中国材料大会 2024
暨第二届世界材料大会
CMC 2024 & WMC 2024

July 8-11, 2024
Guangzhou, China

A06-纳米材料合成及光/电催化应用
A06-Nanomaterials Synthesis and Photo/Electro-catalysis Applications

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Chinese Materials Research Society

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A06.纳米材料合成及光/电催化应用（国际会场）

分会主席：孙再成、徐浩兰、张加涛、张华彬

会议报告：

量子点表面的氟化处理

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铅卤化物钙钛矿纳米晶体（PNCs）因其出色的光电特性而备受关注，广泛应用于发光二极管（LED）和背光显示器。由于合成化学的巨大进展，PNCs 的光致发光量子产率（PLQY）在室温下可轻松达到 90%以上，从而显著提高了 LED 和背光显示器的性能。然而，光发射的热猝灭是制约 PNCs 在电致发光和下转换 LED 中应用的关键瓶颈之一。此外，LED 操作期间不可避免地产生焦耳热，促使钙钛矿纳米晶体中的离子迁移，严重损害器件性能。鉴于上述问题，我们将简要概述我们在抑制 PNCs 热猝灭方面的最新进展。我们报道了一种氟化物后合成处理，可产生具有较内部纳米晶核更宽能隙的富含氟的表面，抑制载流子俘获，提高热稳定性和高效电荷注入。重要的是，在 343 K 下仍保留了近 80％的室温 EQE，而标准 $CsPbBr_3$ 钙钛矿纳米晶体发光二极管则常常出现在热效应下显著下降的现象。此外，氟化物表面修饰策略还被用于装饰 $CsPbCl_{3-x}Br_x$ PNCs 的表面，抑制相分离并在热条件和电场下稳定 $CsPbCl_{3-x}Br_x$ PNCs。最后，我们将阴离子修饰策略延伸至高温固相合成量子点，通过有效修饰表面铅缺陷抑制高温固相合成的 $CsPbBr_3$ PNCs 的 PL 热猝灭。

Plasmon enhanced photocatalysts synthesis and Applications

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Towards the solar photocatalysis applications, due to the large lattice mismatch between metal and semiconductor (lattice mismatch>40%), growth of monocrystalline semiconductor-based plasmonic metal/semiconductor hybrid nanocrystals (core/shell and heterodimer) with modulated composition, morphology and interface strain are prerequisites for flexible control of Plasmon-exciton coupling, efficient electron/hole separation and carriers transfer. We putted forward Reverse Cation Exchange (RCE) induced non-epitaxial growth method. We realized nanoscale monocrystalline growth of the semiconductor shell on Plasmonic metal (Au, Cu etc.) core and composition of semiconductor shell synergistically. The efficient Plasmon enhanced electron/hole separation and hot electron injection have been realized (the hot electron injection efficiency reaches to 48%). Then revolutionary Plasmon enhanced photocatalytic, Photoelectrochemical applications have been realized.

非金属等离子体材料构建及其光催化应用

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表面等离子体共振效应（SPR）是贵金属材料具有的独特光学性质，其在增强拉曼散射光谱、化学生物检测、光电探测等领域具有重要的应用。强 SPR 效应可产生高活性热电子在光催化分解水、有机合成、二氧化碳还原等领域有着重要的应用。贵金属的高昂价格和稀有性制约着金属 SPR 光催化剂的应用，而探索制备具有 SPR 效应的半导体等非金属光催化剂成为理想选择。但非金属 SPR 光催化剂存在载流子浓度低、SPR 效应不稳定的难题，为此我们课题组提出了一系列的解决途径，并构建了 TiO_2/WO_{3-x}, CdS/WO_{3-x}, BP/WO_{3-x} and MoS_2/MoO_{3-x} 等复合非金属 SPR 光催化剂，证明了电子的持续注入可有效提升 SPR 催化效率，同时验证了其在光催化分解水及二氧化碳还原中具有稳定活性。此外，我们探索半导体中构建 SPR 效应的有效途径，提出了富电子能级构造诱导半导体SPR效应的研究思路，并通过在Bi2WO6中构建多种氧缺陷，证明了与钨原子相连的氧缺陷可产生储电子能级，实现载流子富集，诱导 Bi2WO6 产生 SPR 效应，并发现其 SPR 效应在光催化二氧化碳还原产甲烷中具有决定性作用。为厘清非金属 SPR 热电子与光热效应对增强催化反应的具体协同贡献，我们课题组设计合成了非金属 SPR 复合光催化剂 WO_{3-x}/还原氧化石墨烯（rGO），rGO 包覆在 WO_{3-x} 表面稳定了氧缺陷，证明了热电子在增强光催化中的决定性作用，揭示了热电子可加速异丙醇 C-O 键断裂降低异丙醇脱水反应活化能（低至 0.37 eV）的增强催化机制，在全光谱光激发下实现了高选择性（100%）和高效光催化异丙醇脱水产丙烯（437.5 mmol/g/h），催化反应速率提升 180 倍。

Exploring Polyelemental Nanosystems Through Nanoparticle Megalibraries

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The emerging potential of polyelemental nanoparticles in diverse fields has led to an increased demand for combinatorial and high-throughput synthesis that encompass an enormous parameter space of nanoparticles.[1,2] Here, we report a probe-based nanoreactor-mediated method to synthesize polyelemental nanoparticles in a site-specific manner. The method allows one to create nanoparticles consisting of all combinations of desired elements. Important insights into the factors that lead to alloy formation and phase-segregation in polyelemental nanoparticles were obtained, and design rules were established for engineering heterostructures in a single nanoparticle. Further, when combined with massively parallel printing techniques, combinatorial libraries of nanoparticles can be made over large areas, providing a powerful platform to screen polyelemental nanoparticles in a systematic fashion. Based on the synthetic capability, we systematically investigated the thermodynamic phase behavior of immiscible elements in nanoparticles using Au-Rh as a model system. Our results show that their miscibility is increased in nanoparticles by forming solute clusters and single atoms in the particle matrix.[3-5] The two immiscible elements eventually exhibit a phase separation-to-alloy transition in particles with decreased size and become completely miscible in sub-2 nm particles across the entire compositional range. The inverse phase behavior is mainly dictated by the particle size, particle composition, and possible surface adsorbates, highlighting the substantial discrepancy between the bulk and nanomaterials.[5] Collectively, our work not only advances the understanding of the nanoscale thermodynamics of polyelemental systems, but also provides important guidelines for the design of alloy and phase-separated nanostructures that can be useful for catalysis, plasmonics, and other applications.

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光/电介导的自由基反应机制探索与合成应用

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近年来，光、电化学合成策略得到了长足发展，其中自由基中间体常作为反应中的活性物种出现。因此，深入了解自由基中间体的结构、性质对反应路径的探索与设计至关重要。然而，自由基通常具有较高反应活性且不稳定，直接检测存在挑战。通过多种仪器表征手段结合理论计算，我们分别在电化学条件下对磺酰胺氮中心自由基的结构与反应性开展了研究；在光化学条件下对磷中心自由基的产生、加成过程及碳中心自由基与单原子金属中心的作用机制展进行了探索。

有机半导体光催化剂的可控组装与调控

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石墨相氮化碳是一种廉价易得、稳定无毒的有机半导体，具有良好的商业开发和应用潜力。在热力学方面，氮化碳的能带位置可驱动水分解以及有机氧化还原反应的进行，但块体氮化碳（BCN）存在比表面积小、可见光利用率低、光生电子-空穴易复合等问题，不利于在光催化领域中应用。构建具有分级或者超薄结构特征的氮化碳以及功能化复合是克服以上问题的有效途径，通常的“自上而下”策略面临可控性较差、产率低以及步骤复杂等问题。针对以上问题，课题组发展了基于氨基-羟基相互作用的“自下而上”组装策略，实现了在分子水平上调控 CN 的形态和组成，进而提升其光催化效率。以三聚氰胺（Melamine）为前驱体，利用其酸性条件下会部分水解成三聚氰酸（Cyanuric acid）的特点，使用亚磷酸调控其水解速度和超分子组装热力学和动力学因素，合成单斜晶系的六方棒状前驱物。通过热处理，形成原子掺杂与缺陷并存的六方管状石墨相氮化碳（P-TCN）。进而基于超分子前驱体为层状结构的特点，发展了利用分子进行插层获得多孔超薄的氮化碳纳米片、多孔 TiO_2/氮化碳复合体以及单原子铜/氮化碳杂化体的系列方法。并通过引入具有不同 C/N 比和非对称特性的自组装分子，利用酰胺化反应和分子间氢键构建结构新颖的超分子前驱体，进一步热解获得超薄多孔氮化碳集束体。通过对结构、形貌和组成的调控，丰富了氮化碳的活性位点、提高了光生载流子分离效率、拓宽了光吸收范围并调控了能带结构，实现了光生电子和空穴的同时高效利用。所得氮化碳基催化剂用于同步太阳能光催化分解水产氢和选择性有机物氧化，表现出优异的光催化性能和循环稳定性。

光催化材料中电子-空穴的高效利用

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光催化制备清洁能源契合国家的重大战略需求。提升光催化性能的关键是调控催化剂内部较快的光生电荷行为（飞秒-纳秒），以及表面较为缓慢的反应过程（纳秒-毫秒），使之匹配。基于瞬态吸收光谱技术手段，我们一方面围绕光催化剂中电荷动力学表征开展了一系列工作：包括揭示光生电子-空穴进入长寿命“深陷阱态”失活的机理，并通过精准调控催化剂结构，构建了“浅陷阱态”的高活性新材料，以实现光生电荷在水分解中的高效利用；建立了表征和调控界面电子-空穴转移的方法，实现了 100％选择性的光催化二氧化碳转化制甲醇。另一方面，我们从提高催化剂表面反应速率出发，开发了可在皮秒尺度内吸引质子产氢的富吡啶石墨相碳点，并利用羟基在数百个皮秒内转移表面空穴，提高电子利用率，大幅提高了水分解制氢速率。

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Elemental red phosphorus-based photocatalysts for hydrogen evolution

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Expanding the types of photocatalysts to pure elemental semiconductors represents an ideal pursuit for developing "simple, efficient, low-cost, fully visible light" hydrogen production systems through water splitting. As an ideal carrier for the "simplification" design concept of catalysts, red phosphorus exhibits great potential in the field of photocatalytic hydrogen production from water splitting. As a novel elemental photocatalytic material, the photocatalytic activity of red phosphorus still needs to be enhanced, and studies on its photocatalytic kinetic mechanism are relatively limited. Our research group has conducted modification studies on red phosphorus through strategies such as structure, crystal plane, interface, and defect engineering.[1] We have constructed a series of red phosphorus-based photocatalytic materials using an improved chemical vapor deposition process, for the reaction of photocatalytic hydrogen production driven by visible light. Our studies have optimized the energy level structure, electronic structure, and defect structure of red phosphorus-based photocatalysts to achieve efficient separation of photogenerated electrons and holes, as well as a significant extension of the active charge lifespan, thereby enhancing the photocatalytic application potential of red phosphorus. Combining ultrafast spectroscopy techniques and DFT theoretical calculations, we have revealed the kinetic mechanism of the photocatalytic reaction of red phosphorus-based catalysts, providing an important theoretical and experimental basis for the rational design and development of efficient red phosphorus-based photocatalysts and other elemental photocatalysts in the future.

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海洋光电功能防护材料

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生物污损问题严重影响海工装备的使用寿命，造成巨大的经济损失，威胁海洋安全。特别是在海洋环境水线附近，由于阳光充沛，温度适宜，更有利于微生物膜的形成和发展，导致海工装备材料的生物附着现象更严重，因此，因此如何解决水线附近的生物污损问题尤为紧迫。当前，自抛光防污涂料是目前商用最多防污涂料，其防污机理是自抛光共聚物涂层在使用期限内基体不断受到侵蚀，同时释放防污剂。在静止时，聚合物水解后不能及时溶解，表面更新速度慢，长期使用后抛光速率显著下降，进而导致防污剂难以及时杀死表面附着海生物，防污效果不理想。因此，如何控制防污涂层的自抛光速度以及防污剂的释放速度，提高静态水域下涂层的防污性能，是目前急需解决的关键难题。

全太阳光谱驱动的光催化抗菌材料可充分利用水线附近的太阳光能，提高光催化杀菌性能，且环境友好，是一种很有前途的新型防污剂。光催化抗菌材料可产生活性氧，在涂层中扩散速度明显优于金属离子，因此光响应杀菌速度更快，与离子杀菌互相配合，实现梯度高效杀菌效果。两性离子聚合物链可以溶解在海水中迅速形成自更新的动态表面，在静态水域下也能有效抑制生物污损的粘附。因此，目前提出一种解决思路：将光催化防污材料应用到两性离子防污涂层上，解决静态水域下涂层防污效率差的问题。

氧化亚铜/苝-3，4，9，10-四甲酰亚胺（Cu_2O/PDINH）通过整合 p 型 Cu_2O 和 n 型 PDINH 成功构建异质结构提高光催化抗菌效率。PDINH 将吸收光谱从紫外扩展到近红外，将光利用率提高了 75%。Cu_2O /PDINH 异质结构降低了 Cu_2O 的环境污染风险，实现了全太阳光谱驱动，克服了 Cu_2O 不能产生单线态氧的缺陷。Cu_2O/PDINH 异质结构表现出优异的长期和光催化抗菌活性，由于铜离子的灭菌和全太阳光谱驱动 ROS 的连续产生，抗菌率为>90%。这种无机有机 Cu_2O /PDINH 异质结构在能源和环境方面显示出广阔的应用前景。Cu_2O/PDINH 异质结构具有有效的 ROS 提高和优越的光催化杀菌效率，在环保型海洋防污剂中具有巨大的潜力。

原子级纳米材料的精确制备及电/光能源小分子转化应用

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报告人针对 H_2O, CO_2 和 O_2 等资源小分子稳定而不易活化的难点，巧妙地以纳米材料设计合成为切入点，从纳米催化剂的结构、表界面化学性质出发，设计和调控纳米催化剂的化学组成、形貌和表界面结构，从原子级别构建新催化反应活性中心，探索材料结构和资源小分子活化性能之间的构效关系，揭示新的催化反应机理，全面提升了纳米材料催化性能和稳定性。本报告将从特定小分子催化的原子级纳米材料合成、新型结构的构建以及新型催化机制的创制等方面展开讲述。

Finely defined electron behaviors and high value-added production during photocatalytic CO_2 reduction on 2D surface

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Highly performed photocatalytic CO_2 reduction requires strong photocarrier separation and finely defined reduction pathways. The heterojunction induced interfacial built-in field could efficiently facilitate the separation of photocarriers, and yet the behavior of photogenerated electrons on the reduction side material needs to be further guided for the target production reduced from CO_2, during which the coupling is a key process for achieving high value-added chemicals. And although the surface photocatalysis might have similar pathways to electrocatalysis, the mechanism of activation and selection is not completely understood yet due to its multi-electron involved multi-step reaction, which makes C_{2+} production very challenging.

