

NEWS

## 电化学十大科学问题

# The Top Ten Scientific Questions in Electrochemistry

中国化学会电化学专业委员会

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电化学是研究电能与化学能以及电能与物质之间相互转换及其规律的科学，并已逐渐发展成为跨越基础科学（理论）和应用科学（工程、技术）两大领域的重要学科，呈现出不同领域专家通力协作、研究开创的多领域、跨学科交叉的独特态势。当前，国家“双碳目标”持续强力推进能源、材料、环境、生命健康、信息等领域快速发展，电化学进入了新的黄金发展时期，遇到了前所未有的发展机遇，同时也面临着巨大的挑战。

在这样的大背景下，2023年初，中国化学会电化学专业委员会委托其会刊《电化学（中英文）》向全国一线的电化学及其相关学科的科技工作者发起征集电化学领域重大科学问题的活动。重点围绕电化学基础理论、电化学测试技术与方法、纳米与材料电化学、锂离子电池、钠钾离子电池、有机和多价金属离子电池、锂硫电池、固态电池、金属空气电池、超级电容器、液流电池、水系二次电池、燃料电池、电催化、生物电分析、太阳能电池及光电化学、有机与工业电化学、腐蚀与电镀等电化学18个研究方向，共收到来自3000余名一线科技工作者汇总的89个相关的问题和难题。经过中国化学会电化学专业委员会委员和《电化学（中英文）》编委会主任委员认真讨论、多次复议，最终甄选出电化学10个重大科学问题。这是中国化学会电化学专业委员会首次发布“电化学10大科学问题”，

对电化学学科和电化学工业发展中的关键科学问题和技术瓶颈进行了全面梳理和分析研判。本次征集活动面向广大一线科技工作者的工作实践、思考和视野，调查研究过程全面、深入，甄选出的十大问题代表了电化学学科发展的重要需求和明显趋势。

本次电化学重大问题发布活动，是中国化学会电化学专业委员会发挥在学术上的引领作用的重要举措，也是对电化学科学研究和技术攻关方向的深度思考和指引。作为中国化学会电化学专业委员会会刊，《电化学（中英文）》通过发布“电化学十大科学问题”并汇集电化学各研究领域和企业界的知名专家学者予以简要解读，以期引导广大电化学相关学科及业界进一步关注国家重大需求和国际学术前沿，从学科发展的根基出发，聚焦电化学基础问题和技术难题，攻坚克难，扎实推进电化学学科发展的进程。

《电化学（中英文）》后续将整合和挖掘学术资源优势，根据每一个科学问题邀请相关领域的专家学者撰写系列发展策略（roadmap）文章，展示、推进深度思考，提出解决方案，绘制学科发展路线图，促进在各个方向上实现聚力突破。

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## 1. 如何在微观层次探测或模拟原位/工况条件下复杂电化学界面的动态结构变化,并建立其与宏观电化学性能的关系?

电化学界面在诸多重要电化学应用中扮演着核心角色,是实现物质转化和能源转换的重要反应场所。随着现代社会的高速发展,人们对电化学器件和系统各项性能要求不断攀升,比如储能与动力电池需要更高的能量和功率密度、更高的安全性和更长的寿命,电解水制绿氢和二氧化碳还原电解器需要更低的能耗,芯片大马士革铜互连需要实现低至十纳米级尺寸沟槽的超填充等。对此,我们需在对电化学界面微观结构、作用机制和调控规律有全面、清晰认识的基础上,优化设计电极、电解质材料和界面的理化特性。然而,在原位、工况条件下,电化学界面的复杂度显著增加,且不断动态变化。用来描述稀溶液、近平衡、固-液界面等电化学研究对象的传统双电层、电荷传输和转移

理论,不能适用于以超浓、限域、远离平衡态、固-固界面、固-液-气三相界面等为特征的新型电化学体系。如何探测如此复杂的电化学界面的微观结构和反应过程,对实验表征和计算模拟都是巨大的挑战。我们亟需发展同步辐射、多模态谱学和高分辨动态成像表征等实验方法,从分子水平、高能量、高空间和高时间分辨层次,实时、原位、共位点地获取电化学界面的动态演变过程信息。结合第一性原理计算和多尺度模拟,开发跨尺度电化学界面模型的仿真模拟方法。充分利用人工智能方法,开发规范化、自动化的计算和实验集成平台,加速电化学体系实验和计算数据获取,建立开源共享的计算和实验数据库,进而实现高性能电化学材料与器件理性设计和智能优化。

### How to Detect or Simulate the Dynamic Structural Changes of Complex Electrochemical Interfaces under *In-Situ/Operando* Conditions at the Microscale, and Establish Their Relationships with Macroscopic Electrochemical Performance?

