举足左右，便有“氢”重·第九届全国氢能博士生学术论坛

会议手册及论文摘要集

主办单位：中国科学技术协会
中国可再生能源学会
中国能源研究会
湖北省科学技术协会
武汉市科学技术协会
武汉东湖新技术开发区管理委员会
承办单位：武汉新能源研究院
协办单位：国际铜业协会、中国国际工程咨询有限公司
华中科技大学、武汉理工大学
湖北省新能源发展促进会
湖北省环境科学学会等
时　　间：2021年9月25日-26日

中国·武汉

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会议组织委员会

会议主席：

杨珍珍（武汉理工大学）

副主席：

官树猛（武汉理工大学）

会议秘书长：

张　慧（武汉理工大学）

组织委员会（排名不分前后）

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黄鹏涛（武汉理工大学）
王　毅（武汉理工大学）
刘艺灏（武汉理工大学）
姜攀星（武汉理工大学）
吴　凡（武汉理工大学）
夏　蕾（武汉理工大学）
姚志鹏（武汉理工大学）
时贞勃（武汉理工大学）
黄　蕾（武汉理工大学）
陶嘉逸（武汉理工大学）
刘珍斌（武汉理工大学）
王　爽（武汉理工大学）
罗　昇（武汉理工大学）
刘明俊（武汉理工大学）

学术指导委员会（排名不分前后）

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李宝山 副理事长（中国可再生能源学会）
梁　媛 副秘书长（中国可再生能源学会）
王树茂 秘书长　（中国可再生能源学会氢能专业委员会）
谭金婷 老师　（武汉理工大学）
郭烈锦 教授（西安交通大学）
董丽杰 教授（武汉理工大学）
肖生强 教授（武汉理工大学）
潘　牧 教授（武汉理工大学）
周　芬 老师（武汉理工大学）

鸣谢

潘　牧 教授 （武汉理工大学）
董丽杰 教授 （武汉理工大学）
谭金婷 老师 （武汉理工大学）
周　芬 老师 （武汉理工大学）

前言

氢具有能量密度高、资源丰富、可清洁利用等特点，被视为本世纪最具有发展潜力的新型二次能源。氢能的产业化应用主要包括氢气的制取、储运、利用等环节，如何实现氢气的低成本制取，安全运输以及高效利用是实现氢能大规模应用的关键。

第九届全国氢能博士学术论坛由中国可再生能源学会氢能专业委员会和武汉理工大学主办，并由燃料电池湖北省重点实验室博士研究生组织。本届学术论坛定于2021年9月25日 - 9月26日在武汉东湖国际会议中心举办。论坛将以碳达峰、碳中和为发展目标，就氢气的制取、储存与应用等研究领域的新思维、新方法和新成果进行广泛的交流与研讨，为从事氢能研究的青年才俊提供学习交流平台。

根据会议日程，本届论坛安排了特邀专家学术讲座。口头汇报和墙报展示，并设评优秀口头报告奖和优秀墙报展示奖，以表彰研究水平突出、展示内容丰富、现场讲解清晰的报告（墙报）作者。

在筹办论坛过程中，许多同学在会议论文集的整理和编辑方面做了大量工作，但难免存在疏漏和不当之处，还请各位同学指正并提出宝贵意见。

最后，谨向所有关注和支持本届会议的各级单位和各界人士表示衷心感谢！祝本届全国氢能博士生学术论坛圆满成功。

举足左右，便有“氢”重

第九届全国氢能博士生学术论坛组员会

2021年9月于武汉理工大学

会议须知

为了确保您和他人在会议期间的健康、安全与环保，请您注意以下有关事项：

1. 大会期间，请大家带好口罩，勤洗手，注意间距，做好疫情防护。
2. 请不要携带易爆危险物品进入会场，请自行保管好贵重物品。
3. 会议期间，请您随身佩戴参会代表证，参会代表证用于出入会场及会议期间的自主餐厅。
4. 报告期间，请保持会场整洁、安静，请将手机调至振动或安静状态。
5. 墙报交流期间，保持会场卫生，作会前准备。
6. 请报告者及主持人提前15分钟到达会场，作会前准备。
7. 请严格控制报告发言时间（15分钟），提问时间为5分钟。线上无提问环节，有需要交流可以和会务组联系，会务组会提供联系方式。
8. 墙报展示于9月25日上午张贴至指定地点，9月26日会议结束后撤回。墙报交流时，请作者站立于墙报前讲解、自由交流讨论。
9. 本次会议设有5个优秀口头汇报奖和5个优秀墙报奖。
10. 会议期间的集体活动（合影、晚宴、参观等），请听从工作人员的安排。
11. 会议相关资料（论文摘要集）将统一上传至***举足左右，便有“氢”重***微信群。
12. 大会期间联系人：

    东湖宾馆会场联系人：刘珍斌（13647204228），王爽（18571593196）
    东湖宾馆报到联系人：黄鹏涛（18790887062），姚志鹏（15971447244）
    武汉理工大学报到联系人：夏蕾（13260507996），王毅（17362949744）

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第九届全国氢能博士生学术论坛口头报告程序表

会议时间	9月25-26日			
报到时间	9月24日 12:00-19:00			
报到地点	① 武汉东湖宾馆东湖国际会议中心 ② 武汉理工大学新材所润章楼六楼			
9月25日上午				
9:00-9:50	2021中国“双碳”高峰论坛开幕式（东湖宾馆会议中心黄鹤厅）			
9:50-10:00	发布《“3060”中国光谷宣言》			
10:00-10:15	签约仪式			
10:30-12:30	主旨演讲			
12:30-13:30	午餐（东湖宾馆黄鹂厅）			
9月25日下午（东湖宾馆会议中心武汉厅）				主持人
氢能博士论坛开幕式				杨珍珍
13:30-13:35	中国可再生能源学会副理事长李宝山致辞			
13:35-13:40	武汉理工大学研究生院副院长董丽杰致辞			
13:40-14:10	**低成本高安全氢能储运技术初探**	**蒋利军**	**特邀专家报告**	
14:10-14:40	**燃料电池膜电极研发进展**	**潘牧**	**特邀专家报告**	
14:40-15:00	参会代表合照			

15:00-15:20	M-MO$_x$ (M=Ni, Co)复合催化剂的制备及其催化硼烷氨络合物水解制氢性能研究	何佳桓	浙江大学	尧兢
15:20-15:40	金属氢化物介导的水分解：节约电能及氢气氧气解耦产生	靳汝湄	北京大学	
15:40-16:00	锂激发钒氧化物对镁基储氢材料催化活性	臧佳贺	复旦大学	
16:00-16:20	氧化镨与氧化钛协同催化氢化铝放氢研究	梁龙	中科院长春应用化学研究所	
16:20-16:40	墙报交流			
16:40-17:00	镁纳米晶储氢体系吸放氢动力学性能的改性研究	章浩宇	江苏科技大学	康辉
17:00-17:20	用于静态氢压缩装置的 Ti-Zr-Cr-Fe-V 基合金研究	曹子鸣	浙江大学	
17:20-17:40	氢转移动力学增强的有机液体可逆储氢	谢泽威	北京大学	
17:40-18:00	基于固态储氢的氢燃料电池动力系统热量管理和集成研究	尧兢	西安交通大学	
18:00-19:00	晚餐（东湖宾馆黄鹂厅）			
9月26日上午（东湖宾馆会议中心武汉厅）				主持人
8:00-8:20	适用于高密度储氢装置的 Ti-Zr-Mn-Cr-V 基合金的研究	周盼盼	浙江大学	朱鹏飞
8:20-8:40	不同相结构的钴 (FCC/HCP)对 MgH$_2$ 储氢催化性能的影响	俞海杰	江苏科技大学	
8:40 -9:00	催化层孔径优化对质子交换膜燃料电池氧传输阻力机理的研究	官树猛	武汉理工大学	
9:00-9:20	不同流场下阴极开放式质子交换膜燃料电池工作特性研究	王梓轩	天津大学	
9:20-9:40	质子交换膜燃料电池催化层纳米尺度氧气传输机理	樊林浩	天津大学	
9:40-10:00	Cu 掺杂对中温固体氧化物燃料电池 PrBa$_{0.5}$Sr$_{0.5}$Co$_{2-x}$Cu$_x$O$_3$ 阴极性能的研究	贾伟华	西北大学	
10:00-12:00	**参观武汉“两神山”建设纪实展** **（大巴车接送，车牌号：鄂 ALV703 和鄂 ALV660）**			
12:00-13:30	午餐休息（未来科技城全派自助餐厅）			

9月26日下午（东湖宾馆会议中心武汉厅）				主持人
14:00-14:20	低温环境下 PEMFC 中水的行为特征与启动研究	姜攀星	武汉理工大学	吴凡
14:20-14:40	以生物质为燃料的 SOFC 模拟及系统应用研究	朱鹏飞	西安交通大学	
14:40-15:00	墙报交流			
线上参会汇报专场				
15:15-15:30	Ni_3Fe/rGO 对 MgH_2 储氢性能的协同效应	刘江川	南京工业大学	姜攀星
15:30-15:45	提升燃料电池最大功率密度 48%的液滴动力学理论和微流场实验验证	张若凡	同济大学	
15:45-16:00	机器学习参与高性能燃料电池膜电极组件的设计	丁睿	南京大学	
16:00-16:15	空气暴露对 Ni 催化的 Mg-Al 基氢化物的影响	李淑婧	南京工业大学	
16:15-16:45	闭幕颁奖（颁奖人：田明星总经理，武汉理工氢电科技有限公司）			谭金婷

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第九届全国氢能博士生学术论坛墙报展示程序表

编号	姓名	单位	论文题目
1	唐美华	武汉大学	质子交换膜燃料电池低铂电极的极化行为研究
2	廖宇翔	武汉大学	具有高性能氧还原反应催化活性的 PtNi$_x$Cu$_{3-x}$ 纳米催化剂
3	库尔邦尼沙·卡德尔	北京大学	针对便携式燃料电池的块体海绵硼氢化钠水解制氢催化剂
	林友宇	北京大学	
4	马天明	武汉理工大学	氢气长管拖车泄露事故后果模拟研究
5	李毅	武汉理工大学	多孔泡沫铜对大长径比管道中氢-空气预混气体燃爆特性的影响
6	程长山	江苏科技大学	通过 TiFe 和碳纳米管的作用实现 MgH$_2$ 的优异储氢性能
7	曾子龙	西安交通大学	Photocatalytic hydrogen production versus photocatalyst dimension under concentrated solar light: a case over titanium dioxide
8	任莉	上海交通大学	MOF 衍生的一维多空碳纤维纳米限域氢化镁及吸放氢机理研究
9	李映辉	上海交通大学	中空 ZIF-67@ZIF-8 核壳结构衍生物对 MgH$_2$ 储氢性能的改性研究
10	张瑞宇	北京理工大学	考虑碳沉积效应的阳极支撑合成气燃料电池基本反应动力学模型
11	童欣	北京理工大学	无人机固体氧化物燃料电池推进系统的尺寸设计与仿真
12	李晓晓	北京理工大学	阳极厚度对直接 NH3 固体氧化物燃料电池性能影响探究
13	吴凡	武汉理工大学	燃料电池用超薄非标密封材料压缩率的研究
14	杨珍珍	武汉理工大学	燃料电池金属双极板极端状况下的电化学腐蚀
15	罗夏爽	上海交通大学	热处理制备双壳层 Pt-Ni 合金催化剂用于质子交换膜燃料电池
16	安璐	上海交通大学	一种去合金化的高活性 RuNiO$_x$ 酸性电解水催化剂
17	尚娟	浙江大学	掺氢天然气对低碳钢氢脆增强作用研究
18	李勇	天津大学	基于压力波和中间产物对氢气内燃机爆震机理的研究
19	付振	天津大学	掺氢体积分数对 GDI 发动机燃烧性能的影响
20	高朵朵	武汉理工大学	富硒无定形 NiSe$_{1+x}$ 助剂增强光催化制氢性能与机理研究
21	钟威	武汉理工大学	表面原位硒化构建新型核壳 Ag@AgSe$_x$ 纳米粒子实现高效光催化产氢
22	孟凯	武汉理工大学	Dynamic current cycles effect on the degradation characteristic of a H$_2$/O$_2$proton exchange membrane fuel cell

23	周浩然	武汉理工大学	闭口质子交换膜燃料电池性能研究
24	张继伟	武汉理工大学	不同装配扭矩下 PEM 燃料电池性能实验研究
25	张焱	江苏科技大学	$Zr_{0.4}Ti_{0.6}Co$ 纳米片与碳纳米管协同催化增强 MgH_2 储氢性能
26	宋孟臣	江苏科技大学	金属有机骨架负载的 Ni_2O_5 纳米颗粒对 MgH_2 的储氢性能具有高效的催化作用
27	赵颖燕	南京工业大学	核壳结构 NiCu@C 对 MgH_2 储氢性能的催化改性