Herein, we are proposing a coupling-favorable 2D surface for high value-added production, with which multiple reduction pathways could be activated via the diverse design of adjacent localized states. The multiple reduction pathways are defined to contribute thermodynamically and kinetically coupling-favorable adjacent intermediates. This design is supposed to improve the C_{2+} production such as ethanol during photocatalytic CO_2 reduction, while it also raises a strategy for introducing synergetic diversity on the surface of photocatalysts and other optoelectronic materials.

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半导体基纳米晶的表界面调控合成及其催化性能研究

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半导体异质纳米晶，基于各组分能级之间的载流子迁移和耦合，具有较高的理论光催化和电催化活性，结合材料微结构设计调控合成，活性有望突破现有的性能瓶颈。针对上述异质纳米晶的表界面调控，可以最大化其催化活性：大晶格失配度下异质界面的高有序性，提高内部的载流子迁移效率；表面的缺陷构筑，促进反应底物在表面的吸附活化和载流子富集，改善催化性能。基于此，本报告从液相法制备半导体纳米晶的策略出发，设计合成多种具有可调表界面有序性的半导体基异质纳米晶，诱导载流子的定向迁移和优化表面的吸附活化活性，实现催化性能的显著增强。

Ultra-Small LnYVO$_4$:Eu^{3+} Nanoparticles with Persistent Day-Night Photocatalytic and Sono-Catalytic Actions for Water Disinfection

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Day-night photocatalysts and sonocatalysts have become viable contenders for generating persistent reactive oxygen species (ROS) in the quest for improved materials for environmental applications. We introduce novel day-night photocatalyst based on YVO$_4$:Eu^{3+} phosphor doped with lanthanide ions, which exhibit exceptional efficiency in generating ROS when exposed to both light and ultrasound. These nanoparticles function as highly efficient photocatalysts, with a particle size below 5 nm and a single-phase structure. The nanoparticles contain lanthanide ions that function as producers of reactive ROS, while the Eu^{3+} ions and defects in the nanoparticles contribute to their extended activity. The NdYVO$_4$:Eu^{3+} nanoparticles we have developed continue to generate reactive oxygen species (ROS) for a duration of 12 hours even after light/ultrasound irradiation has stopped. This property allows for prolonged disinfection against pathogens like S. aureus and E. coli. The ability to maintain this ongoing activity was also effectively showcased on industrial ceramic plates that were covered with nanoparticles, thereby emphasizing their potential for being included into current water treatment systems. This research proposes a new method for extremely small photocatalysts and sonocatalysts that can act during both day and night. This mechanism provides energy-efficient and cost-effective options for applications such as water purification and disinfection. Our discovery represents a substantial advancement in the development of adaptable catalysts that can be effortlessly included into existing environmental cleanup systems

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Photocatalytic phosphate mineralization on Na$_2$Ti$_6$O$_{13}$ in urea added solution

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Sodium hexatitanate was reported being used as anode materials in Na ion battery due to its higher energy rate and stability. Its photocatalysis was also highlighted. Photocatalytic phosphate mineralization on sodium hexatitanate nanowire is studied in this work. The Na$_2$Ti$_2$O$_{13}$ nanowire was synthesized hydrothermally on Ti alloy pieces in a high alkali solution. The Ti alloy pieces were immersed in a Ca^{2+}, HPO$_4^{2-}$ and urea contained solution under ultraviolet (UV) irradiation. The surface morphology observation by SEM show wadding shape CaP formed between sodium hexatitanate wires. More CaP under UV irradiation compared to that under dark is obtained by EDS and weight tests. More C and N elements are involved in the calcium phosphate (CaP) which is attributed to the photocatalysis. This C and N are from urea, and no N was found on the pieces under dark. The role of urea in the precipitation of CaP on sodium hexatitanate under UV lighting is pursued. A kind of C-N-O bonded CaP compound may be formed under the help of sodium hexatitanate photocatalysis.

Metal hydroxide nanosheets and composites for alkaline electrocatalysis

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In this talk, I will mainly introduce our recent progress on the controllable synthesis and chemical exfoliation of layered metal hydroxides with various metallic compositions (Fe, Co, Ni, etc.). Taking advantages that these single-layer nanosheets are obtained as a monodispersed colloid suspension, we have developed environmentally friendly wet process that can flocculate, stack, and assemble them as building blocks with different kinds of counterpart materials in a manner like LEGO® games. Superlattice-like nanocomposites were prepared by flocculation with oppositely charged graphene derivatives or MoS_2 nanosheets. Electrochemical characterizations identified the nanocomposites as efficient electrocatalysts in oxygen evolution reaction (OER) in alkaline water electrolysis.

Improving charge transport properties of hematite through morphology engineering

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UNIST

This research addresses the challenges encountered in photoelectrochemical (PEC) water oxidation on hematite photoanodes, with a specific focus on two key issues: the limited hole diffusion length (~4 nm) and poor electrical properties. A solution is proposed through the integration of an efficient overlayer onto the branched structure, which induces a highly porous architecture by leveraging additional reaction interfaces utilizing the Kirkendall effect. This effect is particularly pronounced during high-temperature annealing, especially at the interface between the overlayer and Ti-FeOOH (the hematite precursor), exploiting varying diffusion rates of metal atoms. By introducing additional interfaces on the hematite precursor surface, porosity and pore size are effectively controlled, resulting in a significantly nanoporous structure. Through morphological engineering, the overlayer facilitates heteroatom diffusion (doping) into the hematite lattice, thereby enhancing facile charge transport. The material for the overlayer is selected via density functional theory calculations. The optimized photoanode, coupled with an efficient cocatalyst ($NiFe(OH)_x$), demonstrates a maximum photocurrent density of 5.1 mA cm^{-2} at 1.23 V vs. RHE, a remarkable 3.2-fold increase compared to the reference hematite photoanode. This enhancement can be attributed to the highly nanoporous structure and optimal doping. This study marks a notable advancement in improving the PEC performance of hematite-based photoanodes, paving the way for future applications.

低维金属纳米材料的可控合成及其电催化应用

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催化技术是支撑现代工业发展的重要基石。其中，电催化通过将清洁电能转化为化学能，已成为开发下一代能源系统和装置的核心技术，可以有效地应对日益紧张的全球环境和能源挑战。作为电催化的关键部分，催化剂的结构设计和调控极大地决定了整个系统的产物转化效率和选择性。在本次报告中，我将介绍我们课题组在新型低维金属纳米材料的可控合成及其电催化应用方面的最新进展，主要包括以下三个方面：（1）银-铜 Janus 纳米结构的限域生长及其在高性能串联电催化二氧化碳还原中的应用；（2）非常规相贵金属纳米材料的模板法生长及其在非质子锂-二氧化碳电池中的应用；（3）超薄合金纳米材料的可控合成及其在电催化硝酸盐还原中的应用。

Hydrogen Bonds Induced Ultra-Long Stability of Conductive π-d Conjugated FeCo3(DDA)2 with High OER Activity

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Conductive π-d conjugated metal-organic frameworks (MOFs) have attracted wide concerns in electrocatalysis due to their intrinsic high conductivity. However, the poor electrocatalytic stability is still a major problem that hinders the practical application of MOFs. Herein, we report a novel approach to enhancing the stability of MOF-based electrocatalyst, namely, the introduction of hydrogen bonds (H-bonds). Impressively, the π-d conjugated MOF $FeCo_3(DDA)_2$ exhibits ultra-high oxygen evolution reaction (OER) stability (up to 2000 h). The experimental studies demonstrate that the presence of H-bonds in $FeCo_3(DDA)_2$ is responsible for its ultra-high OER stability. Besides that, $FeCo_3(DDA)_2$also displays a prominent OER activity (an overpotential of 260 mV vs. RHE at a current density of 10 mA cm^{-2} and a Tafel slope of 46.86 mV dec^{-1}). Density functional theory (DFT) calculations further indicate that the synergistic effect of the Fe and Co sites in $FeCo_3(DDA)_2$ contributes to its prominent OER performance. This work provides a new avenue of boosting the electrocatalytic stability of conductive π-d conjugated MOFs. (The work has been published in Advanced Materials, the DOI is 10.1002/adma.202402388)

Bi 基化合物异质结的构建及其电还原性能的研究

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通过两种 Bi 不同价态的化合物复合或与非金属载体复合构建的异质结，是将 CO_2 电还原为 HCOOH 的一种高效率策略，在本个研究内容中，通过简单的制备方法，将不同价态的 Bi 基化合物组合构建成为异质结，加速了 Bi 基化合物界面之间电子转移，且增强了 CO_2 中间体的吸附，加速电还原反应进程。合成的 Bi 基氧化物异质结，在标准氢电极电势下，宽电位区间 400 mV ~ 500 mV 对甲酸的法拉第效率达到 91%以上，在 H 型电解池中，-1.0 V 电压下平均电流响应密度为 21.75 mA/cm^2 ·mg。

具有低热预算（≤ 400 ℃），高剩余极化值(2Pr > 25 μC/cm^2)，高耐久性（109）的 $Hf_xGa_{1-x}O_y$ 铁电电容

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自 2011 年科研人员在基于氧化铪的材料中发现铁电性以来，铪基铁电材料在逻辑和存储领域巨大的潜在价值，引起了科研界和工业界的极大兴趣，并取得显著进展。然而，铪基铁电器件失效特性的提升仍然面临挑战，比如，疲劳特性方面，当前铪基铁电晶体管的重复擦写次数在 105 左右，远小于传统铁电材料如 SBT 等 1010 的重复擦写次数，距离类脑计算、内存等应用产品所要求的 1014 的擦写次数更是相距甚远。为了提高铪基铁电器件的疲劳特性，科研人员做出很多尝试，期望通过优化器件的电极材料、掺杂元素和结构等来改进疲劳效应。其中，HfO_2 掺杂工程是一种提高铪基铁电薄膜疲劳特性最常用的方法，掺杂 HfO_2 通常使用原子层沉积工艺（ALD）生长，可以通过控制沉积循环次数，精确控制薄膜厚度和掺杂浓度，因此是一种最简单和重复性非常好的方法。在众多掺杂元素中，镓（Ga）掺杂 HfO_2（HGO）具有高的击穿电场、低矫顽场和高循环的耐久性，然而，现有报道的 HGO 薄膜，需要经过 600 ℃及以上的高温退火才能产生可接受的剩余极化[1]，而在实际应用中，如此高的热预算与集成电路后段工艺并不兼容。

本研究中，我们通过优化退火工艺，实现了低热预算（≤ 400 °C）的 HGO 铁电薄膜。一方面，通过控制快速热退火时通入的 N_2 流量控制结晶过程中的压强，发现在 400 ℃低温退火时，通入的 N_2 流量越小，HGO 的极化强度越大。另一方面，增加快速退火时间，也可以增强 HGO 的铁电性。基于优化后的 $Hf_xGa_{1+x}O_2$ 薄膜的铁电电容器件展现了超低热预算（≤ 400 °C）、高剩余极化值(2 Pr>25 μC/cm^2)以及高耐久性（109 次循环）特性。此研究为探索具有优异疲劳特性、且与先进技术节点后段工艺兼容的铪基铁电材料提供了思路。

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Monolayered 2D Inorganic Nanosheet-Based Hybrid Catalysts with Versatile Energy Functionalities

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Highly anisotropic 2D nanosheets of layered inorganic solids (metal oxides, layered double hydroxides, metal chalcogenides, metal carbides, metal nitrides, and carbon nitrides) have evoked great deal of research activity because of their unique physicochemical properties and outstanding performances as functional materials. A great diversity in the chemical compositions, crystal structures, and defect structures of inorganic nanosheets provides this class of materials with a wide spectrum of physical properties and functionalities. The monolayered inorganic nanosheets synthesized by exfoliation process can be used as powerful building blocks for exploring high performance hybrid catalysts. Since the crystal defect and interfacial interaction have profound influence on the electrochemical and catalytic activity of hybrid materials, the energy functionalities of 2D inorganic nanosheet-based hybrid materials can be greatly enhanced by defect- and interface-engineering. In this talk, several classes of 2D inorganic nanosheets and their nanohybrids applicable for renewable energy technology will be presented together with the discussion about the relationship between chemical bonding nature and functionalities. The crucial role of interface/defect engineering in optimizing the energy performances of 2D nanosheet-based materials will be highlighted.

过渡金属纳米粒子的结构调控：从二维材料负载的催化剂到能源存储器件

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本报告主要介绍二维纳米材料（如氮化硼、石墨氮化碳）负载的过渡金属纳米粒子的制备及其结构调控。这些催化剂在偶联、选择性加氢和高级氧化反应中显示出良好的活性。此外，本报告还简要介绍过渡金属（Pb、V、Mo 等）纳米材料在太阳能电池和集成光辅助储能装置中的应用。

Abstract：This presentation will mainly introduce the preparation, structural regulation and/or immobilization of transition metal nanoparticles on the two-dimensional nanomaterials (e. g., boron nitride, graphitic carbon nitride). These catalysts showed promising activities in coupling, selective hydrogenation and advanced oxidation reactions. In addition, the applications of transition metal nanomaterials in solar cells and integrated energy storage devices will also be addressed.

高性能光电极的混合微波退火合成

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太阳能光电催化分解水制氢或还原二氧化碳转化为碳氢燃料可有效缓解人类对可再生能源的需求，是实现“碳中和、碳达峰”的理想途径。目前还没有一种光电材料能够满足所有的条件（高效、稳定、价廉）。探索新材料、新结构、以及新的制备技术是实现太阳能高效转换的关键。在导电玻璃基底上制备同时具有纳米结构和高结晶性的光电极材料仍然是一个很大的挑战[1]。一方面，高结晶性可以减少了晶界和缺陷，有利于光生电子/空穴的分离、传输；另一方面，纳米结构化增大了电解液的接触面积，同时缩短了光生电子/空穴的传输距离。

混合微波退火（Hybrid microwave annealing, HMA）耦合了常规加热和微波加热，是一种独特高效的加热方法。我们发展了 HMA 在光电催化方面的应用：1）“HMA 结合模板法”解决了高结晶性和纳米结构共存的难题，实现了 Fe_2TiO_5 光电极的性能突破[2]；2）“HMA 合成梯度掺杂芯-壳同质结”的光电极，发挥掺杂优势的同时解决了过多表面缺陷和更高过电位的问题[3]; 3）“HMA 诱导固相界面反应”构筑了合成条件苛刻的氧化铁新型异质结材料，增强了光电催化性能[4, 5]；4）HMA 高效修复了氮离子植入的二氧化钛, 提高了光电催化性能[6]; 5）HMA 结合 Ta 离子的预掺杂，制备了高结晶性 p-t-n 异质结（$Ta:Fe_2O_3@CaFe_2O_4$）[7]；6）HMA 在 α-Fe_2O_3 纳米棒表面合成了非晶 HfO_x 的空穴存储层[8]；7）HMA 诱导稀土 Eu、过渡金属 Nb 共掺杂赤铁矿光阳极，提升光电流密度的同时降低起始电位。HMA 为光电极材料的掺杂、修复和新型半导体材料的合成提供了新的技术平台。

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Single-Atom Catalysts: Emerging Multifunctional Materials towards Sustainable Energy Conversion

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Increasing demand for sustainable energy has accelerated research on various renewable technologies. Developing catalytic energy conversion technologies for replacing the traditional energy source is highly expected to resolve the fossil fuel exhaustion and related environmental problems. Exploring stable and high-efficiency catalysts is of vital importance for the promotion of these technologies. Single-atom catalysts (SACs), containing single metal atoms anchored on supports, represent the utmost utilization of metallic catalysts and thus maximize the usage efficiency of metal atom.[1] However, with the decreasing of particle size, the surface free energy increases obviously, and tends to aggregate into clusters or particles. Selection of an appropriate support is necessary to interact with isolated atoms strongly, and thus prevents the movement and aggregation of isolated atoms, creating stable, finely dispersed active sites. Furthermore, with uniform single-atom dispersion and well-defined configuration, SACs afford great space for optimizing high selectivity and activity.