The electrochemical interface plays a central role in many important electrochemical applications, serving as an important reaction site for material transformation and energy conversion. With the rapid development of modern society, the requirements for the performances of electrochemical devices and systems continue to be climbed, such as the needs for batteries and fuel cells with higher energy and power densities, higher safety, and longer lifetime, the needs for low energy consumption in  $H_2$ -production and  $CO_2$  reduction electrolyzers, and the needs for achieving Cu superfilling in trenches and vias with multiscale down to 10 nm for chip fabrication (Damascene interconnection). It is thus highly demanded to maximize by design the physicochemical properties of electrode-electrolyte materials and interfaces, based on a comprehensive and clear understanding of the microstructure, mechanism, and

regulations of the electrochemical interface. However, under *in-situ/operando* conditions, the electrochemical interface has extremely high chemical complexity and is under dynamic change. The traditional theories describing electric double layer, charge transport and transfer in relatively simple occasions such as dilute solutions, near-equilibrium conditions, and solid-liquid interfaces, cannot be applied to modern electrochemical systems characterized by highly concentrated solutions, confinement environments, far-from-equilibrium conditions, solid-solid and solid-liquid-gas triple-phase interfaces, etc. How to detect the microstructures and reaction processes of such complex electrochemical interfaces is a great challenge for both experimental characterization and computational simulation. It is urgently needed to develop new experimental methods such as synchrotron radiation characterization, multi-modal spectroscopy and high-resolution

dynamic imaging to obtain dynamic evolution information of electrochemical interfaces at real time, *in-situ*, and on-site conditions, at the molecular level, with high energy, and high spatial and high temporal resolutions. Combining first-principles calculations with multi-scale simulations, simulation methods for cross-scale modelling of electrochemical interfaces can be developed. By fully utilizing

AI methods, we can develop standardized and automated computational and experimental integration platforms to accelerate the acquisition of experimental and computational data for electrochemical systems, establish open source shared computational and experimental databases, and ultimately achieve rational design and intelligent optimization of high-performance electrochemical materials and devices.

## 2. 如何理解和调控金属Li负极成核/生长及枝晶抑制策略?

金属锂因其高理论比容量和低电势, 被认为是下一代高能量密度电池的理想负极材料。然而, 金属锂负极在电化学沉积过程中易形成枝晶, 导致电池的循环性能恶化并带来安全隐患。解析电化学过程中金属锂的成核和生长机制, 并发展有效的锂枝晶抑制策略, 是锂金属电池研究领域的一个重要基础科学问题。目前, 通过电化学原位表征技术与理论模拟方法的结合, 对锂枝晶成核和生长过程已形成初步认识, 构建了相应的枝晶生长模型, 包括空间电荷模型、沉积-溶解模型、异质成核模型等, 提出了三维集流体和人工界面层等枝晶抑制策略。然而, 在实际工况下锂的沉积行为往往受多因素耦合的影响, 现有的理论模

型难以准确预测电池运行中的枝晶生长行为, 且枝晶抑制策略也缺乏广域、长时的有效性验证。在未来, 进一步发展适配金属锂的高时空分辨的电化学原位表征技术, 以获得真实电化学过程中锂成核到生长的跨尺度、多维度精细结构及物态信息, 对于理解枝晶演化过程具有重要意义。同时, 如何系统掌握热力学、传质动力学、应力应变等复杂因素对金属锂电沉积过程的耦合影响规律, 完善锂枝晶成核/生长的精确理论模型, 并据此探索工况条件下开发有效的电解液添加剂, 从根本上调控锂金属成核、生长过程, 解决锂枝晶的安全隐患, 是推动高比能金属锂电池发展的关键。

## How to Understand and Regulate the Nucleation and Growth of Metal Lithium at the Anode, and Develop Strategies for Suppressing Dendrite Formation ?

Metallic lithium (Li), due to its high theoretical specific capacity and low potential, is considered an ideal anode material for the next-generation high-energy rechargeable batteries. However, the Li-metal anode tends to form dendrites during the electrochemical deposition process, which could lead to deteriorated battery cycling and potential safety problems. Unrevealing the nucleation and growth mechanisms of Li-metal anode during the electrochemical process and developing effective dendrite-suppression strategies constitute the critical science problem in the fundamental research of rechargeable Li-metal batteries. Currently, based on the *in situ*

electrochemical characterization techniques and theoretical simulation methods, a preliminary understanding about the nucleation and growth of Li dendrites has been provided. Several models, such as the space charge model, the deposition-dissolution model, and the heterogeneous nucleation model, have been proposed to describe the dendrite propagation mechanism, and the corresponding dendrite-suppression strategies, including the three-dimensional current collector and artificial Li-electrolyte interface, have been developed. However, the Li deposition behavior in practical batteries is usually influenced by multiple factors, and it remains difficult, by

employing the existing theoretical models, to predict the dendrite growth behavior during battery operation. Besides, the effectiveness of the present dendrite-suppression strategies has not been verified in a long-term and wide-area study. In the future, *in situ* and *operando* electrochemical characterization techniques with high spatiotemporal resolution are to be developed to collect information at multi-scales and multi-dimensions, about the evolution of fine structures, phases and physical states for nucleation and growth of Li metal (dendrites) in a real electrochemical process. The advancement in characterization technique is of great significance to understanding the

dendrite evolution in a battery. Meanwhile, attention will be paid on comprehending the coupled influence by multiple factors (including thermodynamics, mass transfer kinetics and stress-strain responses) on the electrodeposition of Li metal, establishing accurate theoretical models for nucleation and growth of Li dendrites, and exploring new strategies of exploring effective additives of electrolyte to regulate Li nucleation and growth under the working conditions, resolving intrinsically the safety issue of lithium metal anode. A joint effort will facilitate sustainable development of high-energy rechargeable Li-metal batteries.

### 3. 如何获得满足固态电池应用需求的高性能碱金属离子固体电解质?

固态碱金属电池具有高比能和高安全的潜在优势,是下一代电化学储能技术的研究热点。然而,受限于固体电解质的性能,固态碱金属电池的发展远滞后于预期。碱金属离子固态电解质按照组成可分为三类:硫化物,氧化物和聚合物,但三种电解质各自均存在明显的优点和短板,现阶段没有一种能全面满足固态电池的使用需求。硫化物电解质的离子电导高,但电化学窗口窄;氧化物电解质的化学和电化学稳定性较高,但因其杨氏模量高,界面适形性差;聚合物电解质质软、可加工性好,但离子电导

率低。因此,探索高离子导电率、宽电化学窗口和优异界面适形性的碱金属离子固体电解质仍是固态电池技术发展的关键。从当前研究进展来看,将柔性电解质(聚合物、塑晶、离子凝胶等)与高强度无机、有机纳米固体材料复合,构建“刚柔并济”的软固态复合电解质是一条值得探索的技术路线。基于此,塑晶-聚合物复合电解质、离子凝胶-有机框架材料(MOF、COF)复合电解质、纳米无机碱金属离子导体-聚合物复合电解质,以及它们之间的多元复合电解质应当受到更多的关注。

### How to Obtain High-Performance Alkali-Metal-Ion Solid-State Electrolytes for Solid State Batteries?

Solid state alkali-metal secondary batteries (SSABs) have received considerable attention as a next-generation electrochemical energy-storage technology with high energy density and safety. However, due to the poor performance of solid state electrolytes, the development of SSABs has lagged far behind expectations. Alkali-metal-ion solid electrolytes can be divided into three categories according to their chemical composition: sulfides, oxides and polymers, nevertheless,

each one has its own merits and demerits, and none of them can fully meet the needs of SSABs at the current stage. Sulfide electrolytes have high ionic conductivities but narrow electrochemical windows. Oxide electrolytes have high chemical and electrochemical stability, but poor shape adaptability owing to their high Young's modulus. Polymer electrolytes have excellent flexibility and good processability, but their ionic conductivities are considerably low. Therefore, advanced solid



state electrolytes with high ionic conductivity, wide electrochemical window and excellent interface shape- adaptability are still the key for the development of SSABs technology. Judging from the current research, a possible route is to construct soft solid-state electrolytes by compositing flexible electrolytes (polymers, plastic crystals, ionic gels, etc.) with rigid

inorganic and organic nano-solid materials. According to this judgement, more attention should be paid to the plastic crystal-polymer composite electrolytes, ionic gel-organic frame material (MOF, COF) composite electrolytes, inorganic ion conductor-polymer composite electrolytes, and their multicomponent composites.

#### 4. 如何发展高能量密度多电子转移反应体系的水系电池?

水系电池以其安全性好、功率密度高、循环寿命长等优势在大规模储能领域发挥着重要作用。高能量密度是电池器件走向小型化、集成化以及轻便化发展目标的技术保障,是未来电池的发展趋势。常见水系电池受限于析氢析氧等副反应造成能量密度较低,难以用做动力电池。传统动力电池由于采用有机电解液带来安全性风险,发展高能量密度水系电池尤为重要。电池的能量密度与电池电压、活性物质的浓度以及活性物质的电子转移数直接相关,尤其是电子转移数的增加可以成倍提高电池的能量密度,因此,开发多

电子转移电化学反应是构建高能量密度电池体系的重要策略。然而,多电子转移反应往往涉及多个中间态产物和中间步骤,许多中间态的稳定性差、存在形式复杂,难以从分子尺度观察其结构组成、界面吸脱附以及电荷转移行为,揭示多电子转移的微观机制。针对多电子转移的复杂过程,明确多电子转移的中间态分子,认识其溶剂化结构特性、电极表面吸脱附、电子转移等微观行为,实现电化学反应过程精准调控,获得多电子反应与膜、电极等关键材料的适配,最终为建立高能量密度水系电池提供理论基础和技术支持。

#### How to Develop Aqueous Battery Systems with High Energy Density and Multi-Electron Transfer Reaction?

Aqueous batteries play an important role in large-scale energy storage due to the advantages of high safety, high power density, and long cycle life. High energy density is the technical guarantee for the goals of miniaturization, integration, and portability of battery devices, and is the future trend of battery development. However, common aqueous batteries are endowed with low energy density due to the side reactions of water electrolysis and are difficult to be used as power batteries, which limits their application scenarios. Traditional power batteries suffer from safety issues due to the flammable nature of organic electrolytes. The energy density of an aqueous battery is highly related to the battery voltage, concentration of redox species, and electron transfer number per redox molecule. Therefore, achieving multi-electron transfer

electrochemical reactions is an important strategy to construct a high energy density battery system. However, the electrochemical kinetic and reversibility of multi-electron transfer reactions are usually poor in aqueous batteries, and there is a lack of profound understanding in their micro electrochemical mechanisms. Multi-electron transfer reactions often involve multiple intermediate state products and intermediate steps. Many intermediate states usually suffer from poor stability, short existence time, and complex forms of existence, making it difficult to observe the structure, interface adsorption and desorption, and charge transfer behavior at the molecular scale, and thus, difficult to revealing the microscopic mechanism of multi-electron transfer. In response to the complex process of multi-electron transfer reactions, it is necessary

to develop new methods for multi-scale, high-resolution, and highly sensitive observation of multi-electron transfer processes, and therefore, to clarify the intermediate state, and understand their solvation structure, electrode surface adsorption and desorption, electron transfer behaviors, as well as to realize

precise control of electrochemical reaction processes, and complete the adaptation of multi-electron reactions with key materials such as membranes and electrodes, ultimately providing theoretical basis and technical support for the establishment of high-energy density flow batteries.

## 5. 如何理性设计低 / 非铂的高效长寿命电催化剂并宏量制备?

电催化剂是燃料电池的关键材料, 直接影响电池成本、性能和使用寿命。铂 (Pt) 基电催化剂由于在大多数溶液中、较宽的电势范围内具有良好的催化活性与稳定性, 目前仍然是聚合物电解质膜燃料电池不可替代的催化剂, 约占膜电极成本的40%左右。然而, Pt是世界上储量稀少的贵金属之一, 全球已探明的Pt储量约为7万吨, 年产量约250吨。即使按照0.125 g<sub>Pt</sub>/kW的现有燃料电池技术水平, 全球预计每

年将消耗900吨Pt, 是现有Pt年产量的3~4倍, 严重制约燃料电池技术的发展。因此, 如何深度解析工况下催化剂失效机制, 通过催化剂组成、形貌及原子排布的精准控制, 结合表/界面及纳米限域、配位环境调控等策略, 设计满足复杂工况应用需求的新型高活性、长寿命低/非Pt催化剂, 开发相应的高效宏量制备方法, 是燃料电池领域亟急需解决的重大科学和工程技术问题。

### How to Rationally Design Efficient and Long-Lasting Low/Non-Platinum Electrocatalysts and Their Large-Scale Production?

Electrocatalysts are crucial materials for fuel cells, directly impacting the cost, performance, and lifespan of the cells. Platinum (Pt)-based electrocatalysts, due to their excellent catalytic activity and stability in a wide range of solutions, are currently irreplaceable in polymer electrolyte membrane fuel cells, constituting approximately 40% of the electrode cost. However, as one of the rare precious metals in the world, Pt reserves are globally identified to be about 70,000 tons with an annual production of around 250 tons. Even at a technological level of 0.125 g<sub>Pt</sub>/kW, it is estimated that global consumption will reach 900 tons of Pt per year, representing a three to fourfold increase over current production

levels, which will severely restrict the development of fuel cell technology. The major scientific challenge in the field of fuel cells is the design of novel, highly active, and long-lasting low/non-Pt catalysts that meet the demands of complex operating conditions. Strategies such as comprehending the mechanisms behind catalyst failure in operational conditions, precisely fine-tuning catalyst composition, morphology, and atomic arrangement, in conjunction with advanced approaches such as surface/interface and nano-confinement, and modulation of coordination environments, are essential. Meanwhile, efficient mass production methods for these advanced catalysts must be devised.

## 6. 如何构筑高效气体扩散电极三相界面、理解传质传荷机制及其过程强化?

三相界面作为电化学反应的场所, 其结构、组成及表面特性对包括燃料电池、电解水、二氧

化碳电还原、电合成等在内的诸多电催化体系性能起着至关重要的作用。气体扩散电极的三

相界面通常由离聚物 (ionomer) 催化剂组成, 为保证催化剂活性的充分表达, 精准地调控催化剂/离聚物界面结构十分必要。发展新型的界面结构, 如三维有序阵列结构、分级孔结构、离聚物梯度分散结构等, 均被证实可有效促进反应物、质子、电子的传递动力学, 同时保障良好的水/热管理。在低催化剂载量条件下, 由于催化剂表面的气体局域传输阻力较大, 不利于反应物的高效传输, 造成过电位增大, 因此低载量下的界面结构精控尤为重要。针对此, 如何发展高比表面积、高石墨化程度的多孔载体或开发高离子电导率、高保水性的自聚微孔离聚物, 在此基础上理性调节催化层中的离聚物分布降低局域传质阻

力, 是亟需解决的科学问题。

此外, 如何理解界面传荷、传质机制中的关键科学问题并反馈电极界面设计对高性能气体扩散电极的构筑至关重要。发展高界面敏感性、高时空分辨率的电化学原位表征技术 (如X射线瞬态吸收光谱、扫描探针显微技术与电化学谱学联用、和频共振光谱、针尖增强拉曼光谱等), 以实现在微观尺度、分子尺度、原子尺度上对界面处的瞬态传质传荷以及反应动力学的解析。借助量子力学、多尺度模拟、大数据分析 & 人工智能等先进方法在原子分子层面深入剖析三相界面结构及其在电化学工况下的动态演变规律, 揭示构-效关系。

## How to Construct High-Efficiency Three-Phase Interface and Gain Insights into Enhanced Charge/Mass Transportation Mechanism within a Gas Diffusion Electrode?

The structure, composition, and surface properties of three-phase interface where electrochemical reaction takes place are significant in determining the performance for a variety of electrochemical energy conversion and storage devices, including fuel cells, water electrolyzers, carbon-dioxide electrolyzers and electrosynthesis. As the three-phase interface in a gas diffusion electrode (GDE) is commonly composed of ionomer and catalyst, how to regulate the ionomer-catalyst structure is a prerequisite to maximize the utilization of catalyst. For instance, an engineering novel interface structure, i.e., a three-dimensionally ordered structure, hierarchically porous structure, and ionomer-gradient distribution structure, is promising to facilitate mass transfer and water/heat management, thus enabling complete performance expression of the as-designed GDE. The delicate design of catalyst-ionomer structure is particularly important for the low catalyst loading GDE, where high local transport resistance associated with the permeation and diffusion of reactants results in considerable overpotential. To this regard, developing porous support materials with high surface area and graphitic degree, and self-polymerized microporous ionomers

with high conductivity and water uptake provide an appealing approach to lower local transport resistance.

In addition, a comprehensive understanding on the key scientific problems associated with charge/mass transfer process in the three-phase interface lays the foundation for the interface structure design and thus the high-performance GDE. It greatly depends on the development of *operando* characterization techniques with high sensitivity and spatiotemporal resolution, which include X-ray transient absorption spectroscopy, sum frequency generation vibrational spectroscopy, scanning probe microscopy coupled with electrochemical spectroscopy and tip-enhanced Raman spectroscopy. These *operando* techniques are helpful to gain insights into transient response of mass/charge transfer and reaction kinetics within the three-phase interface at a micro-atomic scale. Combining with advanced theoretical modelling, such as quantum mechanics, multiscale simulation, big data analytics and artificial intelligence, we could dissect the dynamic evolution mechanism of three-phase interface structure under working conditions, thereby revealing the structure-property relationship at an atomic scale.

## 7. 如何破解生命过程中电子传递、能量/物质转化及其与人类疾病的关系和电化学调控原理?

生命过程通常涉及微观层面的电子传递、能量转换与物质转化,例如:呼吸作用中的电子传递、光合作用中的光子-电子能量转换、细胞信号通路中的分子识别与相互作用、细胞内生物大分子的相分离等。这些过程是生命活动的物理化学基础,其调控紊乱与疾病的发生发展密切相关。迄今为止,对于这些过程及其功能调控的研究尚难以认识其中的微观与分子机制。电化学方法具有优越的灵敏度、选择性和时间与空间分辨率,是研究细胞与分子层面生命过程、揭示细胞氧化还原调控机制、干预生物分子功能的有力工具。围绕电化学测量与调控,目前已建立以电化学生

物传感、生物膜电位与物质解析、电化学及电致发光生物成像、生物单分子电学测量等为代表的多尺度多层次电分析技术。在未来,如何进一步将电化学测量与调控手段与光谱学、显微成像、力学与磁学测量等技术相结合,实现微观到宏观的跨尺度、多维度、多模态的高灵敏表征,认识生物体系的微观特性乃至量子效应,理解生命过程中电子传递、能量/物质转化的本质和氧化还原调控原理,探索相关疾病的致病机制与诊疗新范式,开拓生物分子的功能调控与细胞衰老干预新思路,是针对生命体系的物质科学中具有重要意义的新方向。

### How to Decipher the Relationships among Human Diseases and Electron Transfer, Energy Conversion/Substance Transformation in Biological Processes? And How to Modulate Them with Electrochemical Methods?

Electron transfer and the transformation of energy/substances are commonly involved in biological activities, for example, electron transfer in cell respiration, photon-electron energy conversion in photosynthesis, molecular recognition, and interaction in cell signalling pathway, and phase separation of biological macromolecules. Because the above processes establish the physical and chemical bases for biological activities, the disorders in their regulations are closely related to the occurrence and development of a wide range of diseases. To date, it is still intriguing task to reveal the microscopic mechanisms of these key processes. The methods of electrochemistry feature outstanding sensitivity, selectivity, and spatial/temporal resolution, providing powerful tools for studying biological processes at the level of cells and molecules, demonstrating the mechanism of cell redox processes, and intervening the functions of biological molecules. The multi-scale electro-analytical technologies based on

electrochemical measurement and modulation include electrochemical biosensing, membrane potential and neurotransmitter analysis, electrogenerated chemiluminescence microscopy, single-biomolecule electronic measurement, etc. In the future, combining electrochemical strategies with spectroscopy, microscope imaging, force and magnetic measurement techniques will contribute to multi-scale, multi-mode, and highly sensitive new characterizations of biological systems. This will help us to discover more microscopic properties and even quantum effects in biological systems, to understand the chemical nature and physical principles of electron transfer and the transformation of energy/substances, to explore new paradigms for the diagnosis and treatment of related diseases, and to open new ways for regulating the molecular bio-functions and for intervening the cell aging processes. The efforts will potentially lead to important, new directions in the physical science for biological systems.



## 8. 如何突破太阳能电池能量转换效率的肖克利-奎伊瑟极限?

太阳能电池 (solar cell) 是通过光电效应直接把光能转化成电能的装置。由于绿色环保, 价格低廉, 使用便捷等优势, 太阳能发电目前已经跃居为全球最主要的供电方式之一, 在多个领域中得到了广泛应用。太阳能电池的能量转换效率作为衡量其性能的重要指标, 是指在“标准测试条件”下从太阳光转换为电能的功率百分比。其中, 肖克利-奎伊瑟 (Shockley-Queisser, SQ) 极限由 William Shockley 和 Hans Queisser 在 1961 年首次提出, 即对于任何类型的单结太阳能电池, SQ 极限计算的最大效率为 33.7%。然而, 对于多结太阳能电池, SQ 极限可以达到正常阳光下的 68.7%, 或使用集中阳光下的 86.8%。考虑到多结太阳能电池由多个宽带隙的底部电池和窄带隙的

顶部电池叠加形成, 因此, 如何有效控制上下电池之间的连接层结构以及子电池之间的电荷转移至关重要。

电化学方法由于简单方便, 灵敏度高以及准确性好, 是优化电池制备工艺、调节电池界面与体相结构、分析电学性质与机理的有力手段。围绕电化学沉积与测量, 目前已实现了电池连接层的结构可控、电荷传输与分离复合的相互协调等, 建立了电化学系统-太阳能电池多尺度多层次的集成联动, 将太阳光的捕获、转换和存储一体化, 显著提升了电池的能量转换效率。未来, 如何进一步优化电化学方法探索多结太阳能电池内部结构-性能的关系以及电荷平衡机制, 对开拓新思路突破其效率的 SQ 极限具有重要意义。

### How to Break Through the Shockley-Queisser Limit of Energy Conversion Efficiency in Solar Cell?

Solar cell (SC), as a type of photoelectric device, can directly convert light into electricity. Due to its advantages of environmentally friendly, low cost, and easy-to-manufacture, solar power has become one of the most important power supply systems in the world and has been widely used in various fields. As a key parameter for measuring the performance of SC, the power conversion efficiency (PCE) refers to the percentage of power converted from sunlight into electrical energy under "standard test conditions". The Shockley-Queisser (SQ) limit was first proposed by William Shockley and Hans Queisser in 1961, in which, for single-junction SC, the maximum PCE calculated by the SQ limit is 33.7%. However, for multi-junction SCs, it can reach to 68.7% under normal sunlight, or 86.8% under concentrated sunlight. Considering that these devices consist of multiple wide-bandgap bottom cells and narrow-bandgap top cells, it is crucial to effectively control the structure of connection

layer, and the charge transfer between the upper and lower cells.

Electrochemical method features operational simplicity, high sensitivity, and outstanding accuracy, which serves as a powerful tool for optimizing the preparation process, adjusting the interface and bulk structure, and analyzing electrical properties and mechanisms of SC. To date, focusing on electrochemical deposition and measurement, the control of the structure of connection layers and the regulation of transport, separation, and recombination of charges in SC have been achieved. Importantly, a multi-scale and multi-level integrated electrochemical-SC system has been established to capture solar energy, convert, and store energy, significantly improving the PCE of SC. In the future, how to further optimize electrochemical methods to explore the relationship between performance and structure, and the charge balance mechanism in multi-junction SCs will be of great significance for developing new ideas to push the SQ limit.

## 9. 如何深入揭示腐蚀过程中多步骤电极反应动力学机制，精准调控复杂阳极过程和阴极过程？

我国因腐蚀造成的经济损失高达3.6万亿元/年（占GDP 3.34%），腐蚀无时不在吞噬着人类有限的资源，导致能源浪费、环境污染、质量下降、安全隐患及成本上涨等国计民生问题。腐蚀过程是一个在环境作用下复杂的多电极电化学反应耦合系统，腐蚀过程通常包括腐蚀物种向界面阴/阳极区的传质过程、界面阴/阳极电化学反应传荷过程、阴/阳极短路电池间的电子传递过程及腐蚀产物的传输、随后化学反应、腐蚀产物的形成等。材料腐蚀的形式、动力学行为、机制及规律均与上述反应过程密切相关。如何进一步深入揭示腐蚀过程中多步骤电极反应动力学机制，精准调控复杂腐蚀电池的阳极过程和阴极过程，仍面临极大挑战。传统腐蚀电化学方法通常以整

个电极系统为研究对象，以电信号（电位、电流或电荷）为激励和检测手段，通过解释而获得有关电极过程间接、统计和面积平均的研究信息，尚难以从分子、原子水平及高空间分辨率认识复杂腐蚀过程中多步骤电极反应细节及本质机理，难以精准调控腐蚀多电极耦合系统的阳极过程、阴极过程及相关的控制反应。进入新时代，亟需发展高空间分辨的原位电化学探针方法、高时空分辨的原位谱学方法、工况条件下的原子分辨成像方法及AI技术，多尺度深刻揭示腐蚀电化学体系的界面结构，进而探明腐蚀过程中多步骤电极反应机制和动力学规律，实现对复杂腐蚀电化学耦合系统阴、阳极过程及密切相关反应的精准调控。

## How to Further Reveal the Kinetic Mechanism of Multi-Steps Electrode Reactions for a Complex Corrosion System, and How to Precisely Modulate Anodic and Cathodic Processes, as Well as Their Closely Associated Interfacial Reactions?

Corrosion results in a huge economy loss about RMB3.6 trillion a year in China (GDP 3.34%), it always consumes limited human resources and causes energy waste, pollution, quality problem, safety risk and high cost, etc. Corrosion is a complex coupling system with multi electrode reactions functioned of surrounding environment, involving mass transfer of corrosive species toward cathodic and anodic sites separately, charge transfer of Faraday reactions, electron transfer in short-circuit of corrosion cell, and transport of corrosion products, following chemical reactions and formation of corrosion products, which closely affect the corrosion form, kinetic behavior, corrosion mechanism and its regularity. It remains great challenge to further reveal the kinetic mechanism of multi-steps electrode reactions for a complex corrosion system, and to precisely modulate anodic and cathodic processes, and their closely associated interfacial reactions. Traditional research

methods of corrosion electrochemistry, through electrochemical simulation, measurements of response and theoretical analysis, usually can only obtain indirect, average and statistic information for a corrosion system. It is hard to recognize the details of multi electrode reactions and essential mechanism from molecular and atomic level, and to precisely modulate electrode process and associated reactions as well for a complex corrosion system. In the new era, it needs to develop various *in-situ* electrochemical probes with high resolution, *in-situ* spectroscopic analysis in high temporal-spatial resolution, *operando* atomic imaging, and AI techniques to further reveal interfacial structure of corrosion system at multi-scale. Consequently, all in-depth understanding to mechanism and kinetic regularity will benefit to realize precise modulation of anodic and cathodic processes, and the closely related reactions in a complex corrosion system.

## 10. 如何高效、高选择性电化学精准合成高附加值有机化学品？

在双碳目标驱动下，耦合可再生能源的电化学精准合成有望成为绿色能源向高附加值化学品能量转移的新范式。有机电化学合成一般在油水介质中进行，利用电化学反应原位生成活性氧（或活性氢）将有机物选择性电催化氧化（还原）成高价值的有机分子，涉及多电子（多质子）转移步骤的复杂过程以及分离过程。有机电合成可以完成各种转化—如醇制备醛/酮/酸、羰基化合物加氢制备醇及脱氧偶联产物、炔烃/或烯烃类化合物的选择性加氢、药物分子的电化学氟化修饰等。目前需要解决的是有机电合成基础研究和工业化涉及的一系列问题：如有机电催化体系的化

学键选择性断裂与生成机制，介质和表界面效应，电催化剂（电极）的调控规律和规模化制备，油/水界面物质分配、转移及相平衡规律，有机电合成反应器的物质与能量传递规律，波动性电能驱动的有机电合成装置的动/静态响应特性与协调匹配机制等。未来需要发展亲油/亲水双界面催化层构筑技术，高效、高催化活性、高选择性、长寿命的工业电催化剂（电极）的可控制备技术，高效、高性能、低能耗的电催化有机合成反应器设计、放大、产品分离技术和集成工艺，实现可再生电力驱动的高附加值有机化学品的高效、高选择性电化学生产。

### How to Electrochemically and Precisely Synthesize High Value-Added Organic Chemicals with High Efficiency and High Selectivity ?

Motivated by carbon peaking and carbon neutrality goals, the precise electrochemical synthesis in conjunction with renewable energy sources is expected to establish a novel paradigm in the realm of green energy conversion toward high-value chemical energy. Organic electrochemical synthesis generally occurs in an oil-water milieu, using *in-situ* electricity to generate reactive oxygen (or reactive hydrogen). This process selectively electro-catalyzes the oxidation (or reduction) of organic compounds into high-value organic molecules. This intricate process encompasses multi-electron (multi-proton) transfer stages and separation procedures. Organic electrosynthesis is proficient in various transformations, including the derivation of aldehydes/ketones/acids from alcohols, the hydrogenation of carbonyl compounds to prepare alcohols and deoxygenated coupling products, the selective hydrogenation of alkyne/olefin compounds, and the electrochemical fluorination modification of drug molecules. Presently, several challenges confront the industrialization of organic

electrosynthesis, such as the selective breaking and formation mechanisms of chemical bonds in organic electrocatalytic systems, medium and surface-interface effects, the regulation rules and large-scale preparation of electrocatalysts (electrodes), material distribution and transfer at the oil/water interface, phase equilibrium rules, the material and energy transfer rules of organic electrosynthesis reactors, and the dynamic/static response characteristics and coordination matching mechanisms of organic electrosynthesis devices propelled by fluctuating electrical energy. Future efforts should be devoted to concentrate on developing lipophilic/hydrophilic dual-interface catalytic layer construction technology, and controllable preparation of high-efficiency, highly catalytic activity, highly selective, and long-life industrial electrocatalysts (electrodes), as well as the design, amplification, product separation technology, and integrated processes of efficient, high-performance, low-energy-consumption electrocatalytic organic synthesis reactors to realize efficient and highly selective electrochemical production of high-value organic chemicals driven by renewable electricity.