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M-MO$_x$ (M=Ni, Co)复合催化剂的制备及其催化硼烷氨络合物水解制氢性能研究

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摘要：硼烷氨络合物水解被认为是一种安全有效的制氢方法，但未能开发出经济、稳定且高活性的催化剂限制了硼烷氨络合物的进一步工业化应用。在此，利用一维立方棒 $MMoO_4$ (M=Ni, Co) 水合物前驱体，制备得到一维多孔 MoO$_x$ 纳米棒负载的 Ni/NiO 纳米异质结和具有多维度结构自支撑的 Co@$Co_2Mo_3O_8$ 复合催化剂。以 $NiMoO_4$ 为前驱体的 Ni/NiO@MoO$_x$ 性能更为优异，具有最佳 Ni/NiO 重量比（73.96/26.04）的 Ni/NiO@MoO$_x$ 对催化硼烷氨络合物水解表现出最优异的催化活性，在 25 °C 下其转换频率高达 86.29 $\mathrm{mol_{H_2}mol_{Ni}^{-1}min^{-1}}$，放氢速率达到 $10478\ \mathrm{mL\cdot min^{-1}g^{-1}}$（$35947\ \mathrm{mL\cdot min^{-1}g_{Ni}^{-1}}$），这几乎超过大部分非贵金属基和贵金属基催化剂的放氢速率和转换频率。这种 NiO 稳定连接 Ni 和 MoO$_x$ 载体的桥接效应增强了 Ni/NiO 催化剂的耐久性，其催化活性在五次循环中没有显著下降。

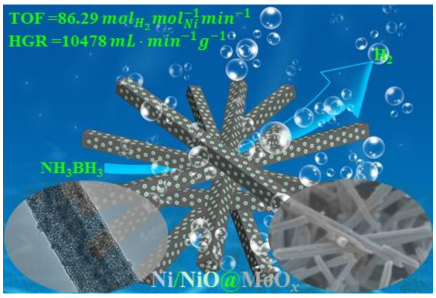

图 1 Ni/NiO@MoO$_x$ 催化硼烷氨络合物水解制氢示意图

Fig. 1 Schematic diagram of the hydrolysis of ammonia borane catalyzed by Ni/NiO@MoO$_x$

关键词：水解制氢；硼烷氨络合物；桥接效应；Ni/NiO 异质结；自支撑 Co@$Co_2Mo_3O_8$

The fabrication of M-MO$_x$ (M=Ni, Co) composite catalysts and their performance in the hydrolysis of ammonia borane

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Abstract: The hydrolysis of ammonia borane is considered as a safe and efficient method of hydrogen generation. However, the failure to development of inexpensive, stable, and high-performance catalysts impedes its the further industrial application. Here in, Ni/NiO nanoparticles on 1D porous MoO$_x$ nanorods and multidimensional mutual-supported Co nanoparticles on 2D $Co_2Mo_3O_8$ nanosheets are fabricated from 1D $MMoO_4$ (M=Ni, Co) hydrate as the precursor. The performance of Ni/NiO@MoO$_x$ with $NiMoO_4$ as the precursor is much better, and Ni/NiO@MoO$_x$ catalyst with an optimal Ni/NiO weight ratio (73.96/26.04) exhibits an excellent catalytic activity for the hydrolysis of ammonia borane (TOF=86.29 $\mathrm{mol_{H_2}mol_{Ni}^{-1}min^{-1}}$, $10478\ \mathrm{mL\cdot min^{-1}g^{-1}}$, $35947\ \mathrm{mL\cdot min^{-1}g_{Ni}^{-1}}$) at 25 °C, overtaking most values both in noble and non-noble metal catalysts for the hydrolysis of ammonia borane. The bridging effect of NiO steadily connected Ni and MoO$_x$ carrier promotes the great durability of Ni/NiO@MoO$_x$-50H, of which catalytic activity exhibits not significant degradation in the fifth cycle.

金属氢化物介导的水分解：节约电能及氢气氧气解耦产生

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摘要：利用金属氢化物（MH）可逆氢吸放氢的基本性质，我们研究了一个创新性的水分解过程。水首先在金属氢化物电极上还原生成的氢原子被金属氢化物自发的吸收，这个过程在热力学上比直接生成氢气更有利，并且在动力学上可在比可逆氢电位更正的电位上发生。之后在温和的温度（~70℃）下，金属氢化物吸收的氢可以释放出来生成氢气。在镀钯的氢化钇薄膜电极上，与理想的析氢催化剂相比，使用低品位热电能可实现高达 25kJ 每物质的量的氢气的节能。金属氢化物介导的水分解也会自动导致解耦的氢气和氧气生成，可以通过使用由镀钯的 $LaNi_{4.5}Al_{0.5}$ 粉末组成的电极来证明。金属氢化物介导的水分解结合了两种经典的储氢应用：镍氢电池的电化学吸氢和气相储氢的热脱氢，为传统金属氢化物研究开辟了一个诱人的新应用领域。

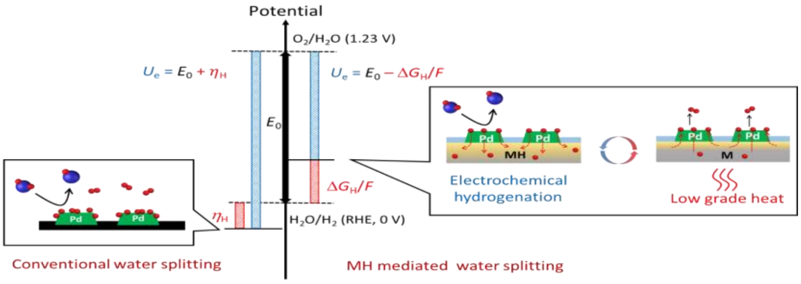

图 1 传统电解水制氢及金属氢化物介导的水分解机理及热力学示意图

Fig. 1 The mechanisms and thermodynamics of H_2 generation from conventional and metal hydride (MH) mediated water splitting.

关键词：水分解；金属氢化物；制氢；储氢；电催化

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Metal Hydride Mediated Water Splitting: Electrical Energy Saving and Decoupled H_2/O_2 Generation

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Abstract: Reversible hydrogen absorption/desorption, the very fundamental property of metal hydrides (MH), can be utilized to innovate the water splitting process. On an MH electrode, the H generated from water reduction is spontaneously absorbed by MH, which is thermodynamically more favorable compared to direct H_2 formation and can be achieved above the reversible hydrogen electrode potential. The absorbed hydrogen can be released to give H_2 at mild temperature (~70℃) using low grade heat Electrical energy saving up to 25 kJ (mol H_2)$^{-1}$ compared to an ideal hydrogen evolution catalyst can be achieved on a Pd coated yttrium hydride thin film electrode. The MH mediated water splitting also automatically leads to decoupled H_2/O_2 generation, which is demonstrated by using an electrode composed of Pd coated $LaNi_{4.5}Al_{0.5}$ powder. The MH mediated water splitting combines two classical hydrogen storage applications: electrochemical hydrogen absorption in Ni-MH batteries and thermal dehydrogenation in gas phase hydrogen storage, which opens an appealing new application field for conventional MHs.

锂激发钒氧化物对镁基储氢材料催化活性

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摘要：镁具有较高的理论储氢容量（7.6 wt%），是一种理想的储氢材料。然而，由于 MgH_2 固有的热力学稳定性和迟滞的动力学性能，制约了 MgH_2 在车载储氢方面的实际应用。本研究使用富锂钒基氧化物 Li_3VO_4 为催化剂，显著提升了 MgH_2 的储氢性能，使其初始脱氢温度降低了 100 ℃左右，并能在近室温下迅速达到饱和吸氢状态。Li_3VO_4 对 MgH_2 的催化机理得到了深入的探讨，碱金属 Li 的存在可以激发过渡金属 V 的催化活性，同时抑制了 O 的活性，从而避免了 Li_3VO_4 与 MgH_2 反应分解，抑制了 MgO 的产生并保持了高价 V 的催化活性。这一发现为其他富锂过渡金属氧化物作为催化剂的研究提供了一定的理论指导。

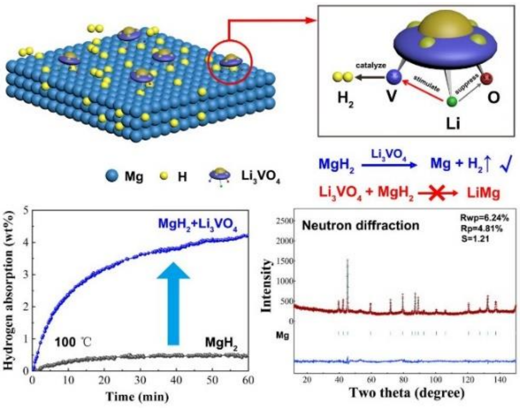

图 1 Li_3VO_4 催化 MgH_2 储氢机理示意图

Fig. 1 Schematic diagram of the hydrogen storage mechanism of MgH_2 catalyzed by Li_3VO_4

关键词：储氢；氢化镁；Li_3VO_4；催化机理；中子衍射

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Lithium triggers the gas-solid catalytic reaction of vanadium oxide on magnesium based hydrogen storage materials

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Abstract: Magnesium-based hydrides are promising hydrogen storage materials, however, little progress has been achieved in improving hydrogen storage performance under ambient condition, consequently impeding further commercial application. Herein, lithium rich transition metal, Li_3VO_4 has been employed to catalyze the hydrogen storage reaction of magnesium-based hydrides, enabling a fast and full hydrogenation of Mg at lower temperature. The structural stability of Li_3VO_4 upon de/rehydrogenation reaction has been confirmed by neutron diffraction and transmission electron microscope observations. The synergistic catalytic role of Li_3VO_4 has been elucidated as the existence of Li stimulates the catalytic activity of V, and simultaneously suppresses the activity of O. V is the key catalytic active site, while O can react with active Mg to generate MgO which is a passivation layer and could prevent the diffusion of H. These findings will give an opportunity to other lithium rich transition metals in the field of catalyzing hydrogen storage systems.

氧化镨与氧化钛协同催化氢化铝放氢研究

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摘要：氢化铝由于高的储氢量 (10 wt.%) 和低的放氢温度 (150-180°C) 被认为是一种极有前景的储氢材料。进一步通过化学方法优化氢化铝放氢反应是其面向应用的关键一步。本工作通过球磨将氧化镨与氧化钛作为添加剂与氢化铝混合，研究复合材料的放氢性能。结果表明，两种氧化物协同催化性能优于单独催化，初始放氢温度为 50°C, 放氢动力学极大改善。根据表征结果提出了多电子对促进放氢的机理。建立了异质结模型对协同催化作用进行了理论分析。

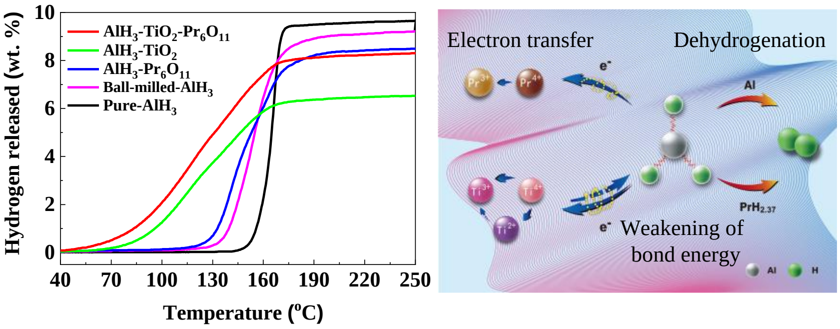

图 1 程序升温放氢和相关机理

Fig. 1 Temperature programmed hydrogen release and the related mechanism

关键词: 轻金属氢化物；氢化铝；放氢反应；协同催化

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Study on the Synergistic Catalytic Desorption of Hydrogen from Aluminum Hydride by praseodymium oxide and Titanium Oxide

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Abstract: Aluminum hydride is considered a very promising hydrogen storage material due to its high hydrogen storage capacity (10 wt.%) and low hydrogen desorption temperature (150-180 ℃). Further optimization of the hydrogen release reaction of aluminum hydride through chemical methods is a key step for its application. In this work, praseodymium oxide and titanium oxide were mixed with aluminum hydride as additives through ball milling to study the hydrogen desorption properties of composite material. The results show that the synergistic catalytic performance of the two oxides is better than that of catalysis alone. The initial hydrogen release temperature is 50℃, and the hydrogen release kinetics is greatly improved. According to the characterization results, the mechanism of multi-electron pairs promoting hydrogen release is proposed. A heterojunction model was established to conduct a theoretical analysis of the synergistic catalysis.