Our research interest focuses on the development of single-atom catalysts with the particular configuration for sustainable energy conversion, including photocatalysis, electrocatalysis, and thermal catalysis.[2] His research also extends to the operando investigation for monitoring the structural evolution of the reactive centers, as well as the mutual interaction between the reactive center and reactant in the catalytic process. The widespread adoption of SACs in diverse catalytic reactions will be comprehensively introduced.[3, 4] By presenting these advances and addressing some future challenges with potential solutions related to the integral development of catalysis over SACs, we expect to shed some light on the forthcoming research of SACs for catalytic energy conversion.

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FeNiO$_x$ modulation for electrocatalysis on water splitting

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NiFeO$_x$ is a kind of electrocatalyst with high activity in oxygen evolution reactions. However, it is unstable with high current density which is still a major challenge restricting its applications. Herein, the work focuses on the stability control of NiFeO$_x$ for working under high current density and explores the methods to introduce the VIB group cations into NiFeO$_x$ to form NiFeMO$_x$ (M=Cr, Mo, W) and enhance the stability with high activity on oxygen evolution reaction via regulating the valence states change of the M cations at large current density. On the as-prepared NiFeMO$_x$, about 3V of voltage is needed to reach 1000 mA cm-1 of current density in a 1.0 M KOH solution and the stable operation is over 1000 hour.

Defect engineering of nanostructured materials for efficient electrocatalysts

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The defect engineering of nanostructured materials has garnered significant research interest due to its utility in exploring high-performance electrocatalysts. The introduction of crystal vacancies into nanostructured material is found to be quite effective not only in tailoring the electronic and local structures but also in increasing the electrochemical activity. Since crystal defects can serve as efficient adsorption/reaction sites for ions, electrolytes, and catalysis reactants, the defect engineering can provide a versatile means to optimize the electrocatalyst functionality of nanostructured materials. In this talk, diverse examples of defect-engineered nanostructures will be presented along with the correlation between chemical bonding nature and energy functionalities. The various roles of crystal vacancies in optimizing the catalyst performance will be highlighted based on combined in situ/ex situ spectroscopic analyses.

Acidic media enables oxygen-tolerant electrosynthesis of multicarbon products from dilute carbon dioxide in simulated flue gas

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Renewable electricity powered electrochemical CO_2 reduction (CO_2R) offers a valuable method to close the carbon cycle and reduce our overreliance on fossil fuels. However, high purity CO_2 is usually required as feedstock, which potentially decreases the feasibility and economic viability of the process. Direct conversion of flue gas is an attractive option but is challenging due to the low CO_2 concentration and the presence of O_2 impurities. As a result, up to 99% of the applied current can be lost towards the undesired oxygen reduction reaction (ORR). Here, we show that acidic electrolyte can significantly suppress ORR on Cu, enabling generation of multicarbon products from simulated flue gas. Using a composite Cu and carbon supported single-atom Ni tandem electrocatalyst, we achieved a multicarbon Faradaic efficiency of 46.5% at 200 mA cm^{-2}, which is ~20 times higher than bare Cu under alkaline conditions. We also demonstrate stable performance for 24 h with a multicarbon product full-cell energy efficiency of 14.6%. Strikingly, this result is comparable to previously reported acidic CO_2R systems using pure CO_2. Our findings demonstrate a potential pathway towards designing efficient electrolyzers for direct conversion of flue gas to value-added chemicals and fuels.

Bio-inspired mesoporous materials and their applications

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Bio-inspired mesoporous materials are popular multifunctional materials, which have great application potentials in various fields. This is mainly because mesoporous nanomaterials not only have the properties of general porous nanomaterials, such as adjustable pore size, large pore volume, high specific surface area, etc, but also possess many advantages of unique morphologies or structures. It has a broad prospect in catalysis, hydrogen storage, separation and electrochemistry. So far, many methods have been developed to regulate the morphology and structure of mesoporous materials, including spraying, drip, Stober method, colloid assisted assembly, confined assembly and solid state reaction. However, the morphology and mesoscopic structure synthesized by the above methods still cannot meet the needs of the development of the times. At the same time, the research on the synthesis mechanism is not profound enough, and the application research is also very limited. Therefore, it is of great significance to further develop a simple and powerful method to construct bio-inspired porous nanomaterials, to conduct in-depth research on its synthesis mechanism, and to give full play to its application potential.

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电催化中的协同催化

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负载型催化剂广泛用于电催化，尤其是多元金属（金属氧化物或金属氢氧化物）负载型催化剂，多组分之间的协同对其催化性能及稳定性至关重要，本文针对电催化：提出利用贵金属-贵金属（过渡金属）-过渡金属氢氧化物相关物种协同效应（如图 B），构筑具有新型纳米结构的多元金属催化剂。以高效电催化甲醇、乙醇氧化和电解水析氢为模型反应，设计合成了 $PtRu/Ni(OH)_2/C$ 和 $Pt_1Cu/Ni(OH)_2/C$ 等一系列多元金属催化剂。并进一步采用原位拉曼与原位红外及 DFT 计算证明了催化剂在电催化中的协同作用机理[1-6]。

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Structurally-integrated nanostructure array electrodes for electrochemical water splitting to produce hydrogen

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With the worsening of the energy crisis and environmental problems, the exploration of sustainable and clean energy source has been urgently desired. Electrochemical water splitting is regarded as a clean and renewable technology for the hydrogen production using electric energy generated from renewable but intermittent energy sources, such as solar and wind. However, water splitting is seriously limited by its low efficiency due to its kinetically sluggish two half reactions including hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Therefore, the development of highly efficient, low-cost and stable catalyst is the critical factor to realize the commercial application of water splitting for hydrogen production. Our group focuses on the design and synthesis of self-supported nanostructure electrodes and their applications in electrochemical water splitting to produce hydrogen. Here we present our recent results on this research area. Firstly, we fabricated a freestanding 3D carbon tubes (3D CTs) grid via anodic aluminum oxide (AAO) template-assisted method, and a series of Pt/Ir/Ru single-atoms were anchored on the 3D CTs as structurally-integrated electrode to realize ampere-level current density HER. Secondly, we developed an in-situ exfoliation method to prepare ultrathin nanosheets on electrodes. A series of transition metal based nanosheet electrocatalysts including biomimetic nanoleaves, ultrathin layered double hydroxides (LDH) nanosheets, and heterostructure nanosheets were synthesized for OER, and the electrocatalytic mechanism was also systematacially studied. Additionally, based on surface plasmon resonance (SPR) effect created by metal nanoparticles, a metal/semiconductor/metal “sandwich structure” nanopatterned photoanode was fabricated to realize high-efficiency photoelectrochemical water splitting by a multiple enhanced mechanism.

涉氢小分子活化转化催化新材料

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氢氧燃料电池（HOFCs）被认为是新兴的“绿氢”经济的基石技术，可以实现从氢到电的转化。虽然质子交换膜燃料电池（PEMFCs）作为 HOFCs 的成员之一，在过去十年中已被用于氢动力汽车，其中一个非常关键的问题是 CO 等杂质气体导致的催化剂中毒，现阶段，氢气主要来源于天然气和甲醇等碳氢化合物的水蒸汽重整、水煤气变换反应等，CO 通常占氢燃料的 1%。因此开发低成本和高效的抗 CO 中毒的氢氧化反应（HOR）催化剂显得十分必要。目前，PGMs 基催化剂是 HOR 的最佳选择，但 PGMs 的低储量和低利用率严重限制了其广泛应用。此外，PGM 基催化剂的表面容易受到微量 CO（10 ppm）的毒化。因此，如果可以大大提高 PGM 基催化剂对 HOFCs 中的 CO 的耐受性，就可以减轻对高纯氢的需求。

为了提高 PGM 基 HOR 催化剂的 CO 耐受性，研究人员探索了各种方法，如掺杂，合金化，异质结构工程等被广泛提出以提高催化剂的活性和耐久性。虽然这些策略已经取得了一些里程碑式的成就，但大多数只能部分解决 HOR 的性能问题，如活性、持久性或 CO 在酸性、碱性或中性介质中的抗毒性。据报道，通过将 PGMs 催化剂的尺寸降低到原子水平，有可能抑制 CO 在 PGMs 纳米颗粒上的吸附，同时提高原子利用效率，从而提高 PGMs 催化剂的 HOR 性能。然而，人们发现活性位点的电子结构的变化会对最终的催化性能产生巨大的影响。调制方法的细微变化可以极大地改变被调节电子结构的结果。调制方法的细微变化会极大地改变被调节电子结构的结果。因此，具有优异电化学性能的原子分散 PGM 基催化剂仍有很大的探索和开发空间。

本报告从两个方面阐述作者的研究兴趣：首先，我们采用了一种含有预制的钴原子的氮掺杂多孔碳框架固定铂原子，钴原子调控铂原子电子结构，获得全 pH 下高 HOR 活性和耐久性的铂钴双单原子催化剂[1]。此外，我们采用空间限域策略构筑了多尺度活性位点，获得近原子尺度的 PtEr 合金团簇和原子级分散的 Pt/Er 位点的双功能催化剂，该催化剂中 Er 原子的掺杂调节了活性中心电子结构，使得该催化剂在 HOR 和 HER 反应都有非常优异的活性和稳定性，在作为质子交换膜电解槽阴极和燃料电池阳极具有较大应用潜力[2]。综上，我们提出同时调制活性中心微观环境来调节催化剂活性中心电子结构的策略，极大的优化了催化剂的性能的策略[3-6]。

关键词：原子级分散催化剂；电催化；氢反应；抗 CO 毒化

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电化学合成氨反应的催化剂设计与电堆放大

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电驱动硝酸盐还原合成氨作为传统哈伯-博施工艺的替代方案已得到深入研究，但其规模化应用需要在工业电堆的高槽电压、大电流密度及浓电解液条件下长期运行。报告人通过催化剂构效设计调控铜基催化剂在电化学合成氨反应中的活性及选择性，调控其氢转移反应速率来解决催化剂在高浓电解液环境中受硝酸盐毒化的问题，进而通过反应器设计和过程参数优化，并结合流体动力学模拟等手段研究电堆内部多尺度物理化学行为，对电堆优化升级，实现低能耗、高选择性的电化学合成氨规模化生产。

纳米高熵材料的制备及其在能源催化中的应用

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纳米高熵材料(HEMS)在能源催化领域显示出广阔的应用前果，但因成分复杂且种类繁多，缺乏可靠的合成方法及精准设计策略。针对以上难题，发展了激光扫描烧蚀策略，实现常温常压下系列零维 HEMS 包括合金、氧化物、硫化物、磷化物、硼化物、每化物、金属单原子的制备。基于 Brewer-Engel 价键理论与 d 带中心理论，建立了高效电催化 HEMs 的主元筛选原则;所合成低贵金属载量高熵合金显著降低电催化全解水反应活化能，获得低过电势。利用快速共沉淀及 CO_2-H_2 活化策略成功制备具有超高内能和丰富自由体积的二维 HEMS;明确了二维 HEMS 结构形成的主元准入条件。二维高熵金属玻璃实现了 100%CO_2 光热甲烷化转化，转化速率达 0.49 mol g^{-1} h^{-1}。

Construction Nanostructure by Controllable Cation Diffusion Kinetics

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Cation exchange reaction has emerged as a powerful protocol to tailor the structure of semiconductor nanocrystals for photoelectricity, energy applications and so on. The absence of the underlying cation diffusion mechanism at nanoscale hindered the precise construction nanostructures by cation exchange reaction. Herein, except for the traditional organic phosphine ligands, thiol ligands, surface vacancies and guest cations were demonstrated to control the cation diffusion kinetics, leading to the single-doping and dual-doping structure. Additionally, the diffusion rate difference between host and guest cations were controlled by changing the ratio of host and guest cations, which enabled the controllable Kirkendall effect for continuous evolution from solid nanorods to nanotubes and ultimately to hollow nanodisks.

界面工程调控吸附行为促进高效电催化转化

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The construction of heterogeneous interfaces can regulate the charge balance between different components and optimize the adsorption behavior of catalyst on reactive species. Combined with the electrocatalytic processes of biomass oxidation and hydrogen evolution, this report introduces three kinds of heterogeneous components of cathode and cathode catalytic materials with high efficiency and analyzes their catalytic enhancement mechanisms.(1) The CuO-PdO composite was designed, and a series of in situ characterization, electrochemical tests and theoretical calculations were performed to elucidate the promoting effect of heterogeneous interface and the internal mechanism of performance improvement in the electrooxidation of biomass platform molecule 5-hydroxymethylfurfural (HMF). (2) The Ag-Co(OH)$_2$ composite was designed and prepared, and the tandem catalysis effect and adsorption enhancement mechanism of the material in the electrooxidation reaction of HMF were analyzed through a series of in-situ characterization, electrochemical testing and theoretical calculation. (3) The Ni-CeF$_3$ and Ni-VN double heterogeneous interfaces were designed and constructed to regulate the adsorption behavior of the catalysts to the intermediates H* and OH$^-$ respectively, thus accelerating the reaction rates of different elementary elements in the total hydrogen evolution reaction.These ideas provide a constructive guidance for the design of efficient multi-component electrocatalysts in the future.

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多功能锑掺杂二氧化锡薄膜透明导电和光电催化及电催化性能的研究

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Sb 掺杂 SnO$_2$ (ATO)由于其优异的光电性能，在各种光电器件中得到了广泛的研究和应用[1, 2]。然而，较宽的能隙(3.6 eV)限制了其光催化活性仅限于紫外光区[3]。因此，需要有效的修饰来缩小带隙，从而捕获更多的光能。化学取代掺杂已被作为一种有效的方式来修饰 SnO$_2$[4, 5]。在多种掺杂的 SnO$_2$ 材料中，掺杂 Sb 不仅可以通过调整 SnO$_2$ 的电阻率、载流子浓度和迁移率来方便地提高 SnO$_2$ 的电导率，还可以增加 SnO$_2$ 的可见光吸收[6]。采用真空热蒸发沉积法对 Sn-Sb-Sn 薄膜进行阳极氧化，制备了不同锑掺杂量的 ATO 薄膜。锑的掺入使 SnO$_2$ 的形貌结构和光电性能发生了明显的变化。在掺杂样品中，5%Sb 掺杂 ATO 实现了 0.8 mA cm^{-2} 的最高光电流密度。同时，Sb 的掺杂将杂质能级引入 SnO$_2$ 的能带，扩大了样品对太阳光的响应范围。与未掺杂 SnO$_2$ 在可见光下几乎没有响应相比，5%Sb 掺杂 ATO 在可见光下实现了 0.3 mA cm^{-2} 的光电流密度。5%Sb 掺杂 ATO 还取得了最高的光电催化产氢和降解甲基橙性能，5%Sb 掺杂 ATO 的光电催化产氢率为 951 μmol cm^{-2} h^{-1},甲基橙降解率为 3 小时降解 70%。10%Sb 掺杂 ATO 取得了最好的电催化产氢率 μmol cm^{-2} h^{-1}，以及最好的透明导电性，其 FOM 优值为 0.55，电阻率为 1.59*10^{-2} Ω·cm，方阻 136 Ω/□。电学和光学分析表明，适当的 Sb 掺杂可以有效调节 SnO$_2$ 能带结构，提高其载流子浓度和载流子迁移率，从而大大提高 ATO 的光学和电学及光电性能。具有合适 Sb 含量的多功能 ATO 可能是光电器件中光电催化、电催化和透明导电膜的理想候选材料。

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LSPR 增强光电催化 CO_2 还原用异质催化剂的构筑

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数百年来，化石燃料的持续开采使得大气中的 CO_2 浓度逐年上升，同时也带来如全球变暖、环境恶化等问题，减少 CO_2 的排放，降低全球 CO_2 的浓度是全人类的任务。其中用光电催化的方法还原 CO_2，不仅能够减少 CO_2 的浓度，还可以将其转化为高附加值的产物如甲烷、乙烯等，在一定程度上缓解能源危机。光电催化 CO_2 还原至高附加值产品可以将过量的 CO_2 循环回可重复使用的碳形式，是一种非常有前景的方法。本文通过构筑 LSPR 增强异质纳米晶，在可见光照的条件下实现高效光电催化 CO_2 转化（PECR），其含碳产物的选择性高达 100%，通过改变 PECR 过程的反应条件，实现多电子还原产物 CH_4、C_2H_4 以及 C_2H_5OH 的生成。该研究为开发新型的 PECR 催化剂，提高催化剂性能提供了一条有效的途径。

Epitaxial growth of highly atomically ordered Pt-Fe nanoparticles from Carbon nanotube bundles as durable oxygen reduction electrocatalysts

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Intermetallic Pt-based nanoparticles have displayed excellent activity for the oxygen reduction reaction (ORR) in fuel cells. However, it remains a great challenge to synthesize highly atomically ordered Pt-based nanoparticle catalysts, because the formation of an atomically ordered structure usually requires high-temperature annealing accompanied with grain sintering. Here we report the direct epitaxial growth of well aligned, highly atomically ordered Pt_3Fe and PtFe nanoparticles (<5 nm) on single-walled carbon nanotube (SWCNT) bundles films. The long-range periodically symmetric van der Waals (vdW) interactions between SWCNT bundles and Pt-Fe nanoparticles play an important role in promoting not only the alignment ordering of inter-nanoparticles, but also the atomic ordering of intra-nanoparticle. The ordered Pt_3Fe/SWCNT hybrid catalyst showed enhanced ORR catalytic performance of 2.3 fold higher mass activity and 3.1 fold higher specific activity than commercial Pt/C. Moreover, the formation of interlocked interface and strong vdW interaction endow the Pt-Fe/SWCNT catalysts extreme long-term stability in potential cycling and excellent anti-thermal sintering ability.

Designing Metal-Oxide-based Catalysts by In Situ Resource Utilization on Mars for Efficient CO_2-to-CH_4 Conversion via Proton Transfer Strategy

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For large-scale conversion of CO_2 into CH_4 on Mars, designing metal-oxide-based catalysts for electrochemical CO_2 reduction reaction from elements rich in Martian ores is an ideal approach. However, the CO_2-to-CH_4 conversion involves multiple proton-coupled electron transfer processes, and requires H_2O dissociation to provide protons, which would preferably bind with carbon-containing intermediates rather than forming H_2. Here we employed a cation defect confinement strategy to construct Cu atomic centers on MgAl layered double oxides (LDO), and the resulting Cu_1/MgAl-LDO catalyst in flow cell could achieve a Faradaic efficiency as high as 73.6% for CO_2-to-CH_4 conversion at the current density of 380 mA cm^{-2}. Comparison experiments and in situ spectroscopies confirmed the synergistic catalysis mechanism between atomic Cu sites and the neighboring Mg-O and Al-O sites in the step of intermediate protonation for form CH_4. We demonstrate that introducing Mg-O species is a powerful means to promotes H_2O dissociation, and the Al-O species have a proper *H adsorption energy to suppress hydrogen evolution reaction. This work gains more insights into the rational design of CO_2-to-CH_4 conversion catalysts by the proton transfer strategy.

基于二维材料的微纳催化器件

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二维材料及其各类衍生物具有高比表面积、富含活性位点与电输性能优秀等特点，已在电化学各领域引起了广泛的关注，是极具潜力的高性能催化材料。深入解析二维材料的催化活性位点并进一步探索催化机理，是提高其催化性能的必经之路。然而，二维材料通常晶体结构多样且形貌尺寸复杂，使得有效评估其催化性能以及分析催化活性位点成为难点。与此同时，微纳电催化器件是近期兴起的一种新型电化学研究方法，主要通过在电化学芯片上构筑结构明确、界面清晰的微纳电化学器件，实现针对单一纳米结构的定性定量电化学测量，并解析复杂界面的催化过程于机理。因此，微纳催化器件被广泛用于研究基于二维材料及其异质结的新型催化剂，在评估二维材料的催化性能、定位活性位点与探索新型催化机理方面发挥了重要作用。本次报告将详细阐述微纳催化器件的关键技术，研究方法以及应用场景，并进一步结合报告人近期基于二维催化剂的电催化水分解制氢的研究，详细介绍微纳电催化器件在分析二维单晶纳米片的催化活性位点以及优化器件性能上中的突出作用，并建立了二维过渡金属硫化物及磷化物的化学组分/界面性质与催化性能的构效关系。

Rapid Self-reconstruction of Pre-electrocatalysts for Efficient and Stable Large-current-density Water/Seawater Splitting

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Reasonable design of electrocatalysts with rapid self-reconstruction for efficient oxygen evolution reaction (OER) under commercially demanded current density is highly desired. Herein, ultrathin Fe-modified Ni hydroxysulfide (Fe-NiSOH) nanosheet arrays were grown in situ on Ni foam via a simple two-step oxidation strategy for efficient and stable large-current-density water/seawater oxidation. Systematical insights including experimental and theoretical analysis reveal that in-situ S leaching from the electrode boosts its self-reconstruction, and results in more ready generation of highly active Ni^{4+} species, which is benefited from their reduced formation energy. Owing to its excellent physical and chemical properties, the Fe-NiSOH catalyst only requires low overpotentials of 207, 240, and 268 mV in alkaline water to deliver current densities of 10, 100, and 500 mA cm^{-2}, respectively, and can work stably for 1100 hours under commercially demanded current density of 500 mA cm^{-2}.[1] Furthermore, it also exhibits excellent seawater oxidation activity and superior resistance to Cl^- corrosion since it can run stably at 500 mA cm^{-2} for over 900 hours. In addition, functional bimetal (Co and Fe) has been designed specifically to modify nickel phosphide (denoted as CoFe-Ni_2P) for boosting seawater splitting. These in situ generated CoFe-NiOOH species remarkably inhibit the adsorption of Cl^- ions but selectively adsorb OH^- ions, which contributes to excellent performance of the CoFe-Ni_2P electrode for large-current-density seawater splitting. Impressively, a flow-type anion exchange membrane electrolyzer assembled by the CoFe-Ni_2P/Ni-felt bifunctional electrode is demonstrated to be operated stably at an industrially large current density of 1.0 A cm^{-2} in 6 M KOH seawater electrolyte for 300 hours. [2]

电解水催化剂表界面的原子级合成与调控

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氢气已成为推动全球能源持续发展和构建低碳经济的关键能源载体之一。开发经济高效且性能稳定的催化剂，有助于推动氢能经济发展。鉴于多数催化反应发生在材料的表面或界面，原子级调控活性位点是设计高效低成本催化剂的关键，同时有助于深入理解材料结构与性能间关系。本研究通过原子级调控过渡金属催化剂的表界面结构，优化了电解水反应过程。通过设计超薄纳米网筛结构，其提供丰富的表界面活性位点精准沉积了超小铂纳米颗粒，有效提升了氢析出反应性能。此外，通过原子精度构建磁性界面结构，在外磁场下实现自旋极化促进的氧析出反应（OER）动力学过程，并在原子尺度下探究磁场促进的水氧化反应机理，构建了关联磁性与 OER 活性的模型，为设计高活性 OER 催化剂提供了新思路。

金属硫化物纳米材料的设计及其在电催化硝酸盐合成氨中的探索

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氨（NH_3）是既一种重要的化工原料，同时也是一种高能量密度的能量载体。相比与传统的工业制氨方式，电催化硝酸盐制氨（NO_3^-RR）高效、低能耗、无污染，同时可以作为废水处理的有效方式，成为了一种可持续合成氨极具前景的方法。然而，NO_3^-还原制氨的过程中涉及多种含氮中间体的吸附和转化，反应机制复杂。因此，设计并制备有效调控反应中间体的高性能催化剂具有重要的科学意义。金属硫化物在晶型、成分、形貌上的多样性及其与电化学性能的关联性，为化学合成创造新型催化剂材料提供了难得的机遇。围绕新型金属硫化物纳米材料的设计及其在电催化 NO_3^-RR 制氨中的探索，我们揭示了金属硫化物：（1）在电化学活化下，硫的可控溶出可以实现催化剂重构，（2）硫元素可以有效调控含氮中间体的吸附和转化，促进活泼氢在催化剂表面的生成；（3）硫可以通过锚定金属阳离子，实现高效，高稳定性催化反应，为 NO_3^-还原制氨反应拓展了一类新型高性能催化剂并提出了新的反应机制。

Electrocatalytic Materials Design Toward Catalytic Conversion of Energy Small-Molecules

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Catalytic conversion of energy small-molecules is an important approach to utilizing the renewable energy. Using electricity generated from renewable energy to drive electrocatalytic conversion of energy small-molecules is a key approach to developing sustainable clean energy technologies. However, electrocatalytic reactions involve complex processes of chemical bond activation and directional reconstruction, which include intricate dynamic evolution of the surface structure, accompanied by the coupled process of mass transport and charge transfer. Therefore, how to achieve rational design and precise synthesis of catalytic materials, dynamic regulation of the catalytic reaction process, and enhancement of electrocatalytic system activity has become a critical scientific issue facing the field of electrocatalysis. This presentation will focus on electrocatalytic materials and devices toward catalytic conversion of energy small-molecules, progressively discussing precise design of catalytic materials, dynamic regulation of structures and properties, and optimization of catalytic systems. The specific content includes the following three aspects: 1) proposing a new “ship in a bottle” nanoconfinement structure, developing high-performance electrocatalytic materials, and addressing the long-standing challenge of the trade-off between catalyst activity, stability, and selectivity; 2) developing a new strategy for dynamic regulation of confined interfaces, dynamically optimizing the electrocatalytic energy conversion efficiency, and overcoming the limitations in understanding the reaction behavior and structural evolution of electrocatalysts; 3) proposing a new concept of multi-atomic catalytic active region, breaking through the bottleneck of the catalytic activity of isolated active sites, and achieving industrial-level electrocatalytic performance.

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The new integrated devices of photo rechargeable battery based on new compatible electrode

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The integrated device of photo echargeable secondary battery with the functions of photoelectric conversion, energy storage and output is a new way to collect, store and transmit solar energy resources efficiently. At present, the poor matching of electrode materials and device structures leads to low photoelectric conversion efficiency and poor cycle performance. Therefore, this study focuses on the development of dual-function compatible electrode materials with photoelectron conversion and storage, and the design and construction of a new structure of integrated optoelectronic devices. At the same time, the generation, storage and transport mechanism of electrons, holes and ions during the charging and discharging of electrode materials in the operation of integrated devices are explored, which lays a theoretical and experimental foundation for the research and development of photorechargeable batteries.

Resonance of $KNbO_3$ nanofibers is effectively stimulated by ultrasound with low frequency and low power to enhance piezocatalytic activity

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Ultrasound is commonly employed as a source of mechanical energy in piezocatalysis, where it serves as an external excitation inducing the piezopotential that drives surface chemical reactions on the catalysts. The augmentation of mechanical energy generally amplifies the piezoelectric potential on the surface of the piezoelectric catalyst, thereby augmenting its piezoelectric catalytic activity. However, increasing the input of mechanical energy results in elevated equipment energy consumption, particularly for ultrasound generators. Therefore, it is imperative to develop a methodology capable of imparting significant mechanical energy to the piezoelectric catalyst while minimizing energy dissipation. In general, the resonance frequency is where the largest amplitude is accessible. Therefore, excitation of the matching piezocatalyst at this frequency should result in a higher level of piezocatalytic activity and an improvement in energy conversion efficiency. In this study, we proposed that the length of piezoelectric $KNbO_3$ nanofibers be fixed to match the low-frequency ultrasound (LFUS), and calculated the length of the $KNbO_3$ nanofibers at low-frequency resonance through simulation. The Piezocatalytic activity of $KNbO_3$ nanofibers at matched and unmatched natural and ultrasonic frequencies was investigated. Even at a reduced ultrasound power of 25 W, a notably high piezocatalytic activity was observed under the resonance, offering strong evidence for resonance-enhanced piezocatalysis. This work presents a fresh way for LFUS-activated piezocatalysis to achieve efficient degradation, which is of practical significance in energy-saving water treatment.

Energy efficient water production through composite hydrogels

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Water is the basis for the existence and continuation of all life on Earth. The water resources on Earth are extremely huge (ca. 1.46 × 1016 cubic meters). However, 99.97% of the water exists in the form of seawater or deep groundwater that is difficult to collect, and only less than 0.03% can be easily used by humans. Due to geographical and climate constraints, the shortage of freshwater is of concern to 2.8 billion people in 48 countries all over the world especially in Africa, the Middle East, and Oceania, and the affected population may rise to 4.0 billion based on reasonable predictions. Consequently, the discovery of the next-generation freshwater production technologies with low-cost, high-water production rate and ease of installation and use is considered a promising solution to this global challenge and has attracted increasing attention all over the world.

The Solar Driven Interfacial Evaporation (SDIE) system is a floating device mounted on the surface of the sea in which a hydrogel with customized features is integrated (Fig. 1). By incorporating a photothermal additive into the hydrogel matrix, SDIE can greatly increase the evaporation rate of seawater. Our team has developed a series of new hydrogel materials that enable higher freshwater production efficiency by tuning the hydrogel structure on the nanometer, micron, and millimeter scale. These systems offer excellent water production performance and high solar-to-steam conversion efficiency compared to state-of-the-art materials.

二维材料可控生长及物性调控

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二维纳米材料独特的结构及量子限域效应使该类材料在信息与能源等领域具有广泛的应用前景。可控制备高质量二维材料并对其进行有效的物性调控是研究其性质及应用的前提。目前，化学气相沉积(CVD)在大规模制备二维纳米材料方面表现出巨大潜力，但该方法涉及多元素跨尺度下热力学及动力学的系统协同调控问题，深入理解二维纳米材料的CVD机理及物性调控将为其可控制备与应用提供坚实的理论基础。

本次报告将从多尺度理论模拟的角度讲述报告人在二维材料 CVD 可控制备及物性调控机理方面取得的一些研究进展，包括: (i) 二维原子晶体的生长动力学机制及多尺度模拟方法的开发；(ii) 制备晶圆级单晶二维材料的机制；(iii) 二维材料结构与物性调控。

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Multifunctional mesoporous carbon materials assambly from nanoemulsion

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Carbon-based mesoporous materials are popular mesoscopic structural materials, which have great application potential. This is mainly because mesoporous carbon materials not only have the properties of general mesoporous materials, such as adjustable pore size of 2-50 nm, large pore volume, high specific surface area, etc., but also have their own unique properties, such as light weight, rigid skeleton, good electrical conductivity and chemical stability. It has a broad prospect in catalysis, hydrogen storage, separation and electrochemistry. So far, many methods have been developed to regulate the morphology and structure of carbon-based mesoporous materials, including spraying, drip, Stober method, colloid assisted assembly, confined assembly and solid state reaction. However, the morphology and mesoscopic structure of mesoporous carbon nanospheres synthesized by the above methods still cannot meet the needs of the development of The Times. At the same time, the research on the synthesis mechanism of mesoporous carbon nanospheres is not profound enough, and the application research is also very limited. Therefore, it is of great significance to further develop a simple and feasible synthesis method to construct functional mesoporous materials, to conduct in-depth research on its synthesis mechanism, and to give full play to its application potential. After a long period of exploration, we found that the introduction of hydrophobic organic small molecules into micellar synthesis system, namely the construction of nano-microemulsion system, can give the synthesis method more powerful functions. Based on this idea, systematic studies have been carried out on the development and synthesis of novel mesoporous carbon materials, the design of novel morphologies, the regulation of mesoscopic structures and the functionalization of carbon skeletons. Meanwhile, the applications of these materials in energy storage and catalysis are studied.

过渡金属氧化物电极多面体调控

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金属氧化物（MxOy）由金属-氧（M-O）配位多面体的结构单元组成，其晶体结构由多面体单元以共用顶点、边或面的方式相互联结而成。因而，M-O 多面体的排列方式、构型及配位环境是影响其晶体结构和物性的关键，对多面体实现精准调控可成为提升金属氧化物电极材料电化学储能性能的高效方法。本研究围绕电化学储能过渡金属氧化物电极材料设计、结构调控和表界面改性等基础科学问题，聚焦金属氧化物多面体调控。在锰、钴氧化物中实现了多面体取向和排列调控、多面体的构型调控以及多面体的配位调控，有效提高了锰基和钴基电极材料的结构稳定性，提升了离子输运性能，并应用与锂/钠电池中，表现出优异的电荷存储性能。该研究为金属氧化物电极的多面体调控提供了新思路和新方法，为新型高性能储能电极材料的开发提供了理论基础。

Implementing the material genome by size-selected atomic cluster beam technology

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The US government launched the Materials Genome Initiative (MGI) for discovering, manufacturing, and deploying advanced materials twice as fast and at a fraction of the cost compared to traditional methods through the high-throughput computing, synthesis and characterization strategy. However, in this three-steps strategy, synthesis cannot be engineered due to a significant portion of materials may not be combined for even ten years, which has become an important technical bottleneck of the MGI.

Atomic cluster is an aggregate of atoms. Their remarkable physical and chemical properties depend sensitively on the number of atoms they contain and differ dramatically from the corresponding individual atoms and bulk solids, such as ferroelectricity, low melting point, catalysis, sensing and superconductivity. Thus makes cluster an important platform for the implementation of the material genome. Moreover, the cluster research field features a mass selected ion beam source, essentially a "inevitable synthesis" technology, which enables the control of atoms one by one and the generation of clusters with specified atomic number and structure. Therefore, it is possible to realize the creation of 100,000 new clusters and material genome by using this "inevitable synthesis" technology. This is also a dream of the cluster researchers since the Nobel laureate Smalley, when the production rate of this technology was ultra low that it takes 1000 years to accumulate 1mg of C60.

Shenzhen Creatom Technology Co., Ltd. (CREATOM) has developed cluster ion beam technology. A micro-milliampere cluster ion source has been built to achieve the manufacturing capacity of grams of cluster new materials every day. Based on which a material gene database of 100,000 kinds of cluster new substances will be established to search for the cluster materials that have excellent performance in special metals, high-performance catalysis and other aspects.

In situ Extreme Micromechanics－Recent Innovations and Prospects

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Alemnis

In situ SEM micro- and nanomechanical testing is an indispensable technique for materials design as well as for fundamental mechanics research. Many new protocols and testing geometries beyond traditional nanoindentation now enable the study of microstructure－property relationships, material intrinsic behaviour including orientation-dependence and plasticity, fracture dynamics, or the performance of novel micro-3D-printed metamaterials, to name but a few.

Thanks to its versatility, in situ SEM-based micromechanics is contributing to numerous scientific domains, including thin films and coatings, metallurgy, glasses and ceramics, semiconductors, biomechanics, or architectured materials. Performing micromechanical tests in situ in a SEM offers two important advantages: (1) unmatched control, stability, and positioning accuracy, and (2) the possibility to perform unique correlative experiments based on, for example, the combination of mechanical data with direct imaging or EBSD measurements.

An increasingly important branch of micromechanical testing can be found in the simulation of real-world, extreme operation conditions, such as high temperatures in engines, cryogenic temperatures in hydrogen storage, dynamic loading under shock or impact, high frequency cyclic fatigue, or a combination thereof. Progress in the understanding of material behaviour at such conditions is clearly linked to the availability of laboratory equipment that can perform reliable tests under such conditions.

We present the most recent developments in instrumentation for in situ extreme mechanics testing at the micro and nanoscales. In focus is a testing platform capable of strain rate dependent testing over the range from 0.0001 s^{-1} up to 10’000 s^{-1} (8 orders of magnitude) with simultaneous high-speed actuation and sensing capabilities with nanometer and micronewton resolution, respectively. Furthermore, the challenges and solutions to performing extreme micromechanics over the temperature range from -150 ℃ to 1000 ℃, and the inherent advantages of using small volumes of sample material will be discussed. Finally, we present examples of such extreme micromechanical in situ tests and discuss future research directions in the field of extreme micromechanics.

Functional photothermal materials for interfacial solar evaporation

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Interfacial solar evaporation is a cost-effective and sustainable technology for clean water production since it only uses solar light as the energy source. The working mechanism of interfacial solar evaporation involves sunlight absorption, photothermal conversion, heat localization and interfacial water evaporation. To facilitate real-world applications, it is required to improve the energy efficiency of interfacial solar evaporation. Energy management during solar evaporation is one of the most important and effective strategies to improve energy efficiency. The ideal solar evaporation system should have minimum energy loss by radiation, convection, and conduction while having maximum extra energy gain from the surrounding environment. This can be realized by rationally designing the structure and configuration of the photothermal materials and evaporators. This presentation will introduce a novel design of photothermal evaporators to simultaneously decrease energy loss, lower evaporation enthlapy, increase light absorption and energy harvesting from the surrounding environment and energy recycling for solar steam generation.

UiO-66（Zr）中的缺陷化学及其高效室温氧化脱硫性能

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Desulfurization of fuel oil is an indispensable step to obtain clean energy source. Design of metalorganic frameworks (MOFs) with densely dispersed and precisely configured defects as delicately-tailored active sites, opens a new door to boost the catalytic activity for targeted reactions. In this work, we first introduce a solvent-free route to obtain highly defective UiO-66(Zr) in one step and further demonstrate several strategies to tailor the type and configuration of the defective nodes. The catalysts displayed extraordinary activity for the oxidative removal of sulfur compounds at room temperature.

Wet-chemical synthesis of metal nanomaterials with unconventional crystal phases and their catalytic properties

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Metal nanomaterials have excellent intrinsic catalytic activity, high electrical conductivity and high stability, making them promising catalyst materials. However, conventional colloidal synthesis mainly focuses on the morphology and composition control of nanocrystals. This report will introduce some interesting discoveries we have recently made in the aspect of crystal phase control. For example, traditional Au nanomaterials have the same face-centered cubic (fcc) crystal structure as bulk gold, while we have developed unconventional 4H/fcc heterogeneous Au nanorods with high yield. Au nanorods in these unconventional crystal phases have high thermal stability and can serve as high-quality seeds for epitaxial growth. Therefore, we further prepared unconventional 4H/fcc core-shell nanostructures, in which Au was coated with other catalytically active metals (such as Pd and Cu). The catalytic performances of these new crystal phase metal nanomaterials in ethanol electrooxidation and carbon dioxide electroreduction were studied. In a latest work, we used Pd-based nanocrystals of different crystal phases as seeds, further deposited Pt surfaces of different crystal phases by colloidal epitaxial growth, and carried out phase-dependent performance analysis of Pt surfaces in organic heterogeneous catalytic reactions. These works demonstrate a new strategy to design and synthesize the crystal phase of metal nanomaterials by wet-chemical method, and explore the effect of crystal phase regulation on various properties of metal nanomaterials.

Design of surface plasmonic metal nanostructures

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Based on the unique properties of surface plasmonic metal nanostructures, the interface effects and coupling effects between metal nanostructures were revealed through the design and construction of metal nanoparticle structures, and their applications in energy and environmental catalysis were further explored. By combining the "top-down" direct-ink-writing 3D printing technology with the "bottom-up" assembly technology, the multi-scale (nanometer-micron-macro) ordered structures of surface plasmonic nanomaterials are constructed. The influence of catalytic reaction is further studied based on the enhancement of surface plasmon, which lays a theoretical and experimental foundation for the practical application of surface plasmonic nanostructures.

Atomistic Mechanisms of Ring Formation During Catalyzed Carbon Nanotube Growth

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In order to realize controllable preparation of high-quality carbon nanotube (CNT), it is crucial to understand the atomistic details of its growth mechanism. In this study, the entire on-substrate chemical vaporization deposition (CVD) growth process of CNT, from initial catalyst melting to steady-state growth, was captured by reactive molecular dynamic (MD) simulations with few artificial constraints. We systematically investigated the evolving behaviors of carbon atoms and identified the major types of ring defects and their associated time scales. In addition, two characteristic formation paths of the six-membered rings were found: they can be obtained from direct close of carbon-chains on the catalyst surface, or healed from metastable non-six-membered-rings. Interestingly, though the average time cost for the formation of rings via the first path is much lower, more six-membered rings were actually formed via the second path, due to a significant reduction in the activation energies mediated by the introduction of an intermediate state.

铜基多元硫属纳米晶的精准合成及光催化性能研究

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纳米科技的快速发展有力地推动了纳米光催化剂的设计与开发； 其中，半导体纳米光催化剂也受到越来越多的研究者关注。然而，目前已报道的大部分半导体光催化剂的光吸收范围有限，不能全面的吸收太阳光，这将极大地限制太阳能光催化制氢应用。因此，迫切需要开发在可见光区具有高吸收系数的新型半导体纳米材料作为光催化剂。由环境优化元素组成的铜基多元硫属化合物具有优异的可见光吸收性能和适合于太阳光吸收的能带结构。此外，铜多元硫属化合物可以通过合金化等方式来调控能带结构，进而提高其可见光的吸收能力。基于此，我们通过表面工程、同质异相结构和掺杂等方法来进一步优化铜基多元硫属化合物纳米材料的光催化性能，制备高效光催化剂。

DDAB 基铯铅溴钙钛矿纳米晶的尺寸调控及白光发光二极管的应用

陈雪莲
西安石油大学

胶体金属卤化铅钙钛矿纳米晶具有优异的光学性质，在发光二极管照明和太阳能电池等领域展现出极大的应用潜力。纳米晶的光学性质主要依赖于其尺寸/尺寸分散性和形貌，通过控制纳米晶的尺寸/尺寸分散性和形貌，可提升其光电性能。精准调控纳米晶的尺寸/尺寸分散性对提高其光学性质至关重要。然而，由于胶体金属卤化铅钙钛矿纳米晶属于离子型晶体，其形成能较低，往往存在合成过程中尺寸不可控的问题，严重限制其在光电和光伏领域的工业化应用进程。

基于此，本文采用配体调控/钝化策略，通过室温平衡控制法合成油酸（OA）封端的铯铅溴纳米晶（OA-$CsPbBr_3$ NCs），在 OA-$CsPbBr_3$ NCs 合成的不同不同阶段引入强配体双十二烷基二甲基溴化铵（DDAB），获得了一系列不同尺寸的 DDAB-$CsPbBr_3$ 纳米晶立方块。DDAB-$CsPbBr_3$ 纳米立方块的尺寸在 6.5 ~ 9.9 nm 之间可调。随着 DDAB 添加时间的延长，纳米立方块的光致发光量子产率（PLQY）从 62.81% 显著提升至 98.58%，荧光寿命从 5.47 ns 延长到 19.45 ns。同时，纳米晶立方块的稳定性也得到了显著提升，在普通环境下储存 4 个月其荧光强度仍保持 80%以上，在紫外光照射 2 h 后其荧光几乎没有衰减，在乙醇和甲苯的混合相中最长能保持 65 min。与 OA-$CsPbBr_3$ NCs 相比，DDAB-$CsPbBr_3$ NCs 构建的 WLED 器件的 Rg 提升到 106%左右，CCT 最大降低了~ 400 K，光效率提高了近 4 倍，表现出优异的器件发光性能。本工作对制备高效稳定的钙钛矿纳米晶具有一定参考意义。

墙报展示：

A06-P01

Ruthenium–Nickel Nanoparticles with Unconventional Face-Centered Cubic Crystal Phase for Highly Active Electrocatalytic Hydrogen Evolution

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Ru-based nanomaterials is the promising alternative to Pt electrocatalysts for green hydrogen energy generation, and crystal phase engineering could significantly push their catalytic performance to newer limits. However, controllable phase regulation on Ru-alloys remains challenging, and elucidating the crystal phase-related electrocatalytic performance is of great significance. Herein, we successfully synthesize RuNi nanoparticles with the unconventional face-centered cubic (*fcc*) phase via a facile route. Comprehensive transmission electron microscopy confirms the structural features of the *fcc*-RuNi and electrochemical analyses indicate the impressive electrocatalytic hydrogen evolution reaction of *fcc*-RuNi. The anomalous *fcc*-RuNi nanoparticles possess an extraordinarily low overpotential of 16 mV in hydrogen evolution. With the aid of density functional theory calculations, the *fcc*-RuNi nanoparticles are found favorable for intermediates desorption and H_2O dissociation in energetics. This work deepens our understanding on the phase regulation of the Ru-based nanostructures and will advance the phase engineering in broader catalytic applications.

A06-P02

分级镍铁层状双氢氧化物复合电催化剂用于高效析氧反应

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高效的析氧反应电催化剂对于降低大规模水分解过程中的能耗具有重要意义。本工作采用三步法在泡沫镍上制备了分级的Fe掺杂纳米片修饰的NiFe层状双氢氧化物((Ni, Fe)Se@NiFe-LDH/NF)复合电催化剂。分级的(Ni, Fe)Se@NiFe-LDH/电催化剂呈现三维多孔结构，具有较大的比表面积和有效的物质转移，(Ni, Fe)Se纳米片和NiFe-LDH之间的紧密结合保证了良好的电子传递，在碱性介质中表现出优异的OER性能。(Ni, Fe)Se@NiFe-LDH/NF 在 100 mA/cm^2 下的过电位为 253mV，Tafel 斜率为 47 mV/dec。分级的(Ni, Fe)Se@NiFe-LDH/NF具有良好的长循环稳定性。突出的OER性能归功于Fe的掺杂、快速电荷转移以及(Ni, Fe)Se 与 NiFe-LDH 之间的协同作用。本研究为高效制备 OER 电催化剂提供了一种有前途的方法。

A06-P03

Air-promoted light-driven hydrogen production from bioethanol over core/shell Cr_2O_3@GaN nanoarchitecture

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Hydrogen production from biomass and/or its derivatives rather than fossil fuels presents one of the most viable routes toward carbon neutrality. Among a variety of biomass and its derivatives, bioethanol is an increasingly available and economical hydrogen vector with a global annual yield of 109.8 billion liters in 2019, which is formed by fermentation of renewable biomass. Nevertheless, the complex chemical bond network of C-C, C-O, C-H, and O-H poses tremendous challenges for bioethanol reforming to H_2 with high efficiency. Extensive thermal energy is generally required to achieve considerable activity, with virtual limitations of huge carbon emissions, high operation cost, and fierce catalyst deactivation. Over recent years, photocatalysis has emerged a disruptive strategy for green hydrogen production from bioethanol by utilizing the infinite solar energy. Unfortunately, there has been no practical success so far in hydrogen production from bioethanol powered by sunlight, which is associated with the unfavored optoelectronic properties of the photocatalysts existed, and limited understanding of the reaction mechanism. Particularly, for most of the reported studies, it is often operated under an anaerobic condition with the limitations of sluggish kinetics and severe coking since O_2 is conceptually recognized as an undesired quencher of photocatalytic hydrogen production by serving as electron scavenger. The removal of O_2 in the reaction system is the premise of achieving high activity regardless of the photocatalysts utilized.

Herein, we have explored a disruptive air-promoted strategy for exceptionally efficient and durable light-driven hydrogen production from bioethanol by developing a core/shell Cr_2O_3@GaN nanowires semiconducting architecture. Owing to the unique catalytic attributes of Cr_2O_3@GaN, hydrogen is produced at an unprecedented rate of 76.9 mole H_2 per gram Cr_2O_3@GaN per hour with record-high light-to-hydrogen efficiency of 17.6% by only feeding bioethanol and light with the assistance of O_2. The simultaneous generation of aldehydes from bioethanol dehydrogenation enables the process more economically promising. Moreover, by decoupling chemical reactions from photons absorption and charges separation over a favored 1D nanoarchitecture, a distinguished TON of 266,943,000 mole H_2 per mole Cr_2O_3 for light-driven hydrogen production was obtained over a long-term operation of 180 hours. This unexpected performance, to our knowledge, far outstrips state-of-the-art photocatalytic systems for hydrogen evolution from a broad range of liquid hydrogen carriers.

We have extensively conducted operando spectroscopic characterizations, isotope experiments, as well as density function theory calculations to study the critical role of air in the exceptional activity and stability over Cr_2O_3@GaN nanoarchitecture. It is revealed that owing to the unique catalytic properties of the Cr_2O_3@GaN, bioethanol is energetically favorable to be adsorbed on the Cr_2O_3@GaN interface compared to O_2 under an aerobic condition, followed by dehydrogenation toward acetaldehyde and H^+ with the aid of photoexcited holes under light illumination. The released protons are then consumed for H_2 evolution by photogenerated electrons. After that, O_2 can be evolved into active oxygen species. It is beneficial for further promoting the deprotonation and C-C cleavage of the key C_2 intermediate of bioethanol, thus significantly lowering the reaction energy barrier of hydrogen evolution and removing the carbon residual with inhibited bioethanol overoxidation toward CO_2 and H_2O. Overall, the synergy between Cr_2O_3 and GaN, together with O_2, makes a significant contribution toward the outstanding activity and stability of light-driven hydrogen production from bioethanol. In sharp contrast, if the reaction was conducted under anaerobic conditions, it would be limited by high energy barrier with undesirable coke accumulation, thus leads to the sluggish reaction rate and rapid deactivation of the catalyst. Owing to the widespread distribution of air, biomass and sunlight on the earth, this work presents an unprecedented air-promoted strategy for light-driven hydrogen production from bioethanol over a novel and industry-friendly Cr_2O_3@GaN nanoarchitecture.

A06-P04

Self-supported FeNi layered double hydroxide anode with high activity and long-term stability for efficient oxygen evolution reaction

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The layered double hydroxides (LDHs) as efficient OER catalysts have attracted significant attention owing to their high surface-to-bulk ratios, controllably layered structure, and tunable metal compositions. The unique lamellar architectures of FeNi-layered double hydroxides nanoparticles (FeNi-LDHs NPs) with high oxygen evolution reaction (OER) activity and prominent catalytic lifetime were first self-assembled on FeNi foam by a chemical corrosion engineering method. The obtained FeNi-LDHs@FeNi foam (FNF)-2 catalysts composed of FeNi hydroxides without any trace of NiOx species can function as active sites for an efficient OER. Moreover, considering the unique lamellar feature and partial crystallinity of FeNi hydroxides, FeNi-LDHs@FNF-2 can achieve a good balance between available active sites and electronic conductivity, thus endowing it with excellent oxygen evolution activity. This study affords an effective strategy to achieve optimized OER performance with a promising future of larger-scale non-precious materials in the industry.

A06-P05

Lattice doped Ir atoms cooperating with surface-anchored IrOx nanoparticles for acid oxygen evolution reaction

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Water electrolysis by renewable electricity has been considered as one of the most promising routes to producing hydrogen. Proton exchange membrane (PEM) water electrolyzer has been attracting broad interest owing to its advantages including low ohmic resistance loss, high current density, quick response and high product purity. However, the slow four-electron oxygen evolution reaction (OER) kinetics and low electrocatalytic stability in acid limit its application. Iridium (Ir)-based electrocatalysts have demonstrated decent OER kinetics and moderate electrocatalytic stability in acid, but they are scarce and expensive. Hence, maximizing the Ir mass activity meanwhile enhancing the durability to increase the cost-effectiveness of Ir-based electrocatalysts for long-term OER in acid has become an urgent demand for PEM water electrolyzer. Reducing Ir usage while maintaining stability is crucial for acidic OER in grid-scale hydrogen production. In this study, we developed a synthetic method of successive electrochemical deposition and high-temperature thermal shock to produce $IrO_x/Ir\text{-}WO_3$ electrocatalyst with 2 nm IrO_x nanoparticles anchoring on Ir doped WO_3 nanosheets. The $IrO_x/Ir\text{-}WO_3$ electrocatalyst demonstrated a low overpotential of 239 mV to achieve a current density of 10 mA cm^{-2} and a mass activity of 1588 A g_{Ir}^{-1}@1.53 V vs. RHE, as well as enhanced stability compared to IrO_2. It was found that the WO_3 support in the IrOx/Ir-WO_3 catalyst contributes to its stability by providing electrons to retard overoxidation and dissolution of Ir atoms during acid OER. Structural analysis and density functional theory calculations revealed that the adjusted coordination environment of Ir and the optimized adsorption energy of oxygen-containing intermediates also contribute to the enhanced stability as well as the high activity of the $IrO_x/Ir\text{-}WO_3$ catalyst. The $IrO_x/Ir\text{-}WO_3$ electrocatalyst holds great promise for advancing grid-scale hydrogen production via renewable energy sources.

A06-P06

Direct electrolysis of seawater to produce hydrogen

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The layered double hydroxide (LDH) electrocatalyst has excellent activity on oxygenation evolution reaction (OER)and is expected to be used in alkaline water electrolysis for hydrogen production industry. However, the stability of LDH under large current density still has great challenges, especially in the application of direct electrolysis of seawater for hydrogen production. Due to the existence of a certain concentration of Cl^- in seawater, competitive reactions such as CER may occur in the OER process, and the generated active chlorine species may seriously corrode the anode or equipment, limiting the long-term stable operation of the LDH anode. Herein, a corrosion-resistant Ag/NiFe-LDH electrocatalyst for seawater electrolysis at large current density, in which Ag species in the catalyst can have a corrosion-resistance of chloride ions from the anode surface and enhance its robustness in seawater is designed. The selective adsorption of Cl^- by Ag in the OER process on the LDH surface reduces the excessive oxidation of the active center Ni^{2+} or Fe^{3+}, and effectively improves the stability of the catalyst. The optimized Ag/NiFe LDH can operate stably over 168h in alkaline solution with a current density of 1000 mA cm^{-2}. The results show that the stability of the anode is improved by the in-situ formation of AgCl on the anode surface, and the concentration of Cl^- near the anode surface is reduced.

A06-P07

Cr-doped NiFeOx electrode for enhancing stability during oxygen evolution reaction at high current conditions

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The main challenge for green hydrogen production is to achieve with low energy consumption and low cost via electrocatalysis water splitting under industrial-level current density. A type of electrocatalyst that can endure high current density, maintain stability and exhibit high activity has been developed and synthesized for the purpose of oxygen evolution. This paper presents a self-supported electrode composed of $NiFeCrO_x$ electrocatalyst within a nickel-based structure. At the current density of 1 A cm^{-2}, it can run stably for more than 200 hours, and there is no noticeable corrosion on the foam nickel base. In a two-electrode water electrolysis system, driven by a 5 V voltage, the current density reaches 2 A cm^{-2} using a $NiFeCrO_x$ electrocatalyst electrode anode with an area of 1 cm^2 and a nickel foam electrode cathode with an area of 1 cm^2. It can operate steadily for over 100 hours. This study offers a solution to address the technical challenge of maintaining stability in hydrogen production through high-current water electrolysis.

A06-P08

Monolayer Graphitic Carbon Nitride: An Efficient Metal-Free Catalyst for Enhanced Photo- and Electro-Catalytic Performance.

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The exfoliation of bulk graphitic carbon nitride (g-C_3N_4) into monolayer has been intensively studied to induce maximum sur-face area for fundamental studies, but ended in failure to realize chemi-cally and physically well-defined monolayer of g-C_3N_4 mostly due to the difficulty in reducing the layer thickness down to an atomic level. It has, therefore, remained as a challenging issue in two-dimensional (2D) chemistry and physics communities. In this study, an “atomic monolayer of g-C_3N_4 with perfect two-dimensional limit” was successfully prepared by the chemically well-defined two-step routes. The atomically resolved monolayer of g-C_3N_4 was also confirmed by spectroscopic and micro-scopic analyses. In addition, the experimental Cs-HRTEM image was collected, for the first time, which was in excellent agreement with the theoretically simulated; the evidence of monolayer of g-C_3N_4 in the perfect 2D limit becomes now clear from the HRTEM image of orderly hexagonal symmetry with a cavity formed by encirclement of three adjacent heptazine units. Compared to bulk g-C_3N_4, the present g-C_3N_4 monolayer showed significantly higher photocatalytic gen-eration of H_2O_2 and H_2, and electrocatalytic oxygen reduction reaction. In addition, its photocatalytic efficiency for H_2O_2 production was found to be the best for any known g-C_3N_4 nanomaterials, underscoring the remarkable advantage of monolayer formation in optimizing the catalyst performance of g-C_3N_4.

A06-P09

Bifunctional electrocatalyst Spinel oxide Co_2GeO_4 and Ni_2GeO_4 with high oxygen evolution reaction and oxygen reduction reaction activity

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Bifunctional catalysts for oxygen evolution reduction (OER) and oxygen reduction reaction (ORR) are key renewable-energy technologies including metal-air batteries and water splitting. In this work, a solid-state sintering approach was employed to prepare spinel-structured bimetallic oxides Co_2GeO_4 and Ni_2GeO_4 with remarkable bifunctional catalytic activity. Compared to Ni_2GeO_4 and Co_3O_4, Co_2GeO_4 demonstrates a larger density of oxygen vacancies, leading to an increased abundance of active sites and superior OER and ORR activities. Electrochemical measurements in alkaline media, the material required a mere overpotential of 263 mV to attain a current density of 10 mA cm^{-2}. Moreover, Co_2GeO_4 exhibited exceptional stability, maintaining a stable potential for 40 hours at a current density of 1 mA cm^{-2}. The calculation revealed that the high stability is attributed to the robust Ge-O bonds, which stabilize the Ge-O4 tetrahedrons within the spinel framework. This study possesses significant potential in guiding the development of highly efficient bifunctional electrocatalysts for both OER and ORR.

A06-P10

Preparation of $Cu_{2-x}S$ nanocrystals and study of photothermal conversion properties

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With the problem of energy utilization and environmental protection becoming more and more serious, efficient photothermal conversion technology has attracted wide attention. $Cu_{2-x}S$ nanocrystals, as a kind of semiconductor material with excellent photothermal conversion properties, have shown broad application prospects in the field of solar energy utilization. However, how to accurately regulate the structure and properties of $Cu_{2-x}S$ nanocrystals is still a key challenge to be solved. In this paper, the preparation of $Cu_{2-x}S$ nanocrystals with different sulfur precursors and their properties in the field of photothermal conversion were investigated. The conversion of Cu_2O to $Cu_{2-x}S$ nanocrystals with different defect structures and adjustable surface photothermal conversion properties was controlled by using different S precursors. By means of XRD, SEM and TEM, it is proved that $Cu_{2-x}S$ nanocrystals have adjustable band gap, which is conducive to expanding the optical absorption range and enhancing the optical absorption intensity. Through the ultraviolet-vision-near-infrared diffuse reflection spectrum,$Cu_{2-x}S$ nanocrystals have excellent solar absorption properties and can effectively convert absorbed light energy into heat energy quickly. The photothermal conversion curves show that the photothermal properties of $Cu_{2-x}S$ nanocrystals synthesized from different sulfur precursors can be regulated. This study provides an experimental basis for understanding the preparation of $Cu_{2-x}S$ nanocrystals and the regulation of photothermal properties, and provides a useful reference for the development and optimization of $Cu_{2-x}S$ photothermal materials.

A06-P11

Highly selective electrocatalytic alkynol semi-hydrogenation over PdCu bimetallic catalyst supported on nickel foam substrate

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Selective hydrogenation plays a crucial role in the chemical industry with widespread applications. Typically, the selective hydrogenation of alkynols to produce corresponding alkenols serves as a vital intermediate in the production processes of pharmaceuticals such as Vitamin A and fragrances. However, traditional thermal catalytic synthesis methods predominantly operate under harsh conditions of high temperature and pressure, inevitably leading to significant energy consumption and environmental pollution. Pd-based catalysts are commonly ued in these processes; nevertheless, Pd single metal interface not only facilitates the formation of alkenols but also promotes over-hydrogenation by-products, thus posing challenges in achieving both high activity and selectivity simultaneously. Herein, we report a wet-impregnation method to prepare a palladium-copper bimetallic catalyst supported on nickel foam substrate for electrocatalytic semi-hydrogenation of alkynols. For the representative substrate of 1,4-butynediol(BYD), the catalyst exhibits excellent BYD conversion (above 99%) and 1,4-butenediol (BED) selectivity (approximately 94%), achieving nearly complete conversion of 20 mM substrate within 1 hour, with the highest Faradaic efficiency reaching 90.27% at -1.10 V vs. Hg/HgO. In-situ spectroscopic and theoretical computational studies indicate enhanced semi-hydrogenation performance due to exothermic alkynol adsorption and alkenol desorption on the PdCu(111) surface. Furthermore, this electrocatalytic semi-hydrogenation strategy is also applicable to various other alkynol substrates.

A06-P12

Construct the photothermal surface of carbon fiber by metal ions etching and their photothermal properties

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As easily accessible renewable and clean energy, solar energy can directly provide thermal energy for human life or production through the photothermal conversion process, that is supplementary energy to enrich the applications of energy structure and alleviate energy shortage. Carbon fiber is a kind of important material for photothermal conversion, which has wide source of raw materials and low cost. However, the flat surface structure of carbon fiber is not conducive to the light absorption and photothermal conversion process, that limits the further improvement of its photothermal conversion performance. Herein, we used Fe to etch the surface of carbon fiber by high temperature, which increased the surface roughness of carbon fiber and formed the surface light trapping structure with efficient light absorption properties. The light absorption rate of the photothermal material in the range of 300-2500 nm is as high as 93% to 98%. Under the light intensity of 4.84kW m^{-2}, the average surface temperature can reach to 178℃, showing the good photothermal conversion performance. We applied the surface structure to photothermal water evaporation, the rate is measured 6.15 kg m^{-2} h^{-1}. This paper provides a simple and universal method to construct the surface trapping structure of carbon-based photothermal materials, which provides a useful reference for the research and development of high-performance carbon-based photothermal materials.

A06-P13

A polyaniline-modified electrode surface for enhancing electrochemical performance

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The structure and properties of electrode surfaces are important for electrocatalysis due to the molecular absorption and mass transport. Therefore, modifying the electrode surface is an effective strategy to improve the performance of some electrocatalytic reactions. Based on the good chemical stability, easy preparation and regulation of conductive polymer, it is possible to modify the electrode surface with conductive polymer to enhance the electrochemical performance of the electrode. Polyaniline was prepared by in-situ polymerization on carbon paper by electrochemical method to modify the surface of the electrode, and the electrocatalytic performance of the electrode was improved by adjusting the parameters of the synthetic polyaniline. The results showed that the growth morphology and dispersion of the electrocatalyst (Pt) were different due to the different thickness of polyaniline with different structure on the electrode surface, and the electrocatalytic performance of hydrogen evolution and ethanol oxidation was also significantly different. The polyaniline modified electrode with a certain thickness has good electrocatalytic performance because of its good hydrophilicity, well-dispersed electrocatalyst and large electrochemical active area.

A06-P14

Synergistic effects of reactive oxygen species in photothermocatalytic VOCs oxidation over Pt/CeO_2/TiO_2

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Cooking oil fumes are similar to cigarette smoke, which contain a large number of carcinogens, which possess a strong potential threat to human health. It has been shown that the long-term exposure to cooking oil fumes can give rise to autonomic dysfunction and increased risk of DNA damage in restaurant cooks. The volatile organic compounds (VOCs) from cooking oil fumes are very complex and do harm to human and environment. Herein, we develop the high-efficiency and energy-saving synergistic photothermocatalytic oxidation approach to eliminate the mixture of heptane and hexanal, the representative VOCs with high concentrations in cooking oil fumes. The Pt/CeO_2/TiO_2 catalyst with nano-sized Pt particles was prepared by the simple hydrothermal and impregnation methods, and physicochemical properties of the catalyst were measured using numerous techniques. The Pt/CeO_2/TiO_2 catalyst eliminated the VOCs mixture at low light intensity (100 mW cm^{-2}) and low temperature (200 ℃). In addition, it showed 25-h catalytic stability and water resistance (water concentration up to 20 vol%) at 140 or 190 ℃. As reported in the previous studies, water vapor and VOCs were competitively adsorbed on the surface of catalysts, thus decreasing catalytic activity. In the present work, the Pt/CeO_2/TiO_2 catalyst possessed excellent water resistance, and even showed a surprising increase in VOCs conversion when water vapor was added. This result demonstrates that the Pt/CeO_2/TiO_2 catalyst possessed practical application value in the photothermocatalytic elimination of VOCs derived from cooking oil fumes.It is concluded that O_2 picked up the electrons from Pt to generate the $\cdot O^{2-}$ species, which were transformed to the O_2^{2-} and O^- species after the rise in temperature. In the presence of water, the ·OH species induced by light irradiation on the catalyst surface and the ·OOH species formed via the thermal reaction were both supplementary oxygen species for VOCs oxidation. The synergistic interaction of photo- and thermocatalysis was generated by the reactive oxygen species.

A06-P15

Mechanistic Investigation into Single-Electron Oxidative Addition of Single-Atom Cu(I)-N_4 Site: Revealing the Cu(I)−Cu(II)−Cu(I) Catalytic Cycle in Photochemical Hydrophosphinylation

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Transition metal catalysis strategy has been widely used in organic synthesis, and has achieved remarkable achievements for medicine, materials, energy and so on. Because the homogeneous catalyst is difficult to separate and recover from the reaction system, which leads to the problem of metal residue and high cost. The construction of heterogeneous catalysts is expected to solve the above problems, but compared with homogeneous catalysts with clear coordination structures, the active center of heterogeneous systems is often difficult to determine, resulting in more challenging mechanism research, which in turn affects reaction design and optimization. Single-atom catalysts can modify isolated active metal atom (or ion) sites on the carrier, providing an ideal platform for revealing the structure-activity relationship at the atomic level.

In this paper, a mild light-induced ligand exchange (PILE) strategy has been developed to construct a Cu-N_4 monoatomic site on carbon nitride carrier. A new Cu(I)-Cu(II)-Cu(I) catalyzed cycle by single-electron oxidation addition process has been demonstrated, which can significantly reduce the high energy barrier while being compatible with alkenes and alkynes. In addition, under light irradiation, the single atom catalyzed hydrophosphinylation reaction have considerable activity with a 1507 h^{-1} TOF . This work will provide new insights into the interactions between single-atom active sites and substrates and help design entirely new reaction modes that differ from homogeneous catalysis.

A06-P16

Regulating the d-band center of Pd based two-dimensional high entropy metalloenes to promote oxygen reduction performance

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Modifying the electronic structure of the central element to regulate the d-band center can optimize the adsorption energy of reaction intermediates and better match with electrocatalytic reactions. Multi-dimensional material design for alloying, from structural and atomic coordination modification to electronic structure. In this work, 2D Pd based high entropy metalloenes (HENs) were designed for ORR, effectively regulating the electronic structure of Pd, increase the d-band width, and makes the ORR performance of PdFeCoNiMo HENs comparable to pure Pt. In addition, the introduction of Pt leads to a redistribution of electronic structure and a strong coupling effect with Pd, causing the center position of the d-band of Pd to be lower than Pt, which is different from previous reports. Here, as an electrocatalyst for ORR, PtPdFeCoNiMo HENs exhibit higher half wave (0.90 V) and excellent stability than commercial Pt/C in 0.1 M KOH electrolyte, with a mass activity (1.40 A mgPt^{-1}) 21 times higher than Pt/C at 0.9 V (vs RHE). It also exhibits excellent activity and stability in 0.1 M HClO4. The electronic structure and ORR mechanism of PtPdFeCoNiMo HENs were revealed through X-ray adsorption spectroscopy (XAS), in situ spectroscopy, theoretical calculations (DFT).

A06-P17

Electrostatic self–assembly parcel structure MXene/Fe_3O_4 nanorings heterogeneous composites with efficient microwave absorption

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Constructing heterointerfaces through heterogeneous interface engineering is regarded as a significant method to achieve efficient microwave absorption (MA). The absent magnetic loss mechanism and high permittivity of $Ti_3C_2T_x$ MXene result in inferior impedance matching, hindering the further improvement of MA performance. Herein, heterogeneous composites of MXene wrapped Fe_3O_4 nanorings (FNRs) are fabricated successfully using electrostatic self–assembly. The heterostructure provides abundant interfaces, heightening interface polarization and reducing permittivity. Meanwhile, FNRs introduce novel interference loss mechanism based on Aharonov–Bohm effect, along with magnetic loss mechanism, which enhance impedance matching and consequently improve MA performance. With the $Ti_3C_2T_x$:FNRs mass ratio of 3:1, the minimum reflection loss (RL_{min}) reaches −52.55 dB at 2.33 mm; with the mass ratio of 1:1, the optimal effective absorption bandwidth (EAB) of 3.48 GHz is attained at 1.42 mm. This work offers a valuable guideline for heterogeneous interface engineering to improve MA properties of two–dimensional materials.

***Keywords*:** Heterogeneous interface engineering; MXene; Fe_3O_4 nanorings; Electrostatic self–assembly; Microwave absorption performance

A06-P18

Impedance matching refinement of nitrogen-doped $Ti_3C_2T_x$ for augmenting microwave absorption efficiency

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The $Ti_3C_2T_x$, due to its expansive specific surface area, myriad surface functional groups (T_x = -OH, -F, -O), and superior electrical conductivity, demonstrates considerable promise in microwave absorption (MA) applications. Nonetheless, the suboptimal impedance matching curtails further enhancement of its MA efficacy. In pursuit of surmounting this limitation, we have synthesized an innovative nitrogen-doped $Ti_3C_2T_x$ (N-$Ti_3C_2T_x$) via a hydrothermal process. The incorporation of nitrogen augments the intrinsic defects within $Ti_3C_2T_x$, thereby bolstering dipole polarization and refining impedance matching. Notably, at a nitrogen concentration of 3.75 at%, N-$Ti_3C_2T_x$ achieves a minimum reflection loss (RL_{min}) of -26.39 dB and an effective absorption bandwidth (RL<-10 dB) of 3.41 GHz, with a thickness of 1.00 mm, underscoring its exceptional MA capabilities. This investigation propels a novel avenue for devising lightweight, $Ti_3C_2T_x$-based composite materials for absorption purposes.

Keywords: N doping, N-$Ti_3C_2T_x$, Impedance matching, Microwave absorption performance

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A06-P19

基于表面形貌的金及金基多元纳米晶电催化活性研究

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1、引言

本研究中通过区分不同低指数晶面对它们电极电势的贡献，致力于揭示具有和不具有高指数晶面的金纳米晶的化学活性与其表面形貌之间的关系；证明金纳米晶与其他金属离子之间的反置换反应，可以成为一种简便有效的制备高性能金基多元催化材料的方法。

2、材料与方法

首先，制备不同尺寸和形貌的金纳米晶；然后，探究了表面配体组成对金纳米晶电极电势的影响；在此基础上，借助不同尺寸和形貌的金纳米晶电极电势的测试以及它们与钯离子间的反置换反应探究金纳米晶的化学活性与其表面形貌之间的关系；最后，探究了一系列具有反置换反应活性的金及金基多元纳米晶作为氧还原电催化剂的催化性能。

3、 结果与讨论

相对于块体金的电极电势，金纳米晶{111}晶面的缺陷可诱发其电极电势发生明显负移；{100}晶面缺陷可诱发电极电势发生正移；而{110}晶面缺陷引起电极电势发生较小负移;这种反常识的表面晶面对金纳米晶电极电势的差异化影响可进一步演变为随着缺陷型{111}晶面占比的增加，金纳米晶展现高反应活性；通过简单的反置换反应所制备的金@钯纳米晶在碱性介质中也表现出优异的氧还原性能（半波电位高于商业 Pt/C 46 mV）。

4、结论

本研究将不同尺寸和形状的金纳米晶表面晶面定量分解为低指数的{111}、{100}和{110}晶面。通过区分不同低指数晶面对它们电极电势的贡献，致力于揭示具有和不具有高指数晶面的金纳米晶的化学活性与其表面形貌之间的关系，有助于全面理解纳米材料表面形貌对其电极电势的影响。同时该初步结果还可作为一个概念证明，即利用纳米材料的低电极电势与其他金属离子之间的反置换反应，可以成为一种简便有效的制备高性能双金属催化材料方法（无还原剂使用）的方法。

5、致谢

本工作得到了齐鲁工业大学培新基金（2023PX054）和齐鲁工业大学人才科研项目（2023RCKY064、2023RCKY071、2023RCKY061）的支持。

A06-P20

A solution-based oxidation-reduction approach for spontaneous construction of nanowire architectures on copper metals

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Copper (Cu) is a critically important functional material with widespread applications in catalysis, battery technology, and sensing. The oxidation-reduction approach serves as an efficient means to modify Cu metals, enabling the creation of nanowire architectures that expand their specific surface area and facilitate the engineering of catalytic active sites. However, the crucial issue is that the reduction process typically requires high-temperature treatment in an H_2 atmosphere, which is laborious and demanding. Here using the dimethylamine methyl borane ($C_2H_{10}BN$) as an efficient reduction reagent, we report a facile solution-based oxidation-reduction approach at room temperature for the direct formation of the nanowire architectures on commercial Cu foams (CF), resulting in a unique three-dimensional (3D) hierarchically skeleton architecture. Moreover, as a typical application, cobalt hydroxide ($Co(OH)_2$) is electrodeposited on the CF with nanowires (CFNW) to form a CFNW/$Co(OH)_2$ electrode for oxygen evolution reaction (OER). The obtained results indicate the nanowire structure significantly increases the contact area between $Co(OH)_2$ and CFNW substrate, resulting in an outstanding OER performance with an overpotential of 175mV at 10 mA cm^{-2} in 1 M KOH. Importantly, this study presents a straightforward modification approach applicable to Cu metals, enabling large-scale production of advanced 3D skeleton Cu materials with diverse applications.

A06-P21

Electrode switch—an efficient induced approach for selfactivation of electrode toward water splitting

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We provide a novel electrode switch (ES) method to improve the stability of the alkaline electrolyzer toward water splitting. The voltage of the alkaline electrolyzer consisting of commercial Ni mesh electrodes utilizing the ES mode exhibits extreme stability because the highly active Ni oxide(hydroxide) with oxygen defects is in situ formed during the hydrogen evolution reaction (HER) polarization process. Electrolyzer can be seen that during the initial 12 h, the voltage gradually increases from 2.4 V to 2.49 V. As the electrodes are switched, an abrupt fall is observed from 2.49 V to 2.23 V, indicating a significant “self-activation” of these electrodes takes place. Furthermore, the decrease in voltage is not heavily dependent on the period of each ES, and a similar phenomenon is also observed as the cycle period is prolonged to 24 h. More importantly, the overall trend of this voltage is decreasing using the ES mode and the ultimate voltage is 2.19 V after 220 h, which is even smaller than the initial value of 2.4 V. Compared with the stability of the electrolyzer reported recently , the ES mode is indeed a very effective approach to enhance the stability of the alkaline electrolyzer.

A06-P22

Nanomaterial with High Curvature Carbon Embedded Interface Electric Field Boosts Acidic 2e- Oxygen Reduction for Hydrogen Peroxide Production

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In acidic environments, the two-electron oxygen reduction electrosynthesis of hydrogen peroxide (H_2O_2) is an efficient and environmentally friendly method for producing stable H_2O_2. However, it remains challenging to find catalysts with selectivity and stability at industry-relevant current densities. In this paper, we propose a novel single-atom catalyst with a Co-N_4 active site fixed on onion-like nanocurvature carbon carriers ($Co_{SA}NC_C$). Using finite element simulation and density functional theory, we demonstrate the presence of a strong interfacial electric field induced by nanocurvature, which causes the D-band center of Co to shift upward towards the Fermi level, thereby optimizing the adsorption of OOH^* intermediates on the catalyst surface. The experimental results show that the Co single-atom catalyst supported on nanocurvature carbon supports achieves Faraday efficiencies of more than 80% and impressively high H_2O_2 current densities of about 300 mA cm^{-2} in acidic media. In conclusion, our study not only reveals the complex relationship between the interfacial electric field and the D-band center but also suggests a novel strategy promising to improve intermediate adsorption in $2e^-$ ORR processes.

A06-P23

Reversed charge transfer to modulate the d-band center of Pd for efficient direct H_2O_2 synthesis

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The direct synthesis of hydrogen peroxide (H_2O_2) from H_2 and O_2 is a promising alternative pathway to the anthraquinone process because it is environmentally friendly and has a high atom efficiency. Experimental and theoretical studies have proven that optimizing the adsorption energy of the key intermediate OOH* on the active site significantly promotes the further protonation of this intermediate and inhibits dissociation of the O-O bond, thus enhancing the activity and selectivity. Tuning the d-band center of the metal by redistributing the charge density of the active sites can effectively optimize the adsorption energy of intermediates, and thus regulate the catalytic performance. Herein, we show that a Lewis acid ($ZnCl_2$ solution) induces abundant oxygen vacancies (O_{vs}) on the surface of TiO_2, which results in a reversal of charge transfer from TiO_2-O_v to Pd nanoparticles, generating an electron-rich Pd configuration. Compared to pristine Pd/TiO_2, Pd/TiO_2-O_v possesses higher H_2O_2 selectivity and productivity, with values of 80.7% and 186 mol kgcat-1 h-1, respectively. In addition, Pd/TiO_2-O_v maintains its stability even after six consecutive reaction runs due to its high resistance to the leaching of Pd species. Theoretical calculations reveal that the reversed charge transfer causes a downshift of the d-band center of Pd, which increases the ability of this species to activate O_2 on the Pd surface and weakens the adsorption of OOH* intermediates. As a result, the Gibbs free energy for the hydrogenation of the key intermediate OOH* is significantly decreased, and the dissociation of O_2 is inhibited. This work reports a reversal of charge transfer tuning the d-band center of the active site for efficient direct H_2O_2 synthesis, which may provide insight for designing high-performance catalysts.

A06-P24

Artificial Intelligence-Assisted Pulsed Electrolysis for Enhancing Acidic Water Oxidation Reaction towards H_2O_2 Production

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Hydrogen peroxide (H_2O_2), an environmentally friendly and indispensable green chemical. The synthesis of catalysts for the preparation of H_2O_2 in acidic environments poses significant challenges. However, pulse electrolysis, the novel electrolysis strategy, is an excellent approaches to address such issues without changing the catalyst composition. Additionally, Machine learning (ML) can independently uncover the potential correlations between programmable parameters features of pulse electrolysis, without being influenced by subjective human opinions, thereby achieving accurate prediction of electrolysis conditions. Herein, for the first time, we combined pulse electrolysis strategy with acidic WOR to prepare H_2O_2 and explored the potential correlation between programmable pulse electrolysis parameters with the assistance of ML technology, ultimately leading to an improvement of 47 times in H_2O_2 yield, 25.9 times in FE%, compared to constant electrolysis. Based on DFT calculations and experimental verification, it has been proven that the generation of H_2O_2 is caused by the 1e reaction pathway in the water oxidation reaction. This study provides a new research perspective and valuable insights from artificial intelligence to address the pain points in the preparation of H_2O_2 via acidic WOR, while also presenting a precedent of utilizing the1e transfer pathways in electrochemical WOR for H_2O_2 production.

会议论文摘要：

静电纺丝构建铁电/光电纤维异质结及其压电光催化性能研究

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铁电材料能够在外界应力作用下发生极化，形成内建电场，并通过引发一系列氧化还原反应实现原位压电催化性能。极化电场力能够驱动光生电子-空穴对反向迁移，通过抑制载流子复合提升光电转换效应。通过静电纺丝技术构筑铁电/光电复合纳米纤维，调控电偶极子的尺寸和结晶度是提升压电催化性能和压电光催化协同效应的有效方法之一。由单畴结构和高结晶度电偶极子组成的铁电纳米纤维，具有更高的局域压电系数，能够实现高效压电催化性能。通过包覆光电半导体构建核壳纳米纤维，在超声波和紫外光辐射共同激励下，能够表现出较高的压电光催化降解速率常数。具有高压电性的电偶极子能够增强力电耦合效应，抑制光生电子-空穴对复合。静电纺丝纳米纤维异质结具有较高比表面积，能够将压电光催化协同效应的活性反应点位限制在一维边界里，有利于界面载流子迁移，已成为铁电和多铁物理与器件领域的重要方法之一。

Configuration-Dependent Hollow Heterostructures for Highly Efficient Photocatalytic Hydrogen Evolution

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Photocatalytic water splitting systems based on semiconductor heterojunctions show great potential for producing hydrogen fuel from renewable resources. Extensive research has been conducted to improve heterojunctions through methods such as element doping, defect regulation, surface modification, and interface engineering. However, studies on the effects of configuration in heterostructures on photocatalytic performance are still insufficient. Herein, configuration-dependent photocatalytic performances are investigated for graphitic carbon nitride ($g\text{-}C_3N_4$) /anatase titanium dioxide ($A\text{-}TiO_2$) hollow core-shell heterostructures. Two types of hollow core-shell heterostructures are ingeniously synthesized with different configurations namely $g\text{-}C_3N_4/A\text{-}TiO_2$ and $A\text{-}TiO_2/g\text{-}C_3N_4$, where $g\text{-}C_3N_4/A\text{-}TiO_2$ denotes a hollow core-shell heterostructure with $g\text{-}C_3N_4$ shell and $A\text{-}TiO_2$ core. Experimental and theoretical calculations show that $g\text{-}C_3N4/A\text{-}TiO_2$ heterostructures have broader light absorption spectra and stronger photocurrent responses compared to $A\text{-}TiO_2/g\text{-}C_3N_4$. Additionally, $g\text{-}C_3N_4/A\text{-}TiO_2$ features improved carrier transport efficiency and more effective electron-hole separation than $A\text{-}TiO_2/g\text{-}C_3N_4$, highlighting the influence of heterostructural configuration on photocatalytic performance. Therefore, the photocatalytic hydrogen production performance of $g\text{-}C_3N_4/A\text{-}TiO_2$ is 1.4 times higher than that of $A\text{-}TiO_2/g\text{-}C_3N_4$. This study underscores a promising configuration-dependent strategy to design heterostructured photocatalysts for efficient photocatalysis.

高温高真空实时应变获取实验

吕方*
安泰科技

【摘要】通过粉末冶金工艺制造方法生产加工 Nb 基合金检测力学用样板，选用国产高真空高温静态万能试验机 CSS44050 进行抗拉强度试验，实验参数设定位移控制 0.85mm/S,实验温度定为 1250℃、950℃两组。在采用 GNCJ-50 高温蠕变持久试验机以 1250℃进行了挂持 150Kg 砝码,实验时长 14H（50400S）的应变数据取值试验，使用接触式与非接触式光学引伸计两种方法进行取值实验。

连续流超声微反应器剥离 MoS_2 纳米片用于电催化析氢

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氢能是一种绿色清洁能源，有望减少化石燃料大肆使用带来了能源和环境危机。电催化水分解是产生环保氢气的一种很有前途的方法，开发高效稳定的催化剂是影响其工业化进程的一个重要影响因素[1, 2]。最近，具有丰富边缘活性位点和多种相结构的二硫化钼(MoS_2)展现出了不俗的催化能力。然而，块状 MoS_2 的惰性基面和不理想的电导率，使其与铂（Pt）族催化剂仍有一定的差距[3-5]。二维（2D）MoS_2 具有独特的表面效应、小尺寸效应和宏观量子隧道效应. 通常表现出更大的表面积和更高的电子传输速率，并具有大量的边缘和缺陷活性位点，这些特性显著提高了 MoS_2 的催化性能[6]。目前合成少层 MoS_2 的手段主要包括 CVD 法和块状 MoS_2 剥离。然而这些合成手段在大规模生产时，其产量较低。

近年来，微反应器由于其微观尺度特性，具有高的热量和质量传递效率。可以实现反应物的快速均匀混。同时，为满足不同产量需求，微反应器可以实现连续生产，相对容易地扩展和调整规模。相较于批量生产，具有更高的生产率和稳定性[7]。本研究采用新型超声微反应器对块状 MoS_2 进行剥离。协同超声空化和微通道的优势，提高了块状 MoS_2 的剥离效率。首先，将块状 MoS_2 与胆酸钠溶于去离子水中搅拌 10 分钟。然后使用蠕动泵以 5 ml/min 的流速将混合溶液通入超声微反应器中进行剥离。持续 1 小时后，将超声后的混合溶液进行离心洗涤。根据 SEM 的表征结果显示，剥离后的少层 MoS_2 具有 200-300 nm 的横向尺寸。电化学测试结果表明，剥离后的 MoS_2 具有更好的催化活性。在 10 mA cm^{-2} 的电流密度下，其过电位为 281 mV,高于块状 MoS_2（319 mV）。

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Crystalline-Amorphous Interface Coupling of NiSe-NiP/NF by layered electrodeposition as bifunctional catalysts for water splitting

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Developing high-active and low-cost bifunctional materials for catalyzing the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) holds a pivotal role in water splitting. Therefore, we have successfully prepared a crystal-amorphous (c-a) coupled NiSe-NiP electrocatalyst on NF (named NiSe-NiP/NF) by layered electrodeposition (The stirring - electrodeposition strategy was adopted in the first step, the second step without agitation). The coupling interface of the crystalline structure with high conductivity and amorphous structure with numerous potential active sites could regulate the electronic structure and optimize the adsorption/desorption of O-containing species. Additionally, sample characterization before and after the OER stability test of NiSe-NiP/NF by Raman spectroscopy confirmed that the active site was NiOOH. Benefiting from these properties, NiSe-NiP/NF required low overpotentials of only 265 mV and 106 mV at 10 mA cm^{-2} to drive the OER and HER in 1 M KOH solutions, respectively, and the NiSe-NiP/NF electrode required a 1.59 V cell voltage to deliver 10 mA cm^{-2} in a two-electrode electrolysis system to catalyze stable water splitting for more than 70 h. This study provides inspiration for other energy conversion reactions in optimizing the performance of catalysts by coupling crystalline-amorphous structures.

Boron-chelated N-methylglucamine on Copper Surface for Boosting CO_2 Electrocatalytic Conversion to Ethylene

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Electrochemical reduction of carbon dioxide (CO_2) to ethylene is a more promising technique compared to conventional industrial processes because of its environmentally beneficial technological merits. However, because there are so many potential reaction pathways, enhancing high selectivity for specific multi-carbon products continues to be extremely difficult. In this work, we establish a semi-metal element doped CuO nanoelectrode in an alkaline electrolyte with the additive N-Methyl-D-glucamine (NMG), which effectuates ethylene activity beyond a Faradaic efficiency of 74%. Our on-site studies reveal that the copper surface with boron-chelated NMG promotes CO_2 transfer and improves *CO coverage. According to a mechanistic analysis, the asymmetrical C–C coupling between *CO and *CHO provides more evidence that the strong proton coupling ability and favorable electron and proton transfer are what cause the far higher selectivity of ethylene. This study offers profound insights into the process of CO_2 to ethylene conversion in addition to an efficient method for designing and building electrolyte microenvironments for highly selective CO_2 to ethylene conversion.

RuCu/B_4C catalyst for promoting electrocatalytic conversion of nitrate to ammonia

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Electrocatalytic reduction of nitrate synthesis of ammonia as a new green environmental protection method, is expected to replace the Haber-Bosch process to synthesize high value-added ammonia. RuCu had a high performance on nitrate reduction because of the high activity of Ru on nitrate reduction and the inhibition of hydrogen evolution by Cu. Hence, constructing RuCu hollow nanoparticles is a possible way to obtain a high atomic utilization, and the interface or porous structure would bring high activity on electrocatalysis. Herein, RuCu hollow nanoparticles were prepared by a hydrothermal reaction and then loaded on a B_4C substrate to construct the RuCu/B_4C catalysts that exhibited high activity on nitrate reduction reaction (NO_3RR) to produce ammonia. The results showed that the synergistic effect between B_4C and RuCu in the catalyst promoted their performance. In detail, RuCu nanoparticles with hollow structures served as the main active centers to transform NO_3^- into NH_3, cooperating with the enhancement of NO_3^- adsorption by the support B_4C. Therefore, RuCu/B_4C synergistically achieved the high yield performance of ammonia.