是正极材料）对碱金属离子的存储特性起着关键性的作用。对于以共价性框架为主的磷酸盐正极材料，仍然面临着电子导电性差、工作电压偏低等挑战。本报告将讨论，针对钠离子电池中磷酸盐正极材料，通过晶格调控（高熵化、高电负性阴离子取代、同构阴离子掺杂、非等价态阳离子掺杂等）、精准碳网络构筑和阴阳离子接力复合材料设计等策略，实现的高电压和高能量密度、长循环寿命和优异倍率等储能性能，并分析了其中涉及的提升机理。

#### FC02-31

### 固态锂电池界面设计与优化策略

杨孟昊

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构筑低阻抗和高稳定的固固界面是提升固态锂电池循环性能的基础科学问题。然而，目前全固态锂电池面临着临界电流密度低和循环寿命较低等问题，这是由于锂金属/固态电解质界面上形成的孔洞等界面缺陷引起的。通过采用大规模分子动力学模拟的方法，本报告介绍了在固体电解质界面上锂金属剥离和沉积过程的原子尺度建模研究。首先，报告人构建了与固态电解质相结合的锂金属剥离和沉积过程模型，详细阐明了锂金属扩散、蠕变和孔洞形成过程，为探讨固固界面失效机制奠定了基础。其次，报告人深入研究了不同固态电解质材料与锂金属形成的共格、半共格和非共格界面结构，采用共格界面结构能够抑制电池失效，揭示了界面结构与孔洞形成之间的关联性。最后，报告人系统建立了固态锂电池稳定运行的界面附着能和施加压力参数图谱，通过选取合适的界面附着能和外部压力等多种新措施都能有效提升固态锂电池的循环性能。

#### FC02-32

### 锂离子电池内外部智能传感技术

金阳

郑州大学

现有商用锂电池采用的易燃的有机电解液，在极端工况或环境下容易发生化学能量剧烈释放造成火灾甚至爆炸事故。安全性是电动汽车和储能大规模推广应用的先决条件，落实电池安全保障措施势在必行。本报告聚焦于实现智能锂电池的多维度内外部智能传感监测技术，介绍用于电池从故障开始到热失控爆发全过程多维特征参量产生机理和探测技术，包括电-热-气-声-压-光等多物理量状态传感监测。

#### FC02-33

### 高比能锂离子电池快充析锂调控

梁正\*

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锂离子电池快充技术是产业界和学术界共同追求的目标。对于工作电位较低的石墨负极而言，快充过程往往伴随析锂，带来安全隐患和容量衰减。锂离子电池快充包含多个过程单元，其决速步骤难以被准确识别且会随循环条件（倍率、荷电状态和温度等）的变化在多个过程之间发生动态迁移，从而导致针对某一个步骤的动力学优化策略效果大打折扣。因此有观点认为在复杂工况下石墨快充析锂很难避免。在这种情况下，将之前聚焦的“抑制快充析锂”转变为“调控快充析锂”，通过一系列调控策略使析锂分布均匀、形貌规则、高度可逆，或许是一个对现有策略的有效补充。

**FC02-34****The Creation of High Performance Energy Storage Materials with Low Packing Factors for “Dual High” Applications**

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The second-minute power replenishment in the fiercely competitive international market urgently requires high-power and high-energy density batteries, and electrode materials with both high rate/capacity ability are the key points. However, “Electronic transport” and “ion migration” are mutually restrictive and difficult to synergize. We propose a theory and method for creating energy storage materials based on multi-scale open structures. The main research topics here include: (1) Proposing the theoretical model of “crystal packing factor ( $PF = SiVi/V_{cell}$ , where  $Vi$  is the ion volume, and  $V_{cell}$  is the cell volume)” to evaluate the constraints of intrinsic multiple physical quantities of materials, and applying the model in the creation of energy storage materials and developing series of novel high performance electrode materials; (2) Proposing the extended concept of “mesoscopic packing factor ( $Me-PF = V_t/V_a$ , where  $V_t$  is the true volume,  $V_a$  the apparent volume)” and creating a “shape preserving” topological ion exchange/etching synthesis to prepare nanoporous single-crystal structured cathode/anode materials with both high-rate and high-capacity performance; (3) Applying the developed high performance electrode materials and developing “dual high” energy storage devices with similar energy density to lithium-ion batteries but two orders of magnitude increased power density. It is expected to provide new understanding and methods for the microstructure design and preparation of high-performance electrode materials for “dual high” applications.

**FC02-35****高镍三元正极材料的界面改性及储锂性能**

左稼暄, 王敬, 张开淋, 杨臻光, 席玉坤, 宋学霞, 钱华明, 张健华, 李喜飞\*  
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高镍三元正极材料 ( $LiNi_xCo_yMn_{1-x-y}O_2$ ,  $x \geq 0.8$ ) 因其较高的放电比容量和较低的成本, 成为当前最具发展潜力的锂离子动力电池正极材料之一, 但其前驱体材料合成难度较大, 对粒径进行精准控制较为困难, 同时高镍三元正极材料在储锂过程中其突出的表界面结构衰退问题造成电化学性能快速降低, 严重制约其规模化应用。针对上述问题, 本报告开展了以下研究工作:

(1) 采用预制母液共沉淀法, 依靠前驱体晶核定向生长实现了对前驱体粒径和致密度的精准控制, 研究了共沉淀过程 pH 值、氨浓度等反应参数对前驱体理化性能的影响规律, 并通过优化固相烧结过程烧结温度、过锂量等参数获得高性能高镍三元正极材料, 0.2 C 下首次放电容量达 225.1 mAh/g, 首次库伦效率达 89.9%。(2) 针对材料在储锂过程中表界面结构衰退问题, 开发了区别于传统金属氧化物包覆层的双金属氧化物包覆层  $NiCo_2O_4$ , 凭借双金属氧化物的高模量、耐蚀性和离子快速迁移特性, 使得材料获得优异的循环性能和较小的电化学极化, 200 次循环材料容量保持率提升 33%。(3) 为进一步缩小包覆层和正极材料界面差异, 在表面包覆基础上进行表面掺杂构筑高离子电子导界面功能层。通过化学气相处理结合空气钝化构筑磷酸盐耐蚀非晶层和高离子电子导过渡层, 显著提升材料的循环稳定性和倍率性能。

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**FC02-36****High Efficiency Perovskite Solar Cells by Vacuum Evaporation**

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Perovskite solar cells are garnering significant interest due to their high photovoltaic performance and economical production costs. However, challenges such as achieving high efficiency in large-area devices and ensuring adequate stability have limited their widespread commercialization. The conventional solution spin-coating technique, commonly used in research settings, faces constraints including small active areas, uniformity issues, and the necessity of toxic solvents. In contrast, vacuum vapor deposition offers a solvent-free approach capable of large-scale, uniform perovskite film deposition, making it a viable option for industrial-scale production of perovskite solar cells. Nevertheless, the efficiency of perovskite cells fabricated using vacuum deposition has been substantially lower compared to solution-based methods, impeding its progress towards industrial application. Our team has innovated the process to surmount the low-efficiency challenge associated with vacuum deposition in perovskite solar cell fabrication, paving the way for the mass production of perovskite photovoltaic modules. This presentation will detail our team's advancements in enhancing the efficiency of large-area perovskite cells through vacuum evaporation, bolstering the stability of perovskite cells, and advancing high-efficiency flexible perovskite solar cells.

**FC02-37****二次离子电池中的磷电化学**

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发展高比能快充电池电极材料，是当前高性能电池的迫切需求和发展趋势。团队聚焦磷负极因其比容量高和导锂快的优势，以化学理论为依据揭示磷负极反应新机理、从材料科学角度理性设计并制备磷基负极材料、从工程化视角优化制备工艺路线、以全电池系统化设计为目标创制基于磷负极的全电池新体系。主要内容：1)揭示溶解新机制，并创制选择性导锂材料和化学吸附材料，利用物理阻隔和化学吸附协同抑制溶解穿梭，提升了其电化学性能；2)电极制备方面，开发了高兼容性粘结剂，创制了具有吸附/转化功能的隔膜，研发了具有抑制磷负极溶解、促进成膜的高兼容电解液体系；3)面向消费电子设备、电动汽车和储能系统的应用需求，研发了基于磷负极的多种电池新体系。

**FC02-38****蒙烯材料与清洁能源**

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苏州大学

Recent years have witnessed a growing interest in employing graphene materials for emerging energy applications. As such, graphene can either be utilized as conductive additives for active components in energy storages to ensure sufficient electrical contact and buffer the severe volume expansion, or as supports for inactive components, i.e., protection/modification layers for current collectors and separators. Despite fruitful progress in the rational design of graphene for such aims, it still proves quite challenging thus far to (i) achieve a uniform distribution of a marginal weight content ( $<5$  wt%) of graphene with tailorable defects for electrode materials or (ii) realize highly functional graphene with versatile pore structures and tunable doping levels for modification of inactive components. In this respect, direct-CVD route serves as a promising solution toward the creation of multifunctional graphene architectures, in stark contrast to the counterparts produced from exfoliation approaches.

In this talk, the state-of-the-art of the direct-CVD route for the controllable synthesis of graphene will be presented; the versatility of direct-CVD graphene shown in energy devices is discussed in terms of differentiated roles.

### FC02-39

#### 聚合物基固态电解质及其固态电池设计

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2 清源创新实验室

目前固体聚合物电解质的低离子电导率和电解质/电极界面的不稳定阻碍了其广泛应用。为应对这些关键挑战，我们采用两条技术路线对聚合物固态电解质进行设计：1) 在传统的 PEO 基聚合物全固态电解质中，我们引入具有双功能的强路易斯酸氟化物添加剂：一方面，路易斯酸和阴离子相互作用可以促进锂盐解离提高锂离子转移效率；另一方面，电解质/电极界面原位生成富 LiF 的界面层，抑制锂金属的不均匀沉积以及 PEO 基质之间持续的不良反应，提升了 PEO 基电解质锂金属电池的界面稳定性和循环稳定性。其次，针对 PEO 室温离子电导率低的问题，发展了新型 PEO 改性方法，实现全固态 PEO 聚合物基固态电池的室温运行。2) 针对传统的固态聚合物电解质存在结晶性高导致其离子电导率低的科学难题，通过紫外光引发聚合交联反应来制备室温耐高压的塑晶酯类聚合物与玻璃纤维复合准固态电解质，该电解质可承受 4.4 V，25°C 离子电导率可达 10.65 mS/cm，匹配复合电解质的固态 LiFePO<sub>4</sub> 电池倍率性能在 10 C 下保持 80 mAh/g，在 300 个循环后仍可维持 124 mAh/g 为初始放电比容量的 85.6%。该类固态聚合物电解质的设计在保证离子电导率的情况下提高了机械性能和电化学稳定性。

**关键词：**聚合物；固态电解质；离子电导率

### FC02-40

#### Electrochemical reaction interface regulation of electroactive metal materials in energy storage

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In the battle to global climate change, China has promulgated a series of policies and is taking solid actions on track to achieve our decarbonization goals, i.e. 2030 carbon peak and 2060 carbon neutral. On this journey, to change our energy structure from fossil fuel dominating to renewable energy dominating is the cornerstone, as the industry development and our better lives all rely on the growing consumption of energy. However, renewable energy sources such as solar, wind and hydropower, all have the characteristics of being intermittent, and the super-large-scale electricity stations from renewable energy are mostly located in western China where energy consumption is not heavy. Under this situation, electrochemical energy storage plays the crucial role on the effective utilization and sustainable exploration of renewable energy. Batteries and hydrogen production via water electrolysis represent two main ways to store the intermittent and/or west-located electricity generated by renewable energy sources, which have been extensively-studied by researchers and with the related technologies well-developed.

Electroactive metal materials which have the intrinsic advantage of being conductive, have been investigated in both batteries and water electrolysis. In recent years, I have studied various types of electroactive metal materials, with the particular interest in the understanding and regulation of their electrochemical reaction interface. In this talk, I will use electrocatalyst Pt<sub>3</sub>Co and metal anodes as the examples to demonstrate how these regulation approaches lead to more efficient electrochemical reaction interfaces, and hence the improved

electrochemical performances in both hydrogen production and metal batteries.

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#### FC02-41

##### Corrosion of doped carbon electrocatalyst examined under operando conditions

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Nitrogen doped carbon is a widely used electrocatalyst developed over the past decades. Yet, it suffers oxidation at high anodic potentials. Because the alkaline electrolyte easily reacts with the acidic gases (CO<sub>2</sub>), the examination of carbon corrosion at operando conditions in base is a long-lasting challenge. We optimized the in-situ cells and used both differential electrochemical mass spectrometry and X-ray absorption spectroscopy to examine carbon degradation at operando conditions. High-accuracy and potential-resolved detection of acidic gases generated during carbon oxidation was enabled. For the first time, we observed the evolution of NO and NO<sub>2</sub> due to denitrogenation. The influence of supported catalyst nanoparticles on the oxidation of carbon was also systematically investigated.

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#### FC02-42

##### Airborne particle emissions emitted from brake materials sliding against grey cast iron disc under urban driving conditions

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Airborne particles emitted from vehicle brakes make up a significant portion of non-exhaust particle emissions in urban areas. Thus, Studying the variation of airborne particles emitted from various brake materials is significant for reducing airborne particles emitted from vehicles. This study investigated the effect of braking conditions on the airborne particles emitted from vehicle disc brakes using Low metallic, semi-metallic, and non-asbestos

organic (NAO) brake materials and grey cast iron as the brake contact pairs. Results show that the coefficient of friction and specific wear rate decrease with increasing contact pressure and sliding rate. Particle number size distribution has a single peak around 100 nm for all brake materials. Generally, total particle number and total particle mass emissions increase with increasing sliding rate and contact pressure. Both sliding rate and contact pressure can significantly affect the particle number and particle mass emissions. There is no particular trend for geometric mean diameter with sliding rate and contact pressure.

#### FC02-43

##### Functional design of porous polymer materials and their performance in lithium metal batteries

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Sun Yat-sen University

In this report, I would like to introduce the important research progress of my research group in the advanced functional structure design of porous polymer materials and their applications in lithium metal batteries in recent years. Specially, we have designed new polymer brushes as building blocks to construct functional porous polymer materials. Such functional porous polymers can not only be used as functional separators, solid-state electrolytes, and artificial SEI protective layers to improve the electrochemical properties of lithium metal anodes, but also as high-performance sulfur cathodes. The representative examples include two-dimensional molecular brush-functionalized porous bilayer composite separators toward ultrastable high-current density lithium metal anodes (Nat. Commun., 2019, 10, 1363), ultrathin, 2D shield-defensive, and single lithium-ion conducting polymeric membrane toward dendrite-free and long-cycling lithium metal battery (Adv. Mater., 2022, 34, 2108437), ultrathin yet robust single lithium-ion conducting quasi-solid-state polymer-brush electrolytes toward ultralong-life and dendrite-free lithium-metal batteries (Adv. Mater., 2021, 33, 2100943), robust all-organic protective layer toward ultrahigh-rate and large-capacity Li metal anodes (Nat. Nanotechnol., 2022, 17, 613), as well as rough endoplasmic reticulum inspired polystyrene-brush-based superhigh sulfur content cathodes toward lithium-sulfur cells with high mass and capacity loading (Adv. Mater., 2023, 35, 2211471).

#### FC02-44

##### 富锂锰基层状氧化物正极材料研究

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#### FC02-45

##### 低温钠/钾离子电池

王华\*

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相对于传统的锂离子电池，钠/钾离子电池除了拥有资源丰富、成本低等优点，在低温领域应用更具优势：

(1) 在同种溶剂中，钠/钾离子的去溶剂化能较锂离子更低，具有更快的界面反应动力学；(2) 钠/钾离子的 Stokes 半径更小，相同浓度的电解液，钠/钾离子体系电导率更高。基于此，我们通过合理的电解液组分设计、电极材料结构优化、电极/电解液界面调控，实现了硬碳负极在低温下高倍率可逆充放电，制备了基于硬碳负极的超低温钠离子、钾离子全电池；发展了低温高比能低温钠/钾金属二次电池以及低温无负极钠/钾电池，实现了 Ah 级软包钠离子电池在 -40° C 下基于全电池 110 Wh/kg 的高能量密度。这些工作体现了钠/钾离子电池在低温环境中的巨大应用潜力。

#### FC02-46

**Development of molecular enhancement electrocatalysts for Hydrogen production****Chunting He\*****Jiangxi Normal University**

Designing efficiently catalytic materials is of great significance for realizing efficient water splitting for hydrogen production and promoting the global carbon neutrality. However, painting a clear physicochemical picture of the catalytic process to achieve accurate synthesis of the catalyst structure remains challenging. Based on molecule-based materials such as structurally regulable metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), we have prepared several highly efficient electrocatalysts through the confinement effect of these porous materials, and developed the concept of molecular enhancement electrocatalysis to remolding the reactivities of various confined active sites. In addition, by establishing series of new catalytic structure models, we have simulated and understood the electronic structure of catalysts, the intermediate sorption, the breaking and recombination of chemical bonds at the atomic level. Our works provide useful guidance for the understanding of catalytic behavior on the organic-inorganic surface/interface and the rational design of new generation energy electrocatalysts.

**FC02-47****Advanced manufacturing and exciton recombination behavior of CsPbX<sub>3</sub> quantum dots****Jizhong Song\*****Zhengzhou University**

Lead halide perovskites, which have quickly grown to encompass the whole optoelectronic research community, such as photovoltaics, light-emitting diodes, lasing and photodetectors, are showing a great promise as a new generation of emitter materials. In addition to their composition independent optoelectronic properties, these emitters in nanocrystal (NC) form have a high photoluminescence (PL) quantum yields (QYs) of up to 100% and narrow light emitting peak with FWHM of about 20 nm, making them particularly attractive for high quality lightings and displays. Among various reported perovskite NCs, inorganic perovskite cesium lead halides (CsPbX<sub>3</sub>, X = Cl, Br, and I) is more promising for practical applications owing to the high thermal stability and low moisture sensitivity comparison with organic-inorganic hybrid counterparts. Herein, I will give a detailed introduction on advanced manufacturing of efficient CsPbX<sub>3</sub> quantum dots and some strategies for the efficient CsPbX<sub>3</sub> quantum dot light-emitting diodes (QLEDs) reported by our group.

**FC02-48****配位氧键能量设计****李峰****中国科学院金属研究所**

电池中的电化学反应发生在电极-电解质界面。所有界面反应过程均与溶剂-溶质相互作用密切相关[1,2]。为了说明溶剂-溶质相互作用之间能量关系对于电化学影响对界面反应的影响,本报告包括了四个内容:(1)通过溶剂-阳离子相互作用实现快速反应铝硫电池[3]。在 Al-S 电池中,电解液中 Al<sup>3+</sup>的配位结构由 Al<sub>2</sub>Cl<sub>7</sub><sup>-</sup>改变为 Al<sub>2</sub>Cl<sub>6</sub>Br<sup>-</sup>, Al<sup>3+</sup>解离活化能降低, Al-S 界面反应加速,性能提高。(2)通过溶剂-阳离子相互作用以减慢反应抑制锂枝晶形成[4]。锂金属负极的醚电解液中,引入新溶剂形成具有强溶剂-Li<sup>+</sup>相互作用的溶剂化结构,锂沉积动力学减慢,抑制了锂枝晶的形成。(3)溶剂-阴离子相互作用实现高稳定性锂金属电池酯电解质中的溶解-沉淀平衡 [5]。在锂金属负极酯类电解液中,引入了新溶剂来替代 DMC,获得了含有游离羰基的新溶剂化结构,游离羰基排斥 NO<sub>3</sub><sup>-</sup>,改变 LiNO<sub>3</sub>的溶解-沉淀动力学,增加其溶解度。(4)固体溶剂-盐相互作用改变溶解度限制[6]。在用于锂金属阳极的酯电解质中,制备了含有解离态 LiNO<sub>3</sub>的中

间层材料，可快速释放和还原，形成稳定的 SEI 膜，提高锂金属负极的长循环稳定性。

**FC02-49****固态电池微纳结构与界面调控**

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High-performance energy storage battery is an urgent demand for the development of new energy electric vehicles, smart grid and other strategic emerging industries. The efficient transport of electrons/ions at the internal interface of the battery is the key to the construction of high-performance batteries. The study of micro-nano scale interface is conducive to the in-depth understanding of the physical and chemical properties and evolution of the interface from a micro perspective. Therefore, based on solid state battery materials and interface regulation, we focus on the design of solid-state battery interface, interface electron/ion transport mechanism and synthesis of key materials. Our work specifically includes the following: (1) By constructing a continuous nanowire network structure to regulate the ion transport at the interface, it is found that the inorganic nanowire / organic polymer interface provides a fast and efficient transport path for lithium ions. (2) The flexible contact interface between electrodes and electrolytes is designed and constructed. The flexible interface provides a three-dimensional channel through electrolyte and electrolyte/electrode interface for ions transport. (3) Based on the above research, some new solid-state energy storage materials are designed, and the application of new energy storage materials in flexible solid-state batteries is realized.

**FC02-50****高性能固态电解质膜的设计**

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**FC02-51****The passivation and elimination of defects in the organic-inorganic perovskite films**

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The types and distribution of defects in organic-inorganic hybrid perovskite thin films, which serve as the active layer, directly determine the performance of perovskite solar cells (PSCs). Understanding the types and distribution of these defects, comprehending their impact on the efficiency and stability of PSCs, and minimizing energy losses due to non-radiative recombination are critical areas of fundamental research in the field of PSCs. To address this, our research team has developed several methods to passivate or directly eliminate defects, for example, using low-dimensional perovskites, chemical polishing and physical polishing.

Firstly, by constructing two-dimensional perovskites on the surface of three-dimensional perovskite thin films, we achieved effective defect passivation and increased the binding strength between grains, thereby enhancing the energy conversion efficiency and mechanical stability of the devices. Secondly, we proposed a two-step chemical polishing strategy that precisely removes impurities from the perovskite thin film surface. Through selective chemical reactions between the polishing agent (octylammonium bromide, OABr) and the unstable components on the perovskite thin film surface, these components are converted into two-dimensional (2D) perovskites, which are then removed through chemical polishing. Additionally, the OABr molecules remaining from the chemical polishing act as passivators, passivating sub-surface defects in the perovskite thin film. This "elimination +



passivation" synergy maximizes the reduction of surface defects in the perovskite thin film. Lastly, a one-step cleaning strategy based on functional polymers was utilized to achieve precise removal of surface impurity phases and effective passivation of sub-surface defects. The strong intermolecular interactions provided by the functional polymers enable effective removal of surface impurities without damaging the perovskite crystal structure. After cleaning, the electron-donating groups (C=O) in the polymers passivate the sub-surface uncoordinated Pb<sup>2+</sup> defects.

Based on these two strategies, we achieved impurity removal and sub-surface defect passivation in perovskite thin films. This synergistic effect significantly reduced interfacial non-radiative recombination and suppressed interfacial ion migration, markedly improving the efficiency and stability of the devices. These two strategies provide strong support for the large-scale industrialization of PSCs in the future.

## FC02-52

### 高稳定性氧电催化剂

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氧还原反应是新能源转换技术如燃料电池和金属-空气电池的核心反应。由于氧还原反应动力学过程较为迟缓, 当前催化剂仍需采用价格昂贵、资源稀缺的贵金属铂作为主要活性组分。催化剂高昂的成本已成为制约燃料电池及许多电化学能源技术商业化进程的重要因素, 研发低成本, 高活性和高稳定的阴极氧还原催化剂是实现众多新能源技术开发和推广的关键。近年来, 贵金属基催化剂的质量活性已经取得了极大的突破, 而对催化剂稳定性, 特别是膜电极及电池器件服役与失效的研究仍然较少。此外, 单原子催化剂由于其独特的电子结构, 均一的活性中心和接近 100% 的原子利用率, 在众多催化反应中均展示出了优异的催化活性, 展现出巨大的应用前景。多元活性中心单原子往往能提供更多种类的活性中心, 且相邻原子间的协同作用也有益于提高其电催化活性, 被认为是单原子催化剂的下一个突破口。然而, 目前的单原子催化剂的研究一般仅限于一元至二元单原子催化剂, 对于多元活性中心单原子催化剂的研究报道很少, 主要是难以实现将不同种类的金属原子稳定的锚定在单一载体上, 极大的限制了单原子催化剂的研究和应用领域。因此, 迫切需要开发一种通用且高效的方法来实现具有多元活性中心的单原子的可控合成方法。

关键词: 稳定性; 氧还原; 燃料电池; 氢能; 低铂

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## FC02-53

### The application of MOF Materials in solid lithium metal batteries

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High-energy and high-safety lithium metal batteries (LMBs) are considered as promising next-generation energy storage devices. Replacing conventional liquid electrolytes with solid electrolytes is expected to improve the stability of LMBs. Metal-organic framework (MOF) has been widely applied in solid electrolytes in recent years because of its high designability, light weight and ordered pore structure. However, there are some problems in solid electrolytes with MOF materials, such as random distribution of MOF fillers in polymer electrolytes, side reactions, low ionic conductivity and low mechanical strength. Herein, high-performance solid electrolytes are

constructed by modulating the structure and designing the functionality of MOF materials. For example, a self-assembly strategy is employed to construct a 3D hierarchically self-assembled MOF conductor, which realizes continuous Li<sup>+</sup> transport and high mechanical strength. Moreover, inspired by the structure and function of the natural leaf, an ultrathin electrolyte with great mechanical flexibility is constructed. The obtained electrolyte eliminates hazardous intercrystalline diffusion of liquid electrolytes in voids and gaps, and simultaneously enables uniform Li deposition and suppresses lithium-electrolyte reactivity, thus resisting dendrite growth and avoiding severe side reactions. These findings will provide research ideas to develop high-performance LMBs.

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## FC02-54

### Development of efficient wide-bandgap perovskites and sub-cell characterization for all-perovskite multi-junction solar cells

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All-perovskite multijunction solar cells promise to deliver power conversion efficiencies (PCEs) beyond the theoretical limit for single-junction devices at low costs. However, the sub-par performance of the wide-bandgap perovskite limits the efficiency gains of tandem solar cells. In this contribution, we unveil localized compositional heterogeneity as a crucial factor in limiting the performance and longevity of wide-bandgap perovskite solar cells. We present our newest mitigation strategies using templated growth of Br-rich perovskites to improve their halide homogeneity and photostability, improving the open-circuit voltage to above 90% of the theoretical limit at 1.8 and 2.0 eV bandgap (1.38 and 1.44 V, respectively). We fabricate efficient all-perovskite double- and triple-junction solar cells, each presenting PCEs beyond 26%.

We also demonstrate a solar-driven water electrolysis system by connecting an all-perovskite tandem solar cell with a water electrolysis cell. A solar-to-hydrogen (STH) efficiency of 17.8% is achieved and maintains over 60% of its initial performance for over 180 hours. Using a suite of sub-cell selective measurement techniques, we explore the efficiency potential and degradation mechanism of tandem solar cells. After aging, additional shunts are introduced in the narrow-bandgap perovskite sub-cell despite the overall optoelectronic quality of the perovskite absorbers unchanged. Cross-sectional SEM and chemical profiling analysis indicate that the decomposition of the perovskite/transporting layer interface is the major factor for device failure. Our results highlight that developing a stable Pb-Sn perovskite/transporting layer interface is critical to further improving the stability of all-perovskite tandem solar cells and PV-assisted applications.

## FC02-55

### 可充放钠电池电极-电解质界面化学研究

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可充放钠电池以其显著的可持续性、经济性成为极具应用前景的电化学储能技术。在电池循环过程中，电解液还原分解在负极表面生成的固体电解质膜 (solid electrolyte interphase, SEI)，对界面稳定性的影响非常关键，首圈充电过程负极表面形成 SEI 膜会消耗活性钠，另一方面，循环过程中 SEI 面临持续生长的问题，这些将大量消耗全电池中有限的活性钠离子，造成不可逆容量损失和内部阻抗增加。针对这些问题，开发了一种安全、实用的钠离子电池正极补钠添加剂，解决了硬炭负极在形成 SEI 膜过程导致首圈库伦效率低，造成全电池能量密度和循环稳定性降低的问题。提出抑制电子泄露稳定碳负极/电解质界面的设计策略，缓解了碳负极循环过程中 SEI 持续生长的问题。另外，提出了双单体原位共聚制备三维网络结构凝胶聚合物电解质的设计策略，稳定了碳负极和金属钠负极表界面，获得了本质安全的可充放钠电池。

**关键词：**钠离子电池；负极；硬炭；金属钠；表界面

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#### FC02-56

##### 柔性印刷能源材料与器件

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#### FC02-57

##### Nickel-Rich Cathodes through Multifunctional Composite Surface Engineering

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Nickel-rich layered oxides are a class of promising cathodes for high-energy-density lithium-ion batteries (LIBs). However, their structural instability derived from crystallographic planar gliding and microcracking under high voltages has significantly hindered their practical applications. Herein, we undertake resurfacing engineering for single-crystalline  $\text{LiNi}_{0.83}\text{Co}_{0.07}\text{Mn}_{0.1}\text{O}_2$  (SNCM) cathode. A passivation shell, comprising a surface fast ion conductor  $\text{Li}_{1.25}\text{Al}_{0.25}\text{Ti}_{1.5}\text{O}_4$  (LATO) layer and a near-surface confined cation hybridization region, is established through co-infiltrating Al and Ti into SNCM, which can profoundly improve structural stability. We show compelling evidence that high-conductivity LATO-overcoat facilitates  $\text{Li}^+$  conduction and resists electrolyte attack. The introduction of strong Al-O bonds and high entropy regions stabilize bulk and near-surface lattice oxygen respectively during cycling with a high cut-off voltage, thus hindering the formation of oxygen vacancies and the occurrence of detrimental volume changing phase transformations, and ultimately suppressing the crystallographic planar gliding and nanocracking. Subsequently, the SNCM through composite surface engineering drastically outperforms the baseline SNCM, exhibiting an ultrahigh 88.9% retention rate of the original capacity at 1.0 C after 400 cycles, and a discharge capacity of 146.8 mAh g<sup>-1</sup> with a 92.6% capacity retention rate after 200 cycles at 5.0 C within a voltage window of 2.7 - 4.3 V. The promising performance

demonstrated by the multifunctional surface coating highlights a new way to stabilize high-energy-density Ni-rich cathodes for LIBs.

## FC02-58

### Advanced characterization methodology for materials structure and reaction mechanism dynamically and precisely visual detection and determination

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We focuses on the common key scientific issues of material field “Advanced characterization methodology for materials structure and reaction mechanism dynamically and precisely visual detection and determination”. The applicant has developed XAS/PDF/XES/XRD/EELS/EXELFS et al. combined with electron microscopy and corresponding energy spectra, molecular vibration spectrum ATR-SEIRAS/DRIFTS/Raman/fs-TA/NMR/PALS et al. to achieve in-situ/operando multi-spectrum for atomically precise materials structure and reaction mechanism dynamically visual detection and determination methodology. The definite holographic "structure activity relationship" regarding the materials structure, valence state and molecule reaction mechanism during in-situ/operando key energy catalytic process was established[1-10]. Through mathematical modeling, DFT calculation and AI machine learning data mining, large materials database regarding the origin and regulation principle of material properties was built, forming “materials structure and reaction mechanism dynamically and precisely visual detection and determination” large materials database driven to accelerate and guide the corresponding object-oriented high performance new materials "Relay iteration" rational design and synthesis general methodology platform.

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## FC02-59

### 一体化固态储能器件：从薄膜到体相

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本报告首先汇报和介绍本课题组在锂离子高盐聚合物固态电解质、硫化物（复合）电解质、正极预锂化等方面的研究进展；进一步设计序构电极（嵌入型氧化物、转换型硫化物、空气电极催化剂）-固态电解质一体化锂电池，通过电解质的原位成膜渗透，极大增加了电极-电解质界面接触面积、减小了界面势垒、增强了界面稳定性，显著提高了器件性能。另外，将介绍一类新型钠离子电池负极材料的储钠机制、准固态钠离子电解质及其一体化钠离子电池的设计。

**关键词：**聚合物电解质；硫化物电解质；锂电池；钠离子电池

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#### FC02-60

##### 高能量、高安全性固态电池

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发展高性能电池技术是我国能源结构转型升级、实现“碳中和、碳达峰”目标的必由之路。广泛使用的锂离子电池不仅能量密度难如人意，氧化物正极与易燃电解液的副反应更使其安全性雪上加霜，严重威胁了锂电池生产、存储、应用、回收整个产业链。针对这一问题，我们提出从锂离子电池化学体系中解耦低容量、含金属锂/氧等高活性物种的电极反应，“釜底抽薪”地根除其对电池性能与可靠性的不利影响。在此基础上，融合富锂无氧的新型高容量硫化锂正极材料与高可靠性的固态电池设计，在实现高能量密度的同时，强化电池在机械、电、热、水氧等滥用条件下的安全性。通过发展兼具高能量、高安全性、高耐候性的新型固态电池，为突破现有电池技术安全性与能量密度“鱼与熊掌不能兼得”的共性瓶颈提供新的思路。

**关键词：**高能量；高安全性；固态电池

#### FC02-61

##### Conversion Anode for Aqueous Zinc Batteries

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Our research focuses on a stable aqueous Zn-based battery with long cycling stability, decent energy density, and ultimate safety performance for large-scale energy storage. To achieve this purpose, we did systematic studies on the Zn metal anode, electrolytes, and new cathode development.

Halogen-powered static conversion batteries (HSCBs) thrive in energy storage applications. They fall into the secondary non-flow batteries and operate by reversibly changing the chemical valence of halogens in electrodes or/and electrolytes to transfer electrons, distinguishing them from the classic rocking-chair batteries. The active halide chemicals developed so far have covered organic halides, halide salts, halogenated inorganics, and organic-inorganic halides rather than the earliest and most widely studied elemental halogens. Aside from this,

various redox mechanisms have been discovered based on multi-electron transfer and effective reaction pathways, contributing to better electrochemical performances and stabilities of HSCBs. We discuss the status of halogen based conversion cathode for zinc batteries and their electrochemical mechanism-performance correlations. We first provide a detailed exposition of the fundamental redox mechanisms, thermodynamics, conversion and catalysis chemistry, and mass or electron transfer modes. We conclude with a perspective on the challenges faced by the community, and opportunities towards practical applications of high-energy halogen cathodes in aqueous zinc ion batteries.

## FC02-62

### **Marangoni Self-Propulsion of Miniaturized Devices for Energy Conversion**

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Marangoni self-propulsion is autonomous motion of liquid or solids driven by a surface tension gradient of either concentration or heat. Conventional Marangoni self-propulsion based on covalent surfactants has the problems of (1) limited motion lifetime as the interface reached saturated adsorption of surfactant molecules, (2) difficulty in motion control such as ON-OFF, trajectory due to the complexity of Marangoni fluid dynamics. Here, we propose a supramolecular strategy of dynamically removing excessive interfacial molecules to maintain the surface tension gradient and prolong the lifetime. The surfactants could either be captured by a molecular recognition process or a supra-amphiphile could act as an alternative. The motion control was realized via a pH-responsive link of Schiff base of supra-amphiphiles, which decompose to be removed to maintain the motion or remain intact to stop the motion. By applying this strategy to the fabrication of a centimeter-scaled miniaturized device, we further regulated the trajectory into rotation and harvested electric energy in the presence of magnetic field. The above strategy provides an active solution to prolong and control Marangoni self-propulsive devices for the advance of intelligent material systems.

## FC02-63

### **2D Graphene in a 3D Architecture: Bicontinuous Nanoporous Graphene for Energy Applications**

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Constructing bulk graphene materials while preserving their inherent 2D properties is crucial for utilizing atomically thin graphene in various devices and engineering applications. Traditional 3D graphene structures, composed of discrete graphene nanosheets, fall short of achieving this objective due to issues such as graphene sheet restacking, weak Van der Waals contacts, and a high density of defects, which substantially compromise the distinctive characteristics of 2D graphene. In recent years, our efforts have led to the successful development of 3D continuously porous graphene by folding single-sheet graphene into a 3D bicontinuous porous architecture. This innovative material not only retains the 2D properties of graphene but also introduces novel functionalities stemming from its 3D structure, establishing a unique category of 3D graphene materials with a myriad of exceptional properties. Our comprehensive studies on this material span from the designable fabrication of 3D nanoporous graphene, with tunable microstructure and physicochemical properties, to exploring its wide range of applications in energy conversion and storage. This presentation will provide an overview of recent advances in overcoming challenges associated with developing 3D continuously porous graphene, highlight the benefits and opportunities that the new materials bring to energy-related applications, and discuss the remaining challenges that

necessitate future research.

#### FC02-64

##### 储能应用驱动二维氧化物结构调控

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电化学电池主要牵涉到的关键问题是离子的存储、传输及转化过程。因此，通过有效途径，促进以上三个与离子相关的电化学过程，均将促进新型电化学器件的性能。申请人利用二维氧化物结构调控有效促进离子存储、离子输运及离子转化，并尝试用其提升电化学储能器件性能。1. 发明了二维氧化物与石墨烯异质组装的方法，获得了高导电性、丰富边缘结构、高金属离子亲和性的复合电极材料，显示优异的离子存储能力。2. 发明了二维氧化物表面孔结构精细调控及垂直排布策略，获得了高锂离子穿透性的三维氧化物修饰层，有效抑制锂枝晶生长。3. 发明了二维氧化物掺杂及导电基体调控策略，获得了高稳定、高活性氧转化催化剂，实现了高性能金属空气电池。

#### FC02-65

##### Interfacial regulation of transition metal sulfide electrocatalysts for alkaline water electrolysis

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Clean hydrogen energy is a promising energy carrier for sustainable energy supply. Green H<sub>2</sub> production from electrocatalytic water splitting consists of two half-cells including HER and OER. Due to sluggish kinetics and unfavorable thermodynamics, the production of hydrogen energy via water electrolysis is highly dependent on electrocatalysts, which are expected to afford high currents at low overpotentials. Considering the practical applications, highly active transition metal-based electrocatalysts are more desirable to perform alkaline electrolyzer due to the low cost and the popularity in industrial fields.

Among them, MoS<sub>2</sub> and WS<sub>2</sub> nanosheets received great attention owing to the unsaturated Pt-like hydrogen adsorption sites and special graphene-like layered structure convenient for electron transfer. But the electrocatalytic activity essentially is determined by edges but not basal planes. Therefore, maximizing the accessible active edges and modulating the conductivity of MoS<sub>2</sub>/WS<sub>2</sub> layers are critical to boost the electrocatalytic performance. Currently, various strategies have been developed in our group to boost the electrocatalytic activity of MoS<sub>2</sub> or WS<sub>2</sub> layers, such as constructing heterointerfaces [1], combining with carbon material [2], forming non-stoichiometric nanocrystals [3], and doping heteroatoms [4]. Also, the intrinsic activity was improved via transforming the crystal structure from 2H phase to 1T phase [5]. These studies provide new insights into optimizing transition metal-based electrocatalysts for water electrolysis.

#### FC02-66

##### Electrolyte design in stabilizing zinc anode

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Li-ion batteries are currently the most commonly used electrical energy storage devices. However, the scarcity of resources and the environmental impact related to the production of Li-ion batteries, as well as the safety issues during their use, severely hinder their wider deployment. Rechargeable aqueous Zn ion batteries (ZIBs) are highly desirable for future applications in large-scale energy storage since they are inexpensive and safe in comparison

with lithium-ion batteries (LIBs). However, the problems of dendrite growth and the related side reactions in zinc anode limit their further development and application. Since the de-solvation process is directly related with water splitting, side reactions and Zn dendrite, thus, the specific de-solvation mechanism is a fascinating research field to figure out the reason of inhibiting side reactions and Zn dendrite. Our research mainly focuses on the de-solvation process of solvated ions ( $[\text{Zn}(\text{H}_2\text{O})_6]^{2+}$ ). We found that some functional chemical groups, amphipathic molecules and carbon quantum dots can help with the de-solvation process and suppress the dendrite growth and side reactions. Additionally, vertically-oriented Zn plating with preferential growth of (100) plane using disodium lauryl phosphate (DLP) as an electrolyte additive is realized. DLP is preferentially anchored on the Zn (002) crystal plane via polar phosphate group, then the deposition of Zn atoms on the (002) plane is shielded by the long alkyl chain, finally promoting the preferred growth of the (100) plane. This unique growth pattern results in ultrastable Zn plating/stripping at super-high current density of  $50 \text{ mA cm}^{-2}$ , with a cumulative capacity of  $8500 \text{ mAh cm}^{-2}$ .

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## FC02-67

### A study on the design and performance of cement-based supercapacitors with an ordered microstructure

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Concrete is the second most consumed material on Earth, after water, with high production and sustained demand. Buildings have a large volume of objects and a long lifespan, but they are also a significant source of electricity consumption. The development of structural energy storage on existing buildings is equivalent to providing movable in-situ power reserves for buildings, which will become an effective means of utilising renewable energy and user-side energy storage. This article presents a composite electrolyte with an oriented microstructure for use in building wall panels. The electrolyte is constructed using magnesium phosphate cement, which forms a rigid cement skeleton. Flexible PAM provides channels for ion transport, while the coupling effect of the solid electrolyte composite components results in ultra-high ion conductivity and multifunctional properties. The electrolyte has been assembled with MXene symmetric electrodes to develop cement-based supercapacitors with high capacity, high energy density, and cycling stability. Finally, a demonstration of cement-based capacitors as building wall panels was conducted, with the objective of providing a feasible exploration for the development of a building power supply.

## FC02-68



**Hybrid anion exchange membrane with a novel quaternary ammonium valence bond/non-valence bond modified covalent organic framework with both ion enhanced conduction and stability for hydrogen production by water electrolysis**

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In view of the increasing global energy use, energy supply, climate, etc. have been negatively impacted. To meet the needs of sustainable development, hydrogen energy has received wider attention as a recognised low- and zero-carbon energy source. Hydrogen production from water electrolysis with anion exchange membranes is particularly important due to the high cost of proton exchange membranes and precious metal catalysts.

Ideal anion exchange membranes (AEMs) need to have high ion selective permeability, low electrical resistance, and good mechanical strength. The challenges are mainly from the following two aspects: (1) Improve the efficiency of hydrogen precipitation from water electrolysis by increasing the ionic conductivity, but this process will cause a decrease in the mechanical properties and stability of membrane materials. The trade-off between ionic conductivity and water absorption and swelling phenomena needs to be resolved. (2) The AEMs system is in a local strong alkaline environment. Therefore, the structure contains functional groups such as amino groups and quaternary ammonium salts that are easily attacked by nucleophilic substances such as OH<sup>-</sup>, leading to the breakage of the membrane molecular chain and the detachment of ion-exchange groups. Therefore, there is an urgent need to overcome the vulnerability of functional groups and polymer backbone to attack by nucleophilic OH<sup>-</sup> and other substances under alkaline conditions.

Numerous studies have shown that the design of AEMs is limited by the trade-off between ionic conductivity and dimensional stability. The construction of "ion-channel" nanostructures to assist transport can combine good ion selectivity with low water absorption and swelling. Covalent organic frameworks (COFs) have attracted much attention due to their large specific surface area, tunable pore size and structure, and easy functional customisation. The design of highly aligned and oriented ion channel structures is facilitated by the selection of advanced multilayer polymeric structures COFs. The strong toughness of quaternary ammonium polyphenylene ether (QAPPO) organic matrix can achieve COF rigid structural transport orbital enriched state and regulate anion transport ability, and the realisation of this property provides a new idea for the design and development of hybrid matrix membranes with high-performance ion-conducting channel structures.

In this paper, we attempted to peel COFs into monolayer nanosheets (SL-COF) by mechanical assistance and other means, and solvent-functionalised SL-COF with PPO, and added a large number of OH<sup>-</sup> quaternary ammonium (QA) cation "springboards", to obtain SL-QACOF@QAPPO, which contains transport sites that can be jumped consecutively. Based on this, the design of SL-QACOF@QAPPO, which combines the toughness of the QAPPO organic matrix with the tunability of the highly dispersed encapsulated SL-QACOF with highly aligned transport sites, with the assistance of ultrasonic and mechanical means, is expected to solve the trade-off between the high conductivity and the strong stability of the AEMs, and to realise an anion-exchange membrane with a higher hydrogen production efficiency.

In this paper, we mainly compared the doping of COFs with different lengths of carbon chains of iodomethane, iodopentane and iodoctane, as well as different structural modifications of trifluoriodomethane, to study the effect of the change of ion transport channels on OH<sup>-</sup> conductivity in SL-QACOF@QAPPO composite membranes, as well as to study the effect of the ion channels on the aggregation degree and selectivity of OH<sup>-</sup> through the different doping amounts of COFs, and to evaluate the effect of the SL-QACOF@QAPPO composite membranes on the aggregation degree and selectivity of OH<sup>-</sup>. Stability of QACOF@QAPPO composite membranes: the dimensional and thermal stability of the composite membranes were judged by measuring their water absorption, swelling rate and thermogravimetric weight.

Secondly, by vacuum impregnating functional ionic liquids into the pores of COFs and comparing with the doping

of quaternary ammonium reagent valence bond-modified COFs, we compared the effects of fixed and movable transport sites on the ion transport mechanism, and used molecular dynamics simulation and Monte Carlo simulation, etc., to predict the transport processes and transfer paths of OH<sup>-</sup> ions in the hybrid matrix membranes as well as the ion transport rate and selectivity and other Performance parameters. Combining the experimental results and simulation prediction results, the dynamic mechanism of OH<sup>-</sup> ion transport applicable to water electrolysis device is established, and the optimal ion channel design method is selected.

The bipyridine groups in the COFs were quaternised and modified and applied in AEMs, so that the COFs skeleton had OH<sup>-</sup>-conducting functional groups, the robust scaffold structure in the COFs could improve the mechanical properties and stability of the AEMs, and the ordered two-dimensional channels and the dense quaternised ion-conducting groups in the channels could improve the electrochemical properties of the AEMs. When 0.25% iodomethane-modified COFs were doped on the membrane substrate, the conductivity was 54.26 mS cm<sup>-1</sup>, which reached about 1.6 times of that of the pure membrane, and when 0.25% fluorine-containing monomer-modified COFs were doped on the membrane substrate, the conductivity could reach 61.54 mS cm<sup>-1</sup>, which was twice of that of the pure membrane. The strength and dimensional stability of the composite membrane were also significantly improved, and its maximum tensile strength was 25.46 MPa, which was an improvement over the performance of the pure QAPPO membrane.

In summary, although there are still some problems in applying COFs to AEMs, their robust scaffold structure and ordered pores can improve the ion channel transport performance of AEMs, so the possibilities of exploring the application of COFs to AEMs are unlimited.

#### FC02-69

##### 铜箔表面疏丙基三甲氧基硅烷膜的电解制备及耐腐蚀性能研究

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#### FC02-70

##### 超声喷丸处理对钛/铝复合板冷轧复合界面复合行为的影响

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#### FC02-71

##### 锂-硫电池中的同位素电化学效应

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同位素效应是指由于质量或自旋等核性质的不同而造成同一元素的同位素原子（或分子）之间物理和化学性质存在差异的现象。尽管核电荷决定了元素的基本的物理和化学性质，但同一元素不同同位素间的性质仍可能存在较大差异，而目前针对同位素电化学性质的研究仍然较少。以锂-硫电池为研究对象，我们初步探索了硫元素稳定同位素（硫-32/硫-34）间的电化学同位素效应。由两种同位素分别形成的八元环分子中，硫-34 比硫-32 形成更强的 S-S 共价键。硫-34 与锂反应活化能更低，反应生成的可溶性多硫化锂具有更强的阳离子-溶剂相互作用和更弱的阳离子-多硫阴离子相互作用，有利于促进多硫化物的溶剂化并阻碍其向负极穿梭（图 1）。因此，基于硫-34 的锂-硫电池表现出更快的正极反应动力学和更好的循环稳定性。基于硫同位素穿梭效应的区别，提出了一种新的稳定硫同位素分离方法，即通过锂-硫电池分离硫同位素。基于该方法得到的同位素分离比相比化学交换法和蒸馏法等传统分离方法高出 1-2 个数量级，为重同位素的低成本提纯制备和应用研究带来新机遇。

## 墙报

## FC02-P01

**A hydrophobic composite coating based on SiO<sub>2</sub>@Cu for droplet energy harvest**

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Raindrop is a clean and widely distributed energy in nature, and liquid-solid triboelectric nanogenerator (LS-TENG) has become a promising way to harvest raindrop energy and convert it into electricity. However, low output performance and complicated fabrication process still limit its practical application. Here, we report a hydrophobic composite coating as triboelectric layer composed of poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) with SiO<sub>2</sub>@Cu and 1H,1H,2H,2H-perfluorooctyltriethoxysilane (FOTS). The addition of SiO<sub>2</sub>@Cu improves the dielectric constant of coating, while the addition of SiO<sub>2</sub>@Cu together with FOTS leads to an increased hydrophobicity, both of which enhance the electrical output performance of LS-TENG. Under the optimal construction condition of PVDF-HFP/FOTS/SiO<sub>2</sub>@Cu triboelectric coating, LS-TENG exhibits an outstanding electrical performance with voltage of 19.3 V and current of 6.8  $\mu$ A from a single waterdrop, which is 2.5 times and 2.8 times higher than that based on pure PVDF-HFP. It shows the ability to light up 27 LEDs and a commercial timer. Besides, all layers in LS-TENG including PVDF-HFP/FOTS/SiO<sub>2</sub>@Cu triboelectric layer and AgNW conductive layer, are fabricated by coating processes of drop-casting and spraying, which gives LS-TENG high scalability, design flexibility and transparency. Therefore, this work provides a novel approach to construct a high-performance and easy-fabrication LS-TENG, and is expected to be widely applied in the field of harvesting droplet energy to power more smart electronic devices effectively.

## FC02-P02

**The solvation structure modification of “water-in-deep eutectic solvent” electrolyte for high-performance aqueous zinc metal batteries**

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Dendrites and side reactions generated by zinc anodes during the cycling process have seriously hindered the development of aqueous zinc metal batteries (AZMBs). In this study, a highly compatible water-deep eutectic solvent (WDES) electrolyte consisting of zinc trifluoromethanesulfonate (Zn(OTf)<sub>2</sub>), propylene glycol (PDO), and water was proposed to improve the stability of zinc metal in AZMB by modulating the electrode/electrolyte interface environment. Experimental and theoretical results showed that PDO reconfigured the hydrogen bonding network, effectively suppressed the reactivity of water, broadened the electrochemical stability window, and reduced the generation of dendrites and by-products. Finally, the Zn//Zn symmetric cell was stably cycled for more than 3000 h. The electrochemical performance of the assembled Zn//V<sub>2</sub>O<sub>5</sub> cell reached 80% specific capacity after 2500 cycles. Therefore, this study provides a new perspective on electrolyte modification strategies for metal-ion batteries.

## FC02-P03

**Dual-ion co-insertion boosting site activity and structural stability of nickel hexacyanoferrate for superior aqueous ammonium ion storage**

Bojie Zhou, Ping Luo\*

Aqueous ammonium ion batteries (AAIBs) are promising candidates for large-scale energy storage because of their low cost, exceptional high safety, and rapid ion diffusion. However, the large ionic radius of  $\text{NH}_4^+$  (1.43 Å) lead to structural damage and limited transport dynamics of cathode materials. Herein, a  $\text{K}^+$  pre-intercalated  $\text{KNiHCF}$  Prussian blue analogues cathode is designed, which could bring the  $\text{NH}_4^+/\text{K}^+$  co-insertion during the cycle. Compared with pure  $\text{NH}_4^+$  insertion, dual-ion co-insertion can effectively improve the electrochemical kinetics and boosting the site activity of the  $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$ . Moreover, the mechanism of two-phase transition during the cycle is revealed and the density functional theory (DFT) calculations prove that  $\text{NH}_4^+/\text{K}^+$  co-insertion alleviates the binding interaction of guest ions to the host materials, which is conducive to ion diffusion and structural stability. Therefore,  $\text{KNiHCF}$  exhibits superior ammonium ion storage performance (63.9  $\text{mA h g}^{-1}$  at 60  $\text{mA g}^{-1}$ ). Compared with other similar cathode, it has excellent cycling stability (77.3% after 3000 cycles at 3000  $\text{mA g}^{-1}$ ). Additionally, assembled  $\text{KNiHCF}$ //activated carbon (AC) hybrid capacitors exhibits an extraordinary capacity retention of 94.9% after 4000 cycles at 1000  $\text{mA g}^{-1}$ . This study provides new insights into the storage mechanisms of AAIBs.

#### FC02-P04

##### Unravelling the Enhancement of Oxygen Vacancies on the Low-Temperature Li-Ion Storage

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Low temperature lithium-ion batteries have attracted considerable attention in extreme environmental applications. However, the poor performance of LIBs at low temperature still limits their development due to slow ion diffusion kinetics in electrode materials. Micron-scale  $\text{V}_2\text{O}_5$  with tunable oxygen vacancy concentrations is prepared by a nucleation-growth phase transition strategy. The experimental quantification indicates that the relationship between the lithium storage performance and the oxygen vacancy concentrations values is linear at temperatures of  $-40^\circ\text{C}$  and above, and exponential at ultralow temperatures below  $-40^\circ\text{C}$ .  $\text{V}_2\text{O}_5$ -300 with rich oxygen vacancies shows a higher rate capability (220  $\text{mAh g}^{-1}$  at 0.05  $\text{A g}^{-1}$  and 103  $\text{mAh g}^{-1}$  at 1  $\text{A g}^{-1}$ ) and a better cyclability (90% capacity retention over 1000 cycles at 0.5  $\text{A g}^{-1}$ ) at  $-40^\circ\text{C}$ . Furthermore, the symmetric full cells exhibit high rate and long cycle performance at  $-40^\circ\text{C}$ . The excellent low-temperature performance indicates that abundant oxygen vacancies in the electrode provide fast ion transport pathways, which are conducive to promoting  $\text{Li}^+$  diffusion kinetics and enabling fast interfacial charge transfer. We demonstrate that the design of oxygen vacancy-rich structures is an effective strategy for the development of advanced electrodes for low-temperature LIBs.

#### FC02-P05

##### Progress in suppressing phase segregation of the wide bandgap perovskites

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The hybrid halide perovskite materials with tunable bandgaps have been regarded as ideal candidates for tandem solar cells. However, during the device operation, halide ions undergo redistribution under illumination, resulting in the formation of two types of perovskites with Br and I enriched, known as photoinduced phase segregation. This issue stems from uneven crystallization and intrinsic defects in perovskite films. Furthermore, the influence of transport layers not only affects perovskite crystallization but also leads to interface charge accumulation during operation. Therefore, comprehending and suppressing phase segregation in hybrid halide perovskites

represent critical challenges in photovoltaics. Initially, we employed a machine learning approach to systematically analyze perovskite composition and transport layer structures, to decipher the underlying causes of photoinduced phase segregation. Subsequently, by introducing functionalized nanocrystals into wide-bandgap perovskites, we anchored the Pb-halide octahedra in situ, thereby enhancing perovskite photostability. Ultimately, we achieved perovskite films that did not segregate for over 5 days. Even after 1000 hours of aging under open-circuit conditions with illumination, these films retained 79% of their initial efficiency.

## FC02-P06

### **Performance study of low-cost amphiphilic ion exchange membranes grafted with poly(norbornene)-based perfluorinated side chain and alkyl side chain links for all-vanadium liquid flow batteries**

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Vanadium Redox Flow Battery (VRFB), as an emerging electrochemical energy storage system, has attracted much attention from the research and industrial communities due to its high safety, environmental protection and design flexibility. One of the core components of the VRFB system is the ion exchange membrane (IEM), which not only affects the energy conversion efficiency, but also affects the reliability and long-term operation cost of the whole system. One of the core components of the VRFB system is the Ion Exchange Membrane (IEM), which not only affects the energy conversion efficiency of the cell, but also relates to the reliability and long-term operation cost of the whole system. The perfluorosulfonate polymer membranes commonly used in current commercial VRFB systems, despite their good chemical and thermal stability, are limited in their large-scale application by their high cost and severe ionic cross-permeability. For example, Nafion membranes, although excellent in proton conduction, have poor ion selectivity and are very expensive. Therefore, finding more cost-effective alternative materials with superior performance has become a hot topic of current research.

As a new membrane material, poly(norbornene) possesses obvious cost advantages over traditional perfluorosulfonate polymer membranes. It not only possesses good ionic conductivity and comprehensive performance, but also maintains low water absorption at high ion exchange capacity (IEC), which is particularly important for maintaining the structural stability of the membrane and avoiding the swelling phenomenon. Taking advantage of the Donnan effect, the quaternary ammonium groups introduced in the amphiphilic ion exchange membranes can effectively repel vanadium ions, significantly reducing the ability of these ions to pass through the membrane, thus improving the ion selectivity of the membranes. In addition, the introduction of long polyfluorinated side chains into the membrane structure was able to form multiple hydrogen bonds, which promoted the formation of ion transport channels and increased the hydrophilicity of the membranes, which indirectly enhanced the chemical and thermal stability of the membranes.

In this thesis, a series of low-cost amphoteric ion exchange membranes (AIEMs) were successfully prepared by using a facile method such as solvent reaction, degassing reaction and solution casting, etc. The effects of different structural side chains, including perfluorinated and alkyl side chains, on the vanadium barrier performance and ion selectivity of the poly(norbornene)-based membranes were also explored, and a comprehensive evaluation of the practical application performance of the prepared membranes in the VRFB system was performed. The effects of different structural side chains, including perfluorinated side chains and alkyl side chains, on the vanadium barrier performance and ion selectivity of the poly(norbornene)-based membranes were investigated, and the performance of the prepared amphiphilic membranes was comprehensively evaluated for practical applications in VRFB systems. The results show that the ion selectivity of the membranes can be significantly enhanced by introducing a specific proportion of perfluorinated long side chains into the quaternised norbornene polymer matrix. The amphiphilic membranes were thoroughly tested for their physical and electrochemical properties, and the VRFB monocells assembled using these membranes demonstrated excellent electrochemical energy storage

performance. The results show that the resulting amphiphilic ion exchange membranes exhibit optimal battery performance when 20 wt% of perfluorinated long side chains are grafted in the poly(norbornene) matrix.

Two novel high-performance AIEMs were prepared by introducing perfluorinated long side chains into the poly(norbornene) matrix. The results show that the introduction of perfluorinated long side chains not only significantly improves the selective permeation of vanadium ions through the amphiphilic ion exchange membranes, but also effectively constructs highly efficient proton transport channels by interacting with sulfonate groups within the membranes. These findings are of great reference value and practical significance for promoting the development of membrane materials for VRFB.

#### FC02-P07

##### **The Molecular Encapsulation Effect for Gel-State Lithium Metal Batteries**

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Gel-state polymer electrolytes with superior mechanical properties, self-healing abilities and high Li<sup>+</sup> transference numbers can be obtained by in situ polymerization of monomers with hydrogen-bonding moieties. However, it is overlooked that the active hydrogen atoms in hydrogen-bond donors experience displacement reactions with lithium metal in lithium metal batteries (LMBs), leading to corrosion of the lithium metal. Herein, it is discovered that the addition of hydrogen-bond acceptors to hydrogen-bond-rich gel-state electrolytes modulates the chemical activity of the active hydrogen atoms via the formation of hydrogen-bonded intermolecular interactions. The characterizations reveal that the added hydrogen-bond acceptors encapsulate the active hydrogen atoms to suppress the interfacial chemical corrosions of lithium metals, thereby enhancing the chemical stability of the polymer structure and interphase. With the employment of this strategy, a 1.1 Ah LiNi<sub>0.8</sub>Co<sub>0.1</sub>Mn<sub>0.1</sub>O<sub>2</sub>/Li metal pouch cell achieves stable cycling with 96.3% capacity retention at 100 cycles. This new approach indicates a feasible path for achieving in situ polymerization of highly stable gel-state-based LMBs.

#### FC02-P08

##### **Artificial heterointerfaces of defect-rich Ni and amorphous/crystalline MoN enable efficient hydrogen evolution reaction**

Wei Peng, Lin Xu, Liqiang Mai

Developing highly-active and robust electrocatalysts for the hydrogen evolution reaction (HER) is extremely desirable for hydrogen production but remains highly challenging. Herein, we reported a rational strategy to fabricate a novel metallic heterostructure composed of defect-rich nickel and amorphous/crystalline molybdenum nitride anchored on a carbon matrix (MoN/Ni@C) as a superior HER electrocatalyst. Owing to the electronic structural modulation of the interfacial synergy of the defects and phase engineering, the MoN/Ni@C exhibits a low HER overpotential of 27 mV at 10 mA cm<sup>-2</sup> and a small Tafel slope of 73 mV dec<sup>-1</sup> in 1.0 M KOH solution, without any distinct attenuation after 180 h of operation. Density functional theory calculation results demonstrate that the interfacial electron transfer leads to a distorted Ni surface incorporation of the MoN phase, achieving the optimal thermoneutral hydrogen adsorption free energies ( $\Delta G^*H$ ) of Mo and Ni active sites. Meanwhile, the amorphous/crystalline structure in the MoN phase exposes more active sites and promotes structural stability. This work provides new insights into designing heterogeneous interfaces of non-noble-metal-based electrocatalysts with superior HER activities.

#### FC02-P09

**New Insights into Phase-Mechanism Relationship of  $\text{MgxMnO}_2$  Nanowires in Aqueous Zinc-Ion Batteries**Zhongzhuo Yang<sup>1</sup>, Xuelei Pan<sup>1</sup>, Yuanhao Shen<sup>1</sup>, Renpeng Chen<sup>1</sup>, Tianzhao Li<sup>1</sup>, Lin Xu<sup>1,2</sup>, Liqiang Mai<sup>1,2</sup>

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In response to the call for safer energy storage systems, rechargeable aqueous manganese-based zinc-ion (Zn-ion) batteries using mild electrolyte have attracted extensive attention. However, the charge-storage mechanism and structure change of manganese-based cathode remain controversial topics. Herein, a systematic study to understand the electrochemical behavior and charge storage mechanism based on a  $3 \times 3$  tunnel-structured  $\text{MgxMnO}_2$  as well as the correspondence between different tunnel structures and reaction mechanisms are reported. The energy storage mechanism of the different tunnel structure is surface faradaic dissolution/deposition coupled with an intercalation mechanism of cations in aqueous electrolyte, which is confirmed by in situ X-ray diffraction, in situ Raman and ex situ extended X-ray absorption fine structure. The deposition process at the cathode is partially reversible due to the accumulation of a birnessite layer on the surface. Compared to smaller tunnels, the  $3 \times 3$  tunnel structure is more conducive to deposit new active materials from the electrolyte. Therefore, pristine  $\text{MgxMnO}_2$  nanowires with large tunnels display an excellent cycling performance. This work sheds light on the relationship between the tunnel structure and  $\text{Mn}^{2+}$  deposition and provides a promising cathode material design for aqueous Zn-ion batteries.