镁纳米晶储氢体系吸放氢动力学性能的改性研究

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摘要：采用湿化学球磨法分别在 20、30 和 40h 的时间内成功地合成了不同碳层的纳米晶镁，根据 Scherrer 公式和 X 射线衍射结果，三种样品的平均晶粒尺寸均小于 30nm。TEM 观察表明，氢化镁颗粒被碳层覆盖。此外，40 小时球磨的镁样品表现出优异的储氢性能尤其是在吸氢方面。制备的样品在接近室温时开始吸氢，并最终在 200℃时吸收 6.8 wt%的氢。样品吸氢的表观活化能（Ea）降低至 26.7 kJ/mol，远低于其他报告的系统。对于脱氢实验，氢化样品在大约 275℃时开始释放氢气，并且在 325℃时在 20 分钟内解吸 6.5 wt%的氢气。有趣的是，制备的样品显示出值得注意的空气稳定性。在空气中放置 60 分钟后，三个样品的脱氢动力学和氢容量基本保持不变，使其有可能用于未来的商业应用。

关键词：储氢；纳米晶镁；碳层；空气稳定性

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Remarkably improved hydrogen storage properties of carbon layers covered nanocrystalline Mg with certain air stability

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Abstract： Different nanocrystalline magnesium with carbon layers were successfully synthesized via a facile wet-chemical ball milling method for 20, 30 and 40 h, respectively. Based on Scherrer formula and X-ray diffraction results, the average crystallite size of all the three samples was below 30nm.TEM observations showed that the hydrogenated Mg particles were covered with carbon layers. Moreover, the 40 h ball milled Mg sample showed outstanding hydrogen storage performance especially in the aspect of hydrogen absorption. The as-prepared sample started to take up hydrogen at nearly room temperature and eventually absorbed 6.8 wt% hydrogen at 200℃. The apparent activation energy (Ea) of hydrogen absorption for the sample was decreased to 26.7 kJ/mol, much lower than that of other reported systems. For the dehydrogenation experiments, the hydrogenated sample could start to release hydrogen at about 275℃ and 6.5 wt% hydrogen was desorbed in 20 min at 325℃.Interestingly, the prepared samples showed noteworthy air stability. Been placed in the air for 60 min, the dehydrogenation kinetics and hydrogen capacity of the three samples were basically unchanged, making it possible to be used in future commercial applications.

$NiTiO_3/TiO_2$对纳米晶 Mg 储氢性能的增强催化作用

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摘要：镁作为一种很有前途的储氢材料，其稳定的热力学和缓慢的动力学阻碍了其实际应用。本文成功地合成了三种不同镍钛摩尔比的 $NiTiO_3$ 样品，并将其掺杂到所制备的纳米晶 Mg 中进行催化。研究结果表明，由于 $NiTiO_3$ 和 TiO_2 在复合材料中的共同催化作用，Ni/Ti 摩尔比为 1:1.1 的 Mg+7 wt%NiTiO3/TiO_2 具有显著的储氢性能。与纳米晶 Mg（69.8±1.2kj/mol）相比，样品不仅在室温下开始吸氢，而且吸氢表观活化能显著降低（52%）至 34.2±0.2kj/mol。此外，氢化样品在 193.2℃左右开始释放氢，最终解吸 6.6 wt%的氢。此外，在 20 个循环中，样品显示出极好的循环稳定性，即吸氢和解吸的动力学性质没有发生明显的衰退，只有 0.3 wt%的氢容量减少。总之，我们的发现可能为研究金属间化合物催化剂在企业储氢材料上的催化作用提供参考。

关键词：储氢；$NiTiO_3/TiO_2$；纳米晶镁

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Enhanced corporate catalysis of $NiTiO_3/TiO_2$ on the hydrogen storage properties for nanocrystalline Mg

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Abstract: As a promising hydrogen storage material, the practical application of magnesium is obstructed by the stable thermodynamics and sluggish kinetics. In this paper, the three kinds of $NiTiO_3$ samples with different mole ratio of Ni to Ti were successfully synthesized and doped into the as-prepared nanocrystalline Mg to catalyze it. The investigation results indicated that the Mg+7 wt% $NiTiO_3/TiO_2$ whose molar ratio of Ni to Ti is 1 to 1.1 showed the prominent hydrogen storage performance due to the corporate catalytic effect of $NiTiO_3$ and TiO_2 in the composite. Not only could the sample start to take up hydrogen at room temperature, but also have a dramatic decrease (52%) to 34.2±0.2 kJ/mol of hydrogen absorption apparent activation energy, compared with that of the nanocrystalline Mg (69.8±1.2 kJ/mol). In addition, the hydrogenated sample began to release hydrogen at about 193.2 °C and eventually desorb 6.6 wt% H_2. Besides, during 20 cycles, the sample revealed the splendid cyclic stability that the kinetic properties of hydrogen absorption and desorption occurred no obvious recession and only 0.3 wt% hydrogen capacity reduced. In brief, our finding might provide reference for the investigation of intermetallic catalysts for corporate catalysis on hydrogen storage materials.

用于静态氢压缩装置的 Ti-Zr-Cr-Fe-V 基合金研究

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摘要：本项研究基于水浴温度区间内工作的静态氢压缩装置，使用感应悬浮熔炼法制备了 $Ti_{0.85}Zr_{0.17}Cr_{1.2-x}Fe_{0.8}V_x$ (x = 0，0.1，0.2)、$Ti_{0.85}Zr_{0.17}Cr_{1.2-y}Fe_{0.7+y}V_{0.1}$ (y = 0，0.1，0.25)、 $Ti_{0.87-z}Zr_{0.15+z}Cr_{0.95}Fe_{0.95}V_{0.1}$ (z = 0, 0.02, 0.04)合金样品，并对其晶体结构与储氢性能展开了系统研究。结果表明，本研究中的合金皆具备 C14 型 Laves 相的匀质单相结构。随合金中 V 含量或 Zr 含量增加，Ti-Zr-Cr-Fe-V 基合金的储氢容量增加，但坪台压显著下降，坪台斜率增大。特别地，V 含量的增加促进了 Ti-Zr-Cr-Fe-V 基合金活化动力学性能的提升。随合金中 Fe 含量增加，Ti-Zr-Cr-Fe-V 基合金坪台压上升，坪台斜率减小，但储氢容量下降。从所研究的 Ti-Zr-Cr-Fe-V 基合金中特别筛选出了 $Ti_{0.85}Zr_{0.17}Cr_{0.95}Fe_{0.95}V_{0.1}$ 合金，其能谱扫描结果与等温吸放氢曲线如图 1。该合金在 293 K 下具备 1.52 wt%的储氢容量与 5.62 MPa 的吸氢坪台，在 353 K 下具备 23.01 MPa 的放氢平台。同时该合金吸放氢滞后较小，放氢时的焓变值较高，为 20.38 kJ/mol H_2。

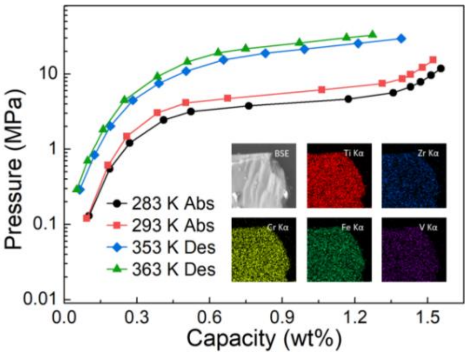

图 1 $Ti_{0.85}Zr_{0.17}Cr_{0.95}Fe_{0.95}V_{0.1}$ 合金的能谱扫描结果与等温吸（Abs）放（Des）氢曲线

Fig. 1 EDS mappings and pressure-temperature isotherms of $Ti_{0.85}Zr_{0.17}Cr_{0.95}Fe_{0.95}V_{0.1}$ alloy

关键词：金属氢化物；Ti-Zr-Cr-Fe-V 基合金；元素取代；氢气压缩；储氢性能

Investigation on Ti-Zr-Cr-Fe-V based alloys for metal hydride hydrogen compressor at moderate working temperatures

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Abstract: $Ti_{0.85}Zr_{0.17}Cr_{1.2-x}Fe_{0.8}V_x$ (x = 0-0.2), $Ti_{0.85}Zr_{0.17}Cr_{1.2-y}Fe_{0.7+y}V_{0.1}$ (y = 0-0.25) and $Ti_{0.87-z}Zr_{0.15+z}Cr_{0.95}Fe_{0.95}V_{0.1}$ (z = 0-0.04) alloys for metal hydride hydrogen compressor at working temperatures of water bath were prepared by induction levitation melting. Their microstructures and hydrogen storage properties were systematically investigated. The results show that all Ti-Zr-Cr-Fe-V based alloys have a single C14 Laves phase structure. As the V or Zr content in the Ti-Zr-Cr-Fe-V based alloys increase, larger hydrogen storage capacity is achieved, while the plateau pressure decreases and the plateau slope factor increases. Conversely, these three properties vary oppositely with increasing Fe content in the $Ti_{0.85}Zr_{0.17}Cr_{1.2-y}Fe_{0.7+y}V_{0.1}$ (y = 0-0.25) alloys. $Ti_{0.85}Zr_{0.17}Cr_{0.95}Fe_{0.95}V_{0.1}$ possesses the best overall properties for the designed hydrogen compressor. It has hydrogen capacity of 1.52 wt% and hydrogenation plateau pressure of 5.62 MPa at 293 K, and dehydrogenation plateau pressure of 23.01MPa at 353 K. Additionally, it possesses relatively low hysteresis and high dissociation enthalpy of 20.38kJ/mol H_2.

氢转移动力学增强的有机液体可逆储氢

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摘要：液相有机氢载体(LOHCs)在储氢材料中具有储氢量高、可逆性好、与油气设备兼容等优势，但在非贵金属催化剂催化下，较慢的吸放氢动力学制约了其商业化应用。以 N-乙基咔唑(NEC)为例，NEC 的可逆吸放氢共涉及 12 个氢原子，因此氢的活化、转移过程十分重要。本课题组针对该问题，提出了过渡金属/金属氢化物(TM/MH)协同催化的设计思路。复合催化剂 Co-B/Al_2O_3-YH_{3-x}可实现 NEC 在 180 ℃、10 MPa H_2条件下 2 h 加氢至 5.5 wt%，以及 12H-NEC 在 200 ℃、0.1 MPa 下 7 h 放氢至 5.5 wt%。通过同位素示踪及动力学同位素效应，本工作证明了过渡金属活化有机底物、金属氢化物增强氢转移的 TM/MH 协同催化机理。进一步地，我们利用化学方法合成了 $LaNi_{5.5}$ 纳米合金，该纳米合金具有稳固的 Ni/$LaNi_5$ 界面，可在单颗粒上实现有机底物的活化以及氢转移的增强。这种结构使得催化剂在保持快速吸放氢的同时具有长循环能力，在 9 次加脱氢反应后催化活性没有明显衰减。这些工作促进了 LOHCs 储氢技术的实用化，并且扩展了金属氢化物催化的研究思路，加深了对氢化物催化机理的认识。

关键词：液相有机氢载体；金属氢化物；氢转移；协同催化

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Reversible hydrogen storage in liquid organic hydrogen carrier with enhanced hydrogen transfer kinetics

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Abstract: Liquid organic hydrogen carriers (LOHCs) show advantages on hydrogen storage capacity, reversibility and compatibility with oil and gas equipment. However, their commercial applications are limited by sluggish hydrogen absorption/desorption kinetics catalyzed by non-noble metals. Taking N-ethylcarbazole (NEC) as an example, the reversible hydrogen absorption/desorption of NEC involves 12 hydrogen atoms, so the process of hydrogen activation and transfer is important. To solve this problem, our group designed and synthesized transition metal/metal hydrides (TM/MH) systems for a synergistic catalysis process. Composite catalyst Co-B/Al_2O_3-YH_{3-x} can achieve the hydrogenation of NEC to 5.5 wt% for 2 hours at 180 °C, 10 MPa H_2, and the dehydrogenation of 12H-NEC to 5.5 wt% for 7 hours, at 200 °C, 0.1 MPa H_2. Through isotope tracing and kinetic isotope effect, the TM/MH synergistic catalytic mechanism was investigated, wherein organics is activated by TM, and hydrogen transfer is enhanced by MH. Furthermore, $LaNi_{5.5}$ nano alloy was synthesized by chemical method, and applicated to hydrogenation/dehydrogenation of NEC/12H-NEC. This nano alloy has a stable interface between Ni and $LaNi_5$, which enables activation of organics and enhancement of hydrogen transfer on a single particle. With this unique structure, $LaNi_{5.5}$ achieves hydrogenation/dehydrogenation of NEC/12H-NEC for 9 cycles, while the activity of catalyst shows inapparent decline. These works promote the practicability of LOHCs hydrogen storage technology, develop the research thoughts of metal hydride catalysis, and deepen the understanding of hydride catalysis mechanism.

二维钒纳米片一种改善 MgH_2 储氢性能的高效催化剂

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摘要：氢化镁（MgH_2）的储氢容量高达 7.6 wt%，而且镁在地壳中资源丰富，同时具有无毒等优点，因此 MgH_2 是一种极具应用潜力的储氢材料。然而，Mg/MgH_2 体系在实际应用中存在热稳定性高、吸附和解吸动力学缓慢等问题。本文采用一种简便的湿化学球磨方法成功制备了二维的钒纳米片（V_{NS}），并证明其对 MgH_2 的储氢性能有很好的改善作用。例如，MgH_2+7 wt% V_{NS} 复合材料在 187.2ºC 时开始释放氢气，比不添加催化剂的 MgH_2 初始放氢温度低 152ºC。在 300ºC 下，MgH_2+7 wt% V_{NS} 复合材料在 10 分钟内释放出 6.3 wt%的氢气，并且完全脱氢的样品即使在室温和 3.2 MPa 的氢压下也能吸收氢气。XRD 和 TEM 结果证实金属钒是促进 MgH_2 脱氢以及再加氢反应的催化单元。本文提供了一种合成具有优良催化性能二维钒纳米片的简便方法，这可能对未来设计和制备用于储氢和其他能源相关领域的层状催化剂有一定的指导意义。

关键词：储氢；氢化镁；二维钒纳米片；催化作用

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Two-dimensional vanadium nanosheets as a remarkably effective catalyst for hydrogen storage in MgH_2

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Abstract: Magnesium hydride (MgH_2), which possesses high hydrogen density of 7.6 wt%, abundant resource and non-toxicity, has captured intense attention as one of the potential hydrogen storage materials. However, the practical application of Mg/MgH_2 system is suffering from high thermal stability, sluggish absorption and desorption kinetics. Herein, two-dimensional (2D) vanadium nanosheets (V_{NS}) were successfully prepared via a facile wet chemical ball milling method, and proved to be highly effective on improving the hydrogen storage performance of MgH_2. For instance, the MgH_2+7 wt% V_{NS} composite began to release hydrogen at 187.2ºC, 152ºC lower than that of additive-free MgH_2. At 300ºC, 6.3 wt% hydrogen was released from the MgH_2+7 wt% V_{NS} composite within 10 min. In addition, the fully dehydrogenated sample could absorb hydrogen even at room temperature under hydrogen pressure of 3.2 MPa. X-ray diffractometer (XRD) and transmission electron microscopy (TEM) results confirmed metallic vanadium served as catalytic unit for facilitating the de/rehydrogenation reaction of MgH_2. This finding presents an example of facile synthesis of two-dimensional (2D) vanadium with excellent catalysis, which may shed light on future design and prepare of highly effective layered catalysts for hydrogen storage and other energy related areas.

基于固态储氢的氢燃料电池动力系统热量管理和集成研究

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摘要：氢能产业链包括制氢、储氢、运氢和用氢等关键环节，其中氢气的储运是限制氢能发展的关键因素之一。相比于传统高压储氢技术，固态储氢方式具有储氢量大、储氢压力低、安全性高等诸多优点，被认为是极具应用前景的储氢技术之一。然而，固态储氢材料吸放氢过程中存在明显的热效应，且该热效应对材料储氢性能具有负反馈效果，因此良好的热量管理对于固态储氢技术应用于氢燃料电池动力系统中至关重要。本研究提出采用相变材料对固态储氢反应器进行热量管理，回收可逆储氢材料吸氢过程中放出的热量用于放氢过程。建立了固态储氢反应器模型，探究了关键物性参数和操作参数的影响规律。提出了储氢反应器连续吸放氢模型，优化了储氢反应器性能。搭建了实验测试平台，验证了氢动力系统的可行性，并将其集成应用于小车平台。研究结果表明，该固态储氢反应器稳定储氢效率达到 60%，能够实现 25 min 续航时间。

关键词：固态储氢；氢燃料电池动力系统；热管理；系统集成；氢能

Thermal management and integration of the fuel cell power system based on the solid-state hydrogen storage

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Abstract: Hydrogen industry chain includes production, storage, transportation and application, among which hydrogen storage and transportation is one of the key factors limiting the development of hydrogen energy. Compared with the traditional high-pressure hydrogen storage technology, solid-state hydrogen storage method has the advantages of large hydrogen capacity, low pressure, and high safety, which is considered as one of the most promising hydrogen storage technologies. However, there is an obvious thermal effect during the processes of hydrogen absorption and desorption of solid-state hydrogen storage materials, which has a negative feedback effect on the hydrogen storage performance. Therefore, a good thermal management is significant for the application of solid-state hydrogen storage technology in hydrogen fuel cell power system. In this study, phase change material is employed for thermal management of the hydrogen storage reactor. The heat released by reversible hydrogen storage material during hydrogen absorption is recycled and used for desorption process. The model of solid-state hydrogen storage reactor is established and the effects of key physical parameters and operating parameters are investigated. Meanwhile, a model of continuous hydrogen absorption and desorption process in hydrogen storage reactor is proposed to optimize the performance of hydrogen storage reactor. In addition, a test bench is built to verify the feasibility of the hydrogen fuel cell power system which is also integrated into a car platform. The results show that the stable hydrogen storage efficiency of the solid-state hydrogen storage reactor can reach 60%, and the running time of 25 min can be achieved in the fuel cell power system.

适用于高密度储氢装置的 Ti-Zr-Mn-Cr-V 基合金的研究

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摘要：针对高密度储氢装置对于储氢合金的技术要求，系统研究了 $Ti_{1-x}Zr_xMn_{1.1}Cr_{0.7}V_{0.2}$ (x = 0.05, 0.06, 0.07, 0.1)以及 $Ti_{0.95}Zr_{0.05}Mn_{1.8-y}Cr_yV_{0.2}$ (y = 0.5, 0.7, 0.9)两系列合金。本文探究了 Zr 部分取代 Ti 以及 Cr 部分取代 Mn 对于 Ti-Zr-Mn-Cr-V 体系合金晶体结构以及储氢性能的影响。结果证明所制备的合金都有着 C14 型 Laves 结构以及均匀元素分布的单相。随着 $Ti_{1-x}Zr_xMn_{1.1}Cr_{0.7}V_{0.2}$ (x = 0.05, 0.06, 0.07, 0.1)合金中 Ti 越来越多地被 Zr 取代，合金储氢容量逐渐增加，平台压力急剧下降。对于 $Ti_{0.95}Zr_{0.05}Mn_{1.8-y}Cr_yV_{0.2}$ (y = 0.5, 0.7, 0.9)合金，随着 Cr 对 Mn 的替代量增加，吸放氢平衡压滞后得到显著改善，而平台压力和储氢能力有不同程度的下降。在上述合金中，$Ti_{0.95}Zr_{0.05}Mn_{0.9}Cr_{0.9}V_{0.2}$ 合金的综合储氢性能最符合高密度储氢装置的技术要求。该成分合金的储氢容量为 1.78 wt%（118.33 kg/m^3），90 ℃下放氢平台压为 9.37 MPa 且有着极低的吸放氢平台压滞后，放氢焓变为 21.64 kJ·mol^{-1}。同时，该合金也表现出优异循环性能。这项工作为钛基合金的成分设计提供了指导。

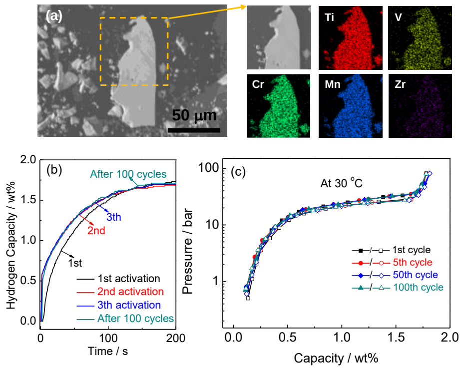

图 1 $Ti_{0.95}Zr_{0.05}Mn_{0.9}Cr_{0.9}V_{0.2}$ 合金的相结构与储氢性能示意图
Fig. 1 Phase structure and hydrogen storage performances of $Ti_{0.95}Zr_{0.05}Mn_{0.9}Cr_{0.9}V_{0.2}$

关键词：金属氢化物；Ti-Zr-Mn-Cr-V 基储氢合金；元素取代；高密度储氢

Development of Ti-Zr-Mn-Cr-V based alloys for high-density hydrogen storage

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Abstract: Two series of $Ti_{1-x}Zr_xMn_{1.1}Cr_{0.7}V_{0.2}$ (x = 0.05, 0.06, 0.07, 0.1) and $Ti_{0.95}Zr_{0.05}Mn_{1.8-y}Cr_yV_{0.2}$ (y = 0.5, 0.7, 0.9) alloys were developed for high-density hydrogen storage units. The effect of partial substitution of Zr for Ti and Cr for Mn on microstructures as well as hydrogen storage performances was systematically investigated. All prepared alloys are determined as a single phase of C14-type Laves structure and uniform element distribution. As Ti is increasingly substituted with Zr in the $Ti_{1-x}Zr_xMn_{1.1}Cr_{0.7}V_{0.2}$ (x = 0.05-0.1) alloys, the hydrogen storage capacity increases gradually, while the plateau pressures decrease drastically. For $Ti_{0.95}Zr_{0.05}Mn_{1.8-y}Cr_yV_{0.2}$ (y = 0.5-0.9) alloys, with the increase substitution of Cr for Mn, equilibrium pressure hysteresis of de-/hydrogenation improves significantly, while the plateau pressures and the hydrogen storage capacity decrease slightly. Among the studied alloys, $Ti_{0.95}Zr_{0.05}Mn_{0.9}Cr_{0.9}V_{0.2}$ is the most suitable for high-density hydrogen storage units with excellent cycling performances. The hydrogen storage capacity is 1.78 wt% in gravimetry and 118.33 kg/m^3 in volumetry. The desorption plateau pressure at 90 °C is 9.37 MPa with extremely low hysteresis, and dissociation enthalpy is 21.64 kJ·mol^{-1}. This work provides a guideline for the alloy composition design of Ti-based alloys.

不同相结构的钴 (FCC/HCP)对 MgH_2 储氢催化性能的影响

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摘要： 氢脱附温度高、反应动力学缓慢是限制 MgH_2 实际应用的主要因素。本研究制备了具有面心立方(FCC)结构和六方紧密堆积(HCP)结构的 Co 颗粒，证明了 Co 颗粒是氢化镁的良好催化剂。FCC 结构的 Co 颗粒对 MgH_2 的催化效果优于 HCP 结构的 Co 颗粒。7wt% Co FCC 和 HCP 颗粒改性 MgH_2 的初始脱氢温度均由 301.3℃降至 195.0℃左右，但 7wt% Co FCC 结构改性 MgH_2 的解吸速率较快，在 325℃10 min 内解吸了约 6.5 wt% H_2。在 70°C、32.5 bar 氢气压力下检测氢吸收，在 150°C 下 40 分钟内再充 6.0 wt% H_2。7wt% FCC Co 改性 MgH_2 的脱氢活化能和吸附活化能分别显著降低至 76.6±8.3 kJ mol^{-1} 和 68.3±6.0 kJ mol^{-1}。研究了 MgH_2+7 wt% FCC Co 在 300℃、325℃、350℃和 375℃时的平台压力，平台压力分别为 1.40、2.80、5.37 和 9.88 bar。MgH_2+7 wt% FCC Co 的氢分解焓（ΔH）为 80.6±0.1 kJ mol^{-1}，比制备的 MgH_2 低 5.8 kJ mol^{-1}，说明 FCC Co 调节了 MgH_2 的热力学性质。前 20 个循环的循环性能表明，MgH_2-FCC Co 复合材料的反应动力学和容量基本没有变化。密度泛函理论计算结果表明，钴颗粒可以拓宽 Mg-H 键，降低氢化镁的分解能。本文可为寻找高效储氢催化剂和其他能源相关研究领域提供参考。

关键词： 储氢；氢化镁；FCC/HCP 钴颗粒；催化作用；密度泛函理论

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The effect of different Co phase structure (FCC/HCP) on the catalytic action towards the hydrogen storage performance of MgH_2

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Abstract: High hydrogen desorption temperature and sluggish reaction kinetics are the major limitations for the practical application of MgH_2. In this study, Co particles with a face centered cubic (FCC) structure and a hexagonal close packed (HCP) structure were prepared facilely and proved to be good catalysts for magnesium hydride. Co particles with FCC structure presented better catalytic effect on MgH_2 than that with HCP structure. Both 7wt% Co FCC and HCP particle modified MgH_2 decreased the initial dehydrogenation temperature from 301.3 °C to approximately 195.0 °C, but 7wt% Co with FCC structure modified MgH_2 has a faster desorption rate, and around 6.5 wt% H_2 was desorbed in 10 min at 325 °C. Hydrogen uptake was detected at 70 °C under 32.5 bar hydrogen pressure and 6.0 wt% H_2 was recharged in 40 min at 150 °C. The hydrogen desorption and absorption activation energy for 7wt% FCC Co modified MgH_2 was significantly decreased to 76.6±8.3 kJ mol^{-1} and 68.3±6.0 kJ mol^{-1}, respectively. Thermodynamic property was also studied, the plateau pressures of MgH_2+7 wt% FCC Co were determined to be 1.40, 2.80, 5.37 and 9.88 bar for 300 °C, 325 °C, 350 °C and 375°C. The decomposition enthalpy of hydrogen (ΔH) for MgH_2+7 wt% FCC Co was 80.6±0.1 kJ mol^{-1} ,5.8 kJ mol^{-1} lower than that of as-prepared MgH_2, which means FCC Co tune the thermodynamic property of MgH_2. Moreover, cycling performance for the first 20 cycles revealed that the reaction kinetics and capacity of MgH_2-FCC Co composite remained almost unchanged. The result of density functional theory calculation demonstrated that cobalt could extract the Mg-H bond and reduced the decompose energy of magnesium hydride. Our paper can be presented as a reference for searching highly effective catalysts for hydrogen storage and other energy-related research fields.

催化层孔径优化对质子交换膜燃料电池氧传输阻力机理的研究

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摘要：在质子交换膜燃料电池（PEMFC）中，氧传输阻力是阻碍电池实现高性能的因素之一。本文采用造孔剂优化催化层(CL)的孔径分布，研究其对氧传输阻力机理的影响，包括分子扩散阻力、Knudsen 扩散阻力和局域氧传质阻力。结果表明，随着孔隙的形成，在高电流密度下电池性能有显着改善，这主要是归咎于其良好的氧传输性能，在低铂条件下，这种优势更加明显。造孔剂的加入使孔径向更大的孔径移动，范围大约为 70-100 nm，同时增加了累积孔体积。进一步的测试表明，孔隙形成后 CL 中分子扩散阻力的降低远大于 Knudsen 扩散阻力。此外，优化后的孔隙结构也会获得更多的有效孔隙，增加了离聚物在 Pt 表面的有效面积，有利于降低低铂负载下的局域氧传质阻力。

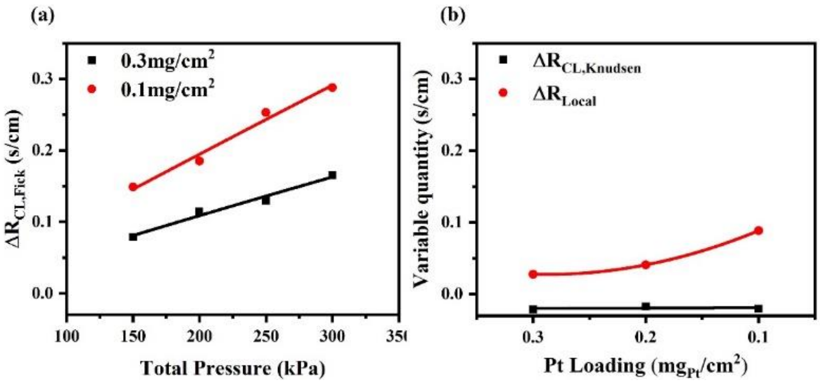

图 1 造孔前后催化层中分子扩散阻力、Knudsen 扩散阻力和局域传质阻力的变化

关键词：孔径优化；造孔剂；氧传输阻力；质子交换膜燃料电池

Influence of pore size optimization in catalyst layer on the mechanism of oxygen transport resistance in PEMFCs

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Abstract: In PEMFC, the oxygen transport resistance severely hinders the cell from achieving high performance. In this paper, pore-forming agents was used to optimize the pore size distribution of the catalyst layer (CL), and to study its effect on the mechanism of oxygen transport resistance, including molecular diffusion resistance, Knudsen diffusion resistance, and local O_2 resistance in CL. The results showed that with the pore formation the cell performance had a significant improvement at high current density, mainly due to its better oxygen transport properties, especially under low platinum conditions. The addition of pore-forming agent moved the pore diameter toward a larger pore diameter with a range from 70 to 100 nm, and also obtaining a higher cumulative pore volume. Further tests indicated that the improvement of molecular diffusion resistance was much larger than that of Knudsen diffusion resistance in the catalyst layer after pore formed. In addition, the optimized pore structure will also get a higher number of effective pores, which resulted in an increased effective area of the ionomer on the Pt surface. The higher effective area of the ionomer was particularly beneficial for the reduction of local O_2 resistance with low Pt loading.

不同流场下阴极开放式质子交换膜燃料电池工作特性研究

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摘要：阴极开放质子交换膜燃料电池（PEMFC）由于其结构简单、寄生功率低而被认为为是无人机和便携式应用上很有前景的替代电源。在这项研究中，通过实验研究了具有不同阴极流场（平行、点阵和金属泡沫）的阴极开放式 PEMFC 的工作特性。通过测试极化曲线和电化学阻抗谱(EIS)分别表征电池性能和电化学阻抗。结果表明，在常规工况下泡沫金属流场具有更好的性能。虽然提高风扇电压可以提供足够的反应气体并去除多余的水分，但过大的空气流速会降低膜水含量并降低电池的运行温度。提高工作温度会改善电池性能，但较高的水分蒸发率会引起欧姆电阻增加。在低电流密度区域，随着阳极背压的增加，电池性能趋于稳定，而在高电流密度区域，随着阳极背压的增加，电池性能下降。

关键词: 阴极开放式质子交换膜燃料电池；流场；电化学阻抗谱；工作特性

Experimental investigation on open-cathode proton exchange membrane fuel cell with different cathode flow fields

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Abstract: The operational parameters of an open-cathode proton exchange membrane fuel cell (PEMFC) with different cathode flow fields (parallel, pin-type, and metal foams) are investigated by experiments. The operational parameters include fan voltage, operating temperature and the anode backpressure. Electrochemical impedance spectroscopy (EIS) and polarization curve are conducted to characterize the cell performance and electrochemical impedance inside the cell, respectively. The results show that the cell with the metal foam flow field has better performance than that with the other flow fields in the baseline conditions. Although increasing the fan voltage could provide adequate reactant gas and remove excess water, too large air flow rate could reduce membrane water content and decrease temperature that is bad for the cell performance. Increasing the operating temperature would improve the cell performance, but the increase of ohmic resistance caused by higher water evaporation rate cannot be neglected. The cell performs stably with increasing the anode backpressure in the low current density region, while the cell performance decreases with increasing the anode backpressure in the high current density region. Understanding of the characteristics of different cathode flow fields in the open-cathode proton exchange membrane fuel cell could provide comprehensive guidelines for the design and operation of the low-power portable PEMFC applications.

低温环境下 PEMFC 中水的行为特征与启动研究

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摘要：低温环境下 PEMFC 的储存/启动能力是制约其商业化应用的主要因素之一。我们首先基于异相成核理论，对低温环境下MEA水的结晶动力学特征参数进行了理论计算，通过模拟仿真揭示了受过冷水结晶诱发时间控制下 PEM 电池低温储存/启动过程中 MEA 冰相饱和度分布规律、对MEA微结构和电池启动性能的影响；然后采用长直流道单电池分区测试方法，研究了低温启动过程中电流密度、温度、气体压力等物理量的演变特征，进而探究了流道及膜电极内部水的形态变化；同时设计实验获得了吹扫条件和方式对电堆残余水的影响关系。基于这些研究结果，制定了优化的电池低温启动控制策略，并进行实验验证，成功实现了电堆-30℃冷启动和-40℃存储，为大功率电堆高效、快速的冷启动提供了理论指导和实验基础。

关键词：质子交换膜燃料电池；冷启动；结晶动力学；分区测试；吹扫

Study on the water behavioral characteristics in PEMFC and Start-up at Low Temperature Environment

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Abstract：The storage/start-up capability of PEMFC in low temperature environment is one of the main factors restricting its commercial application. Firstly, based on the theory of heterogeneous nucleation, we theoretically calculated the crystallization kinetic parameters of water in MEA at low temperature environments, through simulation, the distribution of ice phase saturation in MEA and its effect on microstructure of MEA and start-up performance of fuel cell were revealed during the low temperature storage/startup process of PEMFC under the control of the induction time that supercooled water crystallized; Then, using partition test method for the single cell with long and straight flow channels, the evolution characteristics of physical quantities such as current density, temperature and gas pressure during low-temperature start-up were studied, and then the morphological changes of the water inside the flow channel and the membrane electrode were explored; at the same time, experiments were designed to obtain the effect of purge conditions and methods on the residual water in the stack. Based on these results, an optimized cold start control strategy was developed, and experimental verification was carried out, successfully realized the -30℃ cold start and -40℃ storage of the stack, which provided theoretical guidance and experimental basis for the high-efficiency and rapid cold start of high-power stacks.

质子交换膜燃料电池催化层纳米尺度氧气传输机理

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摘要：低铂载量下，燃料电池阴极催化层中的氧气传输阻力很高，严重影响了燃料电池的性能，阻碍了高性能、低铂载量燃料电池的发展。因此，探究催化层中的氧气传输机理对于燃料电池意义重大。本研究利用分子动力学模拟探究了氧气在电解质薄膜中的传输机理。发现了铂面上存在着离聚物分子紧密排布的致密超薄层，该结构是导致高氧气传输阻力的主要原因，发现氧气分子更容易到达铂颗粒的边和角位置。同时还发现铂表面添加离子流体可抑制离聚物长链的紧密排布，为氧气在致密超薄层中的溶解提供了更大的自由空间，加入离子流体后超薄层中的氧气密度提升了一个量级、氧气传输流量提升了高达 8 倍。

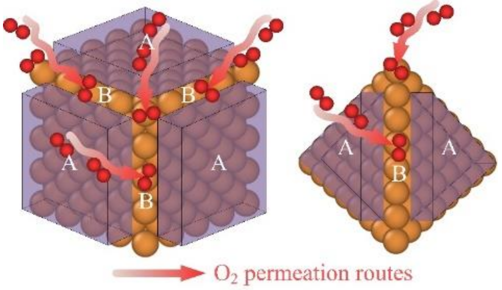

图 1 铂颗粒周围氧气渗透路径

Fig. 1 Schematics of O_2 permeation routes near Pt particles.

关键词：质子交换膜燃料电池；催化层；氧气传输；纳观结构

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Nanoscale oxygen transport in catalyst layer of proton exchange membrane fuel cells

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Abstract: The oxygen transport resistance in the cathode catalyst layer is high, which significantly affects the performance of fuel cells and hinders the development of high-performance and low-Pt-loading fuel cells. Therefore, exploring the oxygen transport in the catalyst layer is of great significance for fuel cells. In this study, the oxygen transport in the electrolyte film is explored using molecular dynamics simulations. It was found that a dense ultrathin layer with tightly arranged ionomer molecules is present on Pt surface, which is the main cause of high oxygen transport resistance. And the oxygen molecules can more easily reach the edges and corners of Pt particles. Moreover, adding ionic liquid on Pt surface can inhibit the tight arrangement of ionomer chains and provide larger free space for oxygen dissolution. The ionic liquid additives can increase the oxygen density in the ultrathin layer by an order of magnitudes and the oxygen flux by up to 8 times.

以生物质为燃料的 SOFC 模拟及系统应用研究

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摘要：为了揭示以生物质气化合成气为燃料的固体氧化物燃料电池的内部工作机理和性能，建立了固体氧化物燃料电池的二维多物理场模型。本研究弥补了以往生物质气化装置与 SOFC 堆耦合研究多停留在系统层面的不足。结果表明，以水蒸气为催化剂的生物质气化合成气为燃料的 SOFC 性能最佳。峰值功率密度可达 10240 $W\cdot m^{-2}$ 左右。随着工作温度的提高，SOFC 的峰值功率密度将会增加。在 1123 K 温度下，峰值功率密度可达 15128 $W\cdot m^{-2}$ 左右。当操作温度为 1123 K 时，水气位移反应的平均反应速率为-29.73 $mol\cdot m^{-3}\cdot s^{-1}$。这说明 WGS 反应在高温下会向相反的方向进行，从而降低了氢的浓度。此外，阳极通量的增加和电池长度的减小导致 SOFC 电流密度的增加。总体而言，该工作可为生物质合成气为燃料的 SOFC 优化和实际应用提供指导。

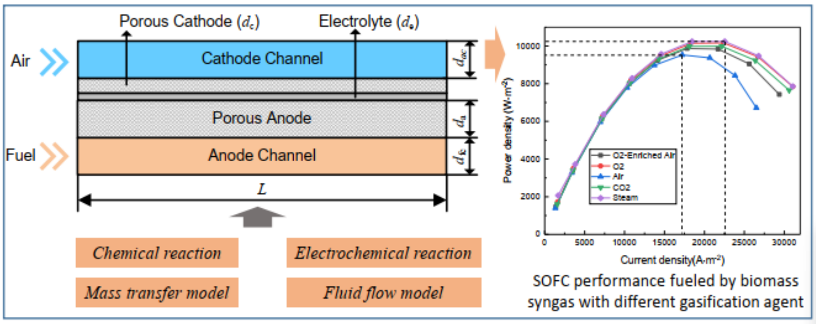

图 1 以生物质为气化合成气为燃料的 SOFC 多物理场建模示意图

Fig. 1 Schematic diagram of SOFC multi-physical field modeling fueled by biomass syngas

关键词：固体氧化物燃料电池；多物理场建模；传质流动耦合；化学反应

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Multi-physics field modeling of biomass gasification syngas fueled solid oxide fuel cell

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Abstract: In order to uncover the inner working mechanism and performance of solid oxide fuel cell (SOFC) with biomass gasification syngas as fuel, a two-dimensional SOFC multi-physical field model is established. This study makes up for the deficiency that the previous studies of coupling biomass gasification unit and SOFC stack mostly stay at the system level. The results show that the SOFC fueled by the syngas produced from gasification of biomass with steam as the agent has the best performance. The peak power density could achieve approximately 10240 $W\cdot m^{-2}$. With the improvement of operating temperature, the peak power density of SOFC will be increased. At the temperature of 1123 K, the peak power density could achieve about 15128 $W\cdot m^{-2}$. The average reaction rate of water gas shift (WGS) reaction is -29.73 $mol\cdot m^{-3}\cdot s^{-1}$ when the operating temperature is 1123 K. This indicates that the WGS reaction will proceed in reverse direction at high temperatures, thereby reducing the hydrogen concentration. In addition, increase in the anode flux and decrease in the cell length lead to the increase of SOFC current density. In general, this work could provide guidance for the optimization and practical application of SOFC using biomass syngas as fuel.

Cu 掺杂对中温固体氧化物燃料电池 $PrBa_{0.5}Sr_{0.5}Co_{2-x}Cu_xO_3$ 阴极性能的研究

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摘要：$(La_{0.75}Sr_{0.25})_{0.95}MnO_{3\pm\delta}$(LSM)、$La_{0.6}Sr_{0.4}CoO_3$(LSC) 和 $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3+\delta}$(LSCF)被认为是全球三种有前景的阴极材料[1]。本文采用 EDTA-柠檬酸法成功合成出了 Cu 掺杂的 $PrBa_{0.5}Sr_{0.5}Co_{2-x}Cu_xO_3$（PBSCCx, x=0,0.1,0.2）材料并将其应用于中温固体氧化物燃料电池阴极。XRD 测试结果表明 Cu 掺杂在不改变材料四方空间群的前提下促使晶格收缩, PBSCCx 与 GDC 也具有良好的热稳定性；热重分析结果证实 Cu 掺杂增加了氧空位浓度，这能有效增加氧传输动力学速率；在 LSCFCx 材料中, $PrBa_{0.5}Sr_{0.5}CoCuO_3$(PBSCC1.0))显示出最佳的电化学性能，在 600 ℃下通过交流阻抗谱法测得 PBSCC0，PBSCC0.5，PBSC1.0 的极化电阻(R_p) 为 1.199 $\Omega\cdot cm^2$，0.735 $\Omega\cdot cm^2$，0.439 $\Omega\cdot cm^2$，这将使得 PBSCC1.0 有潜力成为有希望的阴极材料。

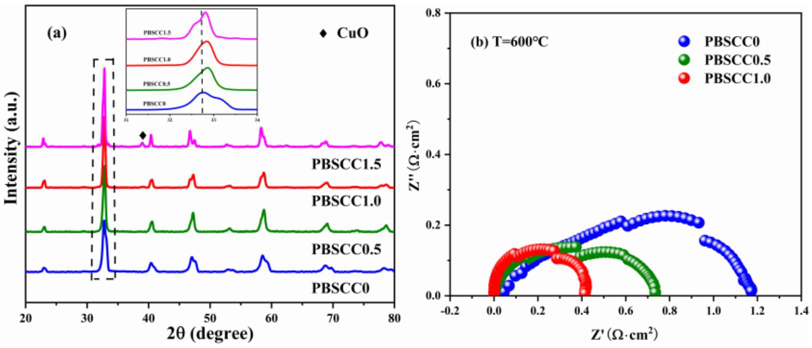

图 1 (a) PBSCCx (x = 0,0.5,1.0,1.5) 的 XRD 相图；(b) PBSCCx (x= 0,0.5,1.0) 阴极在 600 ℃下的电化学阻抗谱

Fig.1 (a) XRD patterns of PBSCCx(x = 0,0.1,0.2,0.3); (b) Electrochemical impedance spectra of the PBSCCx(x= 0,0.1,0.2) cathodes measured at 600 ℃

关键词：固体氧化物燃料电池；阴极；相结构；氧空位；交流阻抗

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The study of Cu doping on the performance of $PrBa_{0.5}Sr_{0.5}Co_{2-x}Cu_xO_3$ cathode for intermedium temperature solid oxide fuel cell

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Abstract: $(La_{0.75}Sr_{0.25})_{0.95}MnO_{3\pm\delta}$(LSM)、$La_{0.6}Sr_{0.4}CoO_3$(LSC) and $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3+\delta}$(LSCF) are the most promising cathode materials for SOFCs[1]. In this work, Cu doped $PrBa_{0.5}Sr_{0.5}Co_{2-x}Cu_xO_3$(PBSCCx, x=0,0.1,0.2) were synthesized through a EDTA-CA complexation process[2]. The lattice parameters of PBSCCx increase as Cu substitution amount reduce without changing its quartet structure, and the LBSCFx cathodes exhibit excellent chemical compatibility with GDC electrolyte; TGA results confirm that the oxygen vacancies promote along with the Cu concentration, which effectively increases the kinetic rate of oxygen transport. $PrBa_{0.5}Sr_{0.5}CoCuO_3$(PBSCC1.0)) demonstrates the best electrochemical performance, the R_p as AC impedance spectroscopy of PBSCC0，PBSCC0.5，PBSC1.0 are 1.199 $\Omega\cdot cm^2$，0.735 $\Omega\cdot cm^2$，0.439 $\Omega\cdot cm^2$ in 600 ℃，which make PBSCC1.0 become one of the potential cathode material.

三元过渡金属硫化物 $FeNi_2S_4$ 空心球对 MgH_2 储氢性能的影响

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摘要：稳定的热力学和缓慢的动力学限制了 MgH_2 的实际应用。在本研究中，我们设计了一种具有空心球结构的三元过渡金属硫化物 $FeNi_2S_4$ 作为催化剂，通过构建 MgH_2/Mg_2NiH_4-MgS/Fe 体系来解决上述问题。值得注意的是，由于源自 MgH_2-$FeNi_2S_4$ 复合材料的 Mg_2Ni/Mg_2NiH_4、MgS 和 Fe 活性物质的协同催化作用，MgH_2 的吸氢和放氢能力得到了显着改善。复合材料在 373 K 下 1 h 吸氢 4.02 wt%，与球磨后的 MgH_2 (0.67 wt%) 形成鲜明对比。在放氢动力学方面，复合材料的初始放氢温度比 MgH_2 低 80 K，脱氢活化能比 MgH_2(178.9 kJ mol^{-1})降低了 104.4 kJ mol^{-1}。该方法为提高 MgH_2 材料的脱氢/吸氢性能提供了一种新的策略。

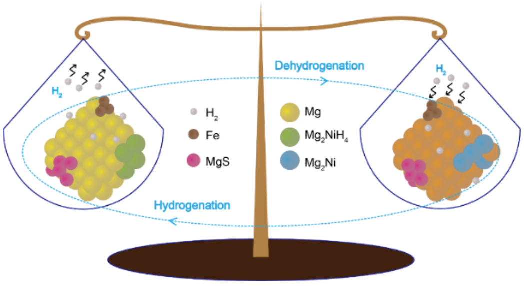

图 1.MgH_2-$FeNi_2S_4$ 复合材料吸氢/放氢过程示意图。

Figure 1. Schematic diagram of the hydrogenation/dehydrogenation processes of the MgH_2-$FeNi_2S_4$ composite.

关键词：储氢材料；MgH_2；$FeNi_2S_4$；储氢动力学；催化剂

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Effect of ternary transition metal sulfide $FeNi_2S_4$ hollow balloons on hydrogen storage performance of MgH_2

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Abstract: The stable thermodynamics and slow kinetics limit the practical application of MgH_2. In this study, we design a ternary transition metal sulfide $FeNi_2S_4$ with a hollow balloon structure as a catalyst to address the above issues by constructing a MgH_2/Mg_2NiH_4-MgS/Fe system. Notably, the hydrogen absorption and desorption of MgH2 has been significant improved due to the synergistic catalysis of the active species of Mg_2Ni/Mg_2NiH_4, MgS and Fe, originated from the MgH_2-$FeNi_2S_4$ composite. The hydrogen absorption capacity of the doped composite at 373 K for 1 h increases to 4.02 wt%, a sharp contrast to the milled-MgH_2 (0.67 wt%). In terms of desorption kinetics, the initial desorption temperature of the composite is 80 K lower than that of the milled-MgH_2, and the fitted dehydrogenation activation energy decreases by 104.4 kJ mol^{-1} compared with the milled-MgH_2 (178.9 kJ mol^{-1}). This method provides a new strategy for improving the dehydrogenation/hydrogenation performance of MgH_2 material.

Ni_3Fe/rGO 对 MgH_2 储氢性能的协同效应

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摘要：相较于单金属材料，双金属催化剂具有独特的物化特性。在此，基于层状双金属氢氧化物（LDH）前驱体，制备了均匀负载于 rGO 表面的 Ni_3Fe（~12nm）纳米粒子（Ni_3Fe/rGO），并研究它对 MgH_2 储氢性能的协同作用。MgH_2-5 wt.% Ni_3Fe/rGO 复合材料在 100℃仅需 100s 达到 6wt.%的吸氢量，而对于掺有单独组分的 Ni_3Fe、Ni/rGO 和 Fe/rGO 的 MgH_2，在 100℃均需要超过 500s 才能吸收 3wt.%的氢。此外，该材料仅在 185℃时开始释放氢气，均低于掺有 5 wt.% Ni_3Fe（205℃）、Ni/rGO（210℃）和 Fe/rGO（250℃）的 MgH_2。结果表明，Ni_3Fe/rGO 复合材料的优越性能归因于 rGO 以及原位形成的活性物种（Mg_2Ni 和 Fe）间的协同效应。同时，这项研究为基于 LDH 前驱体制备高效催化剂提供了创新见解。

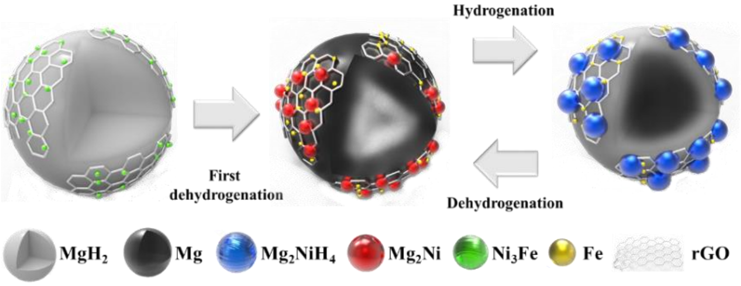

图 1 Ni_3Fe/rGO 对 MgH_2 吸放氢过程的协同作用示意图
Fig. 1 A schematic diagram of the synergistic effect of Ni_3Fe/rGO on the dehydrogenation and hydrogenation of MgH_2

关键词：双金属催化剂；Ni_3Fe/rGO；MgH_2；协同效应

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Synergistic Effect of rGO support Ni_3Fe on Hydrogen Storage Performance of MgH_2

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Abstract: Bimetallic catalysts possess unique physical and chemical properties that distinct from the individual. Herein, a Ni_3Fe nano material (~12 nm) homogeneously loaded on the surface of reduced graphene oxide (Ni_3Fe/rGO) was prepared based on layered double hydroxide (LDH) precursor. Its synergistic effect toward hydrogen storage performance of MgH_2 was studied. The MgH_2-5 wt.% Ni_3Fe/rGO composite could reach 6 wt.% H_2 only within 100 s at 100 °C, while for MgH_2 doped with each individual components Ni_3Fe, Ni/rGO and Fe/rGO all required more than 500 s to uptake 3 wt.% hydrogen under the same condition. The composite started to release hydrogen at 185 °C, much lower than that of the MgH_2 doped with 5 wt.% Ni_3Fe (205 °C), Ni/rGO (210 °C) or Fe/rGO (250 °C). The results show that the synergetic effect among rGO and in-situ formed active species (Mg_2Ni and Fe) is responsible for the catalytic mechanism on hydrogen storage of MgH_2. Meanwhile, this study supplies innovative insights to design high efficiency catalysts based on the LDH precursor.

提升燃料电池最大功率密度 48%的液滴动力学理论和微流场实验验证

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摘要：微流场是改善质子交换膜燃料电池（PEMFC）输出性能的重要策略。阐明微通道中的液滴动力学行为及其对水管理的影响至关重要。基于流体力学模型的理论分析表明，对于相同半径的液滴，由于特征尺寸的匹配，微通道内液滴的最大驱动压差将增加约 560%。在相同的操作条件和膜电极条件下，PEMFC 中的微流场（0.5mm×0.5mm 通道）比 PEMFC 中的正常流场（1mm×1mm 通道）提高了约 48%的最大功率密度。同时，具有微流场的质子交换膜燃料电池可以在不增加空气湿度的情况下获得最优异的性能。它的自增湿特性使其在将来具备取消辅助系统中的增湿设备的潜力。

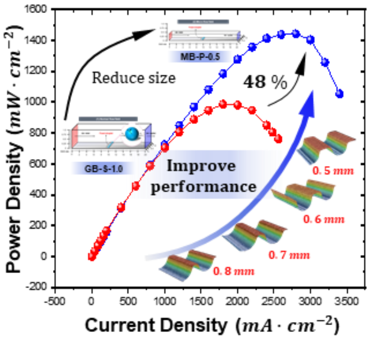

图 1 微流场单电池功率密度变化曲线
Fig. 1 Power density curve of micro flow field single cell

关键词：质子交换膜燃料电池；微流场；双极板；液滴动力学；相对湿度

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Droplets dynamics theory and micro-flow field experiments of improving self-humidifying feature and maximum power density in fuel cells

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Abstract: Micro-flow field is a preeminent stratagem for improving proton exchange membrane fuel cells (PEMFC) output performance. Elucidating the droplet dynamics behavior in the micro-channel and its impact on water management is essential. This work has investigated that, for the same radius droplets, the maximum driving pressure difference of droplets will increase by 560% approximately in micro-channel due to the matched characteristic dimension through theoretical analysis based on the fluid mechanics model. The micro-flow field ($0.5\,mm \times 0.5\,mm$ channel) in PEMFC can promote the maximum power density by about 48% compared to the normal-flow field ($1\,mm \times 1\,mm$ channel) in PEMFC by experiments under the same operating conditions and membrane electrode assembly. Simultaneously, PEMFC with the micro-flow field can obtain the most excellent performance without humidifying the air. Its self-humidification characteristic makes it possible to cancel the humidification equipment in the auxiliary system in the future.

机器学习参与高性能燃料电池膜电极组件的设计

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摘要：在面对多变量、高维度的复杂数据时，人类研究者察觉并归纳获得可靠规律的能力是非常有限的。质子交换膜燃料电池（PEMFCs）同时涉及微观化学反应，介观物质输运和宏观水热管理，跨尺度进行建模指导非常困难。随着人工智能（AI）领域的兴起，训练机器学习算法进行跨尺度数据驱动建模被证明是一种有效的策略。通过实验数据集，我们成功训练了针对非贵金属[1]，贵金属基[2]膜电极的 AI 辅助决策优化模型，能够协助研究人员突破传统试错范式加速材料性能优化。除此之外，为了更好地让研究者与 AI 互动协同进步，我们将可解释方法[3,4]引入用于剖析 AI 黑箱模型，并证实 AI 拥有数据挖掘并获得不同于人类研究者的独特而可靠的见解的能力。

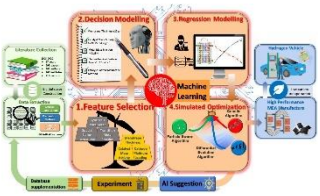

图 1 AI 辅助设计膜电极优化闭环工作流程示意图
Fig. 1 Schematic of AI-aided close-loop MEA optimization workflow

关键词：质子交换膜燃料电池；机器学习；膜电极；人工智能；催化剂

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Machine learning participates in the design of high-performance membrane electrode assemblies in PEMFCs

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Abstract: When faced with multivariate, high-dimensional and complex data, human researchers have very limited ability to detect and generalize to obtain reliable laws. Proton exchange membrane fuel cells (PEMFCs) also involve micro-chemical reactions, mesoscopic material transport, and macro-hydrothermal management. It is very difficult to conduct cross-scale modeling and guidance. With the rise of the field of artificial intelligence (AI), training machine learning algorithms for cross-scale data-driven modeling has proven to be an effective strategy. Through the experimental data set, we successfully trained the AI-assisted decision-making optimization model for non-precious metals [1] and precious metal-based [2] membrane electrodes, which can assist researchers to break through the traditional trial and error paradigm and accelerate material performance optimization. In addition, in order to better allow researchers to interact with AI and make progress together, we introduce interpretable methods [3,4] to analyze AI black box models, and prove that AI has unique data mining and obtains unique and reliable data mining. The ability to insight.

空气暴露对 Ni 催化的 Mg-Al 基氢化物的影响

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摘要：空气稳定性是镁基储氢材料在实际应用中亟需解决的关键问题之一。本文比较研究了空气暴露前后添加微米/纳米 Ni 的 Mg-Al 基合金氢化物的脱氢性能。随着空气暴露时间的增加，$Mg_{90}Al_{10}$-5microNi-air样品的脱氢峰值温度逐渐升高，而$Mg_{90}Al_{10}$-5nanoNi-air样品的低温主导脱氢峰峰值温度稳定在 256 ℃。暴露于空气中 5 天后，$Mg_{90}Al_{10}$-nanoNi-air 样品能够在 300 ℃下 2,800 s 内能释放 5.0 wt.% H_2，保留了优异的脱氢动力学。X 射线衍射（XRD）和扫描电子显微镜（SEM）表明，均匀分散的纳米 Ni 颗粒比微米 Ni 具有更大的与 Mg-Al 合金的接触面积和更高的催化活性，X 射线光电子能谱（XPS）分析表明，空气暴露后只有少量 Ni 转变为 $Ni(OH)_2$，大部分 Ni 以单质态存在。红外光谱（IR）分析表明，球磨中 Ni 的添加能有效地阻止 $Mg(OH)_2$ 的生成。添加纳米 Ni 的 $Mg_{90}Al_{10}$ 在空气暴露后具有优异的低温脱氢性能，归因于均匀分散的单质态纳米 Ni 保留了优异的纳米诱导效应。在球磨过程中，Al 和 Ni 颗粒也有效地包覆 MgH_2，起到了良好的抗空气毒化作用。本研究对开发高活性、高稳定性的储氢材料具有重要的指导意义。

Abstract： Air stability is one of the key challenges to be solved in practical application of magnesium-based hydrogen storage materials. The dehydrogenation properties and microstructure of Mg-Al-based hydrides with micro/nano-Ni added before and after air exposure were compared and studied. With the increase of air exposure time, the peak dehydrogenation temperature of $Mg_{90}Al_{10}$-5microNi-air gradually increased, while the low-temperature peak dehydrogenation temperature of $Mg_{90}Al_{10}$-5nanoNi-air remained unchanged at 256 °C. After being exposed to air for 5 days, $Mg_{90}Al_{10}$-nanoNi-air can release 5.0 wt.% H_2 in only 2,800 s at 300 °C, maintaining quite excellent dehydrogenation kinetics. X-ray diffraction (XRD) and scanning electron microscopy (SEM) show that the uniformly dispersed nano-Ni particles have larger contact area with $Mg_{90}Al_{10}$ and higher chemical reaction activity than micro-Ni. X-ray photoelectron spectroscopy (XPS) analysis shows that after air exposure, only a small amount of Ni was transformed to $Ni(OH)_2$ and most Ni is in the state of simple substance. Infrared (IR) analysis shows that the addition of Ni can effectively prevent the formation of $Mg(OH)_2$. $Mg_{90}Al_{10}$ with nano-Ni added has excellent low-temperature dominant dehydrogenation performance after air exposure, which is attributed to the uniformly dispersed simple state nano-Ni, retaining outstanding nano-inducement. Al and Ni particles also effectively coated MgH_2 during ball milling and played a good role in anti-air poisoning. Studying the effects of air exposure on the hydrogen storage properties is critical for developing applicable hydrogen storage materials.

质子交换膜燃料电池低铂电极的极化行为研究

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摘要：发展高性能的低铂载量质子交换膜燃料电池（PEMFC）是氢能应用体系中的关键技术之一。多孔催化层作为其核心部件，通常由传导质子的离聚物和催化剂（Pt/C）组成，其内部的多相结构是决定气体分子、电子和质子的传输动力学的重要因素。因此，区分催化层中各传输过程引起的极化损失、研究铂载量对各传输过程的动力学特性的影响对优化低铂催化层的结构和提高铂利用率具有指导意义。在本工作中，我们将多种实验表征手段与多尺度模拟结合，在全面考虑催化层内质子的传导、气体在各种孔道中和离聚物薄膜中的传输、以及催化剂表面的电化学反应等多种过程及其耦合的基础上，详细研究了不同铂载量催化层的极化行为。结果显示，在校正催化层中的质子传输阻抗和氧气的大孔扩散传输阻抗，并将电流归一化到单位铂表面积后，不同铂载量膜电极的 Tafel 曲线基本重合。这表明氧气在铂表面的离聚物薄膜中的扩散是一个与催化层铂载量无关的本征过程，并不存在目前普遍认为的低铂催化层中铂表面的局域气体扩散阻抗显著增大的现象。

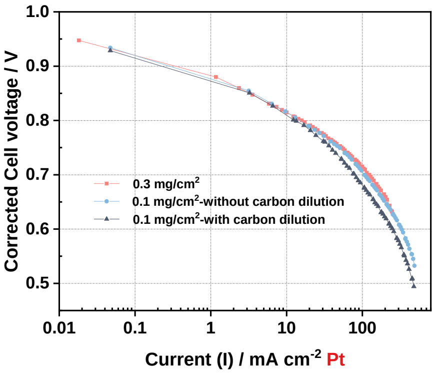

图 1 扣除 $R(H^+)$、HFR 及氧气分子扩散阻抗后的 Tafel 曲线

Fig. 1 Tafel curves after HFR, electrode proton resistance, bulk transport, and hydrogen cross over correction

关键词：催化层；铂载量；传输阻抗；多尺度介观模拟

Deconvolving the Polarization Loss in Low-Pt PEMFC Electrodes

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Abstract: High-performance and low-platinum (Pt) proton exchange membrane fuel cells (PEMFCs) are among the key technologies in the hydrogen energy system. Understanding the Pt-loading effects on the kinetic characteristics of various transport processes in the catalyst layers (CLs) is an effective route to break the usual Pt loading reliance of PEMFC performance. The CLs are comprised of assemblies of ion-conducting ionomers and agglomerates of catalysts (Pt/C), which should form internal porous structures delicately balancing the transport kinetics of the gas molecules, electrons and protons. Due to those various physiochemical processes in CLs are highly coupled, to distinguish the contributions of various processes in a CL to the polarization loss plays a guiding role in the optimization of CL structure and improvement of Pt utilization. In this work, PEMFC electrodes with various catalyst loadings (CL thickness) are fabricated, and the constitutions of their polarization losses are analyzed by a variety of characterization approaches. The results showed that after correcting the polarization losses caused by the proton transport resistance and the molecular diffusion resistance of O_2, very similar polarization curves of platinum surface area-normalized current density against overpotential are obtained, regardless of platinum loadings, which indicates that the diffusion of O_2 in the ionomer film on the platinum surface, the so-called local transport resistance, is an intrinsic property that is independent on the platinum loading of the CL.

具有高性能氧还原反应催化活性的 PtNi$_x$Cu$_{3-x}$ 纳米催化剂

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摘要：质子交换膜燃料电池（PEMFCs）由于其高能量效率以及绿色无污染等优点而被广泛关注[1]。PtCuNi 合金可能具有较高的氧还原反应催化活性[2]。本文通过切换气氛的方法，合成了不同比例的 PtNi$_x$Cu$_{3-x}$ 纳米颗粒。SEM 结果显示， PtNi$_x$Cu$_{3-x}$ 纳米颗粒随着 Ni-Cu 比例的变化而呈现从十二面体到直径的变化。ORR 表征结果表明，不同比例的 PtNiCu 均对氧还原具有优良的催化活性，其中 PtNi$_{1.5}$Cu$_{1.5}$ 氧还原活性最高，半波电势约比商业 20wt%Pt/C 的氧还原催化活性正移 140mv。

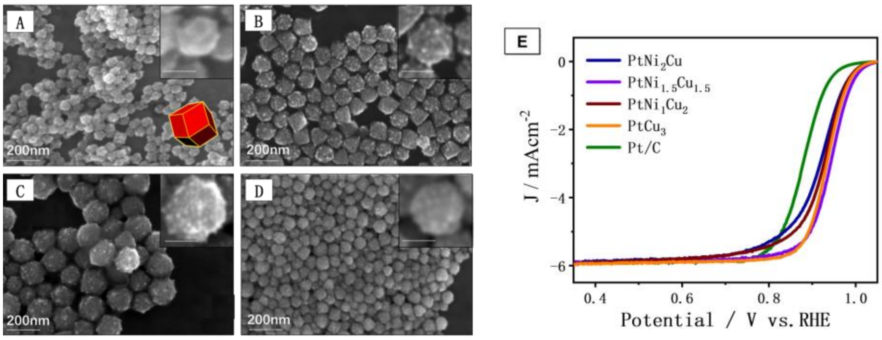

图 1（A-D）：PtNi$_2$Cu（A），PtNi$_{1.5}$Cu$_{1.5}$（B），PtNiCu$_2$（C），PtCu3（D）的 SEM 表征，内嵌图片标度为 50nm；（E）氧还原极化曲线

Fig. 1 (A-D): SEM images of PtNi2Cu (A), PtNi1.5Cu1.5 (B), PtNiCu2 (C), PtCu3 (D) with embedded image scale of 50 nm; (E): Oxygen reduction polarization curve

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PtNiCu nanocatalysts with high catalytic activity for oxygen reduction Reaction

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Abstract: As a clean and efficient energy conversion technology, the large-scale application of fuel cells is limited by the slow kinetics of the oxygen reduction reaction (ORR) and the high price of Pt as a cathode catalyst. PtCuNi alloy may have higher catalytic activity for oxygen reduction reaction [2]. In this work, we used oleylamine as the solvent, protective agent and reducing agent to synthesize PtNi$_x$Cu$_{3-x}$ nanoparticles in different proportions at 270°C by switching the atmosphere. SEM results show that PtNi$_x$Cu$_{3-x}$ nanoparticles changes from the Ni-Cu ratio. The change from the dodecahedron to the diameter. Different proportions of PtNi$_x$Cu$_{3-x}$ nanoparticles were loaded on carbon and electrochemically dealloyed, and then they were electrochemically characterized. ORR characterization results show that P different proportions of PtNi$_x$Cu$_{3-x}$ have excellent catalytic activity for oxygen reduction. Among them, PtNi1.5Cu1.5 has the highest oxygen reduction activity, and its half-wave potential is about 20wt% more than commercial Pt. The catalytic activity of /C for oxygen reduction is moving forward by 140mV.

针对便携式燃料电池的块体海绵硼氢化钠水解制氢催化剂

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摘要：本文研制了一种用于 $NaBH_4$ 水解的将无定形硼化钴纳米颗粒均匀沉积在表面的块体聚乙烯醇缩甲醛(PVFM)海绵催化剂。$NaBH_4$ 的水解局限在海绵孔隙内，没有可见液体，因此简化了制氢体系。该体系在一个轻质的塑料容器中就可以实现约 200 mL min^{-1} 的稳定产氢，而且水解运行过程中体系不受放置方位的限制。反应结束后，只需将残留溶液挤出即可回收催化剂。由于这些独特的优势，块体海绵催化剂非常有希望开发高效、易于操作的 50 W 规模的便携式燃料电池在线制氢系统。

关键词：燃料电池；$NaBH_4$ 水解；块体海绵；在线制氢

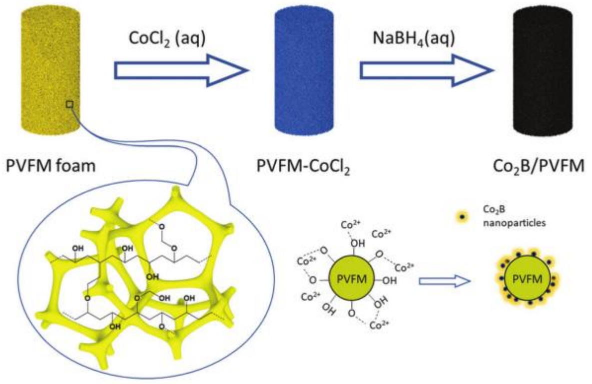

图 1 Co_2B/PVMF 海绵催化剂的制备过程示意图

A monolithic sponge catalyst for hydrogen generation from sodium borohydride solution for portable fuel cells

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Abstract: A monolithic sponge catalyst composed of amorphous cobalt boride nanoparticles homogeneously de-posited on the fibers of a commercial polyvinyl formal (PVFM) sponge is developed for the hydrolysis of $NaBH_4$. The hydrolysis of $NaBH_4$ is confined within the pores of the sponge without visible liquid，which significantly simplifies the H_2 generation system. Steady H_2 generation of about 200 mL min^{-1} can be achieved in a light weight plastic container. There is no restriction on the orientation of the H_2 generation unit during operation. The catalyst can be easily recycled after reaction by simply squeezing out the residual solution. Due to these unique advantages, the monolithic sponge catalyst is highly promising to develop high efficiency, easy to operate onsite H_2 generation systems for 50 W scale portable fuel cells.

氢气长管拖车泄露事故后果模拟研究

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摘要：长管拖车是目前氢气的主要运输方式，相较于其他危险品运输车辆其安全问题没有受到应有的重视。本文将氢气长管拖车视为移动点源，通过构建基于高斯烟团模型的移动场景下氢气扩散模型来量化氢气泄露事故的影响范围。首先，通过数值模拟计算地面氢气的等浓度曲线，然后根据氢气浓度将氢气泄露事故的威胁区域划分为代表不同危害等级的子区域，最后结合气象信息建立考虑风向变化的氢气泄露事故的风险热力图。将上述模拟过程应用在实例中，得到的结果对事故现场的应急处置以及运输路线的合理规划有重要的参考价值。

关键词：长管拖车；氢气运输；泄露扩散；模拟；高斯烟团模型

Simulation study on the consequence of hydrogen leakage accident involving long-tube trailer

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Abstract: Long tube trailer is the main transportation mode of hydrogen nowadays. Compared with other dangerous goods transport vehicles, its safety problem has not been paid much attention. In this paper, the hydrogen long tube trailer is regarded as a moving point source, and the hydrogen diffusion model in the moving scene based on the Gaussian smoke cloud model is constructed to quantify the impact range of hydrogen leakage accident. Firstly, the isoconcentration curve of hydrogen on the ground was calculated by numerical simulation. Then, the threat region of hydrogen leakage accident was divided into several sub-regions representing different hazard levels according to the hydrogen concentration. Finally, the risk heat map of hydrogen leakage accident considering the change of wind regime was established based on meteorological information. The simulation process is applied to an example, and the results are of great reference value to the emergency treatment on the accident site and the rational planning of the transportation route.

多孔泡沫铜对大长径比管道中氢-空气预混气体燃爆特性的影响

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摘要: 氢能作为一种清洁能源，其安全使用对市场化推广至关重要。本研究利用 10PPI、20PPI、30PPI、40PPI 和 60PPI 五种孔径的泡沫铜在单块、大间隔以及连续泡沫铜板材三种实验方案下研究其对长管道（长径比 108）中当量比 Φ=1 的氢-空气预混气体的阻火抑爆能力。研究结果表明：60PPI 连续泡沫铜板材实验方案下，可有效阻止火焰向管道下游传播，上游管道压力仅为 60kPa，火焰传播速度 25m/s。火焰猝熄过程中发现了“负压抽吸”现象。随着泡沫铜孔径减小，冲击波超压与火焰传播速度随之减小。对于单块泡沫铜板，其结构强度较低，抗冲击性能较弱，未能起到阻火作用，在反射激波与火焰的作用下板材断裂；对于大间隔泡沫铜，可有效阻止下游激波与火焰的反射冲击。

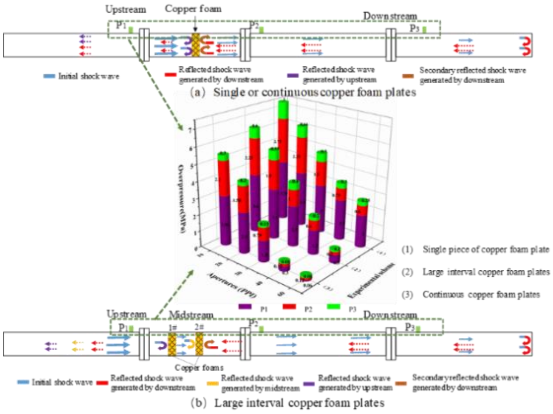

图 1. 不同实验方案下的冲击波传播过程

Fig.1 Propagation process of shock waves under different experimental schemes

关键词：氢气；泡沫铜；DDT；大长径比

Influence of porous copper foam on the explosion characteristics of hydrogen-air premixed gas in a pipe with large aspect ratio

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Abstract: As a kind of clean energy, the safe use of hydrogen is essential to market promotion. In this work, the fire and explosion suppression performance of copper foams with five apertures of 10 PPI, 20 PPI, 30 PPI, 40 PPI and 60 PPI were investigated under three experimental schemes of single piece of copper foam, large interval and continuous copper foams. The experiments were carried out in a circular cross-sectional pipe with aspect ratio of 108 for the premixed stoichiometric hydrogen-air mixtures. The results show that continuous copper foams with aperture of 60 PPI can effectively prevent flame from spreading to the downstream of the pipe and make flame quenching. The phenomenon of "negative pressure suction" was observed in the flame quenching process. The upstream overpressure was reduced to 60 kPa and the flame propagation velocity was 25 m/s. As the aperture of copper foam decreased, the shock wave overpressure and flame propagation velocity decreased. The process of deflagration to detonation transition was effectively inhibited. For a single piece of copper foam, it failed to play a role in fire resistance. Large interval copper foams can effectively prevent the reflection impact of shock waves and block the flame from downstream.

通过 TiFe 和碳纳米管的作用实现 MgH_2 的优异储氢性能

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摘要：多种催化剂对改善氢化镁的储氢性能表现出很高的活性。在此，我们成功地制备了 TiFe 作为一种优良的催化剂，然后通过球磨法掺入氢化镁中，以改善氢化镁在低温下的脱/再氢化性能。与制备的 MgH_2 相比，在 MgH_2 中加入 15wt%-TiFe 后，起始脱附温度可降至 175℃。此外，在 300℃下，10wt%-TiFe 掺杂的 MgH_2 在 10 分钟内释放了大约 6.5wt%的 H_2，并且在 125℃的低温下，在 3MPa 的氢气压力下可以快速吸收 5.3wt%的 H_2。此外，碳纳米管（CNTs）的额外掺入均匀地分布在 MgH2 颗粒的表面，使 MgH_2 + 10 wt%-TiFe + 5wt%-CNTs 复合材料具有出色的循环性能。掺入 TiFe 和 CNTs 后，MgH_2 的氢化激活能从 72.5± 2.7 kJ/mol 降低到 60.7±8.0 kJ/mol。然而，添加 TiFe 和 CNTs 对 MgH_2 的热力学性能影响有限。XRD、TEM、SEM 和 EDS 的分析表明，均匀分布的 TiFe 和 CNTs 在提高 MgH_2 的储氢性能方面分别起到了活性催化单元和防止聚集的作用。

关键词：氢化镁；TiFe 碳纳米管；催化机理

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Achieving superior hydrogen storage properties of MgH_2 by the effect of TiFe and carbon nanotubes

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Abstract: Multiple catalysts have exhibited high activity on improving the hydrogen storage performance of magnesium hydride. Herein, TiFe as a superior catalyst was successfully prepared, and then doped into MgH_2 via ball milling to improve the de/rehydrogenation properties of MgH_2 at low temperatures. Compared with as-prepared MgH_2, the onset desorption temperature could be reduced to 175 ℃ after adding 15 wt%-TiFe to MgH_2. Furthermore, the 10 wt%-TiFe doped MgH_2 released approximately 6.5 wt% H_2 within 10 min at 300 ℃, and 5.3 wt% H_2 could be rapidly absorbed at low temperature of 125 ℃ under hydrogen pressure of 3 MPa. Moreover, the additional doping of carbon nanotubes (CNTs) evenly distributed on the surface of MgH_2 particles, enabling the MgH_2 + 10 wt%TiFe + 5wt%-CNTs composite with outstanding cycling performance. The activation energy of hydrogenation for MgH_2 was reduced from 72.5 ± 2.7 kJ/mol to 60.7 ± 8.0 kJ/mol after doping with TiFe and CNTs. However, the addition of TiFe and CNTs had limited influence on the thermodynamic properties of MgH2. The analysis of XRD, TEM, SEM and EDS indicated that uniformly distributed TiFe and CNTs served as active catalytic unit and aggregation preventer on enhancing the hydrogen storage properties of MgH_2, respectively.

Photocatalytic hydrogen production versus photocatalyst dimension under concentrated solar light: a case over titanium dioxide

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Abstract： Revealing photocatalyst behavior under different light intensities is of significance for the design of photocatalytic reaction system under real solar energy. To this end, we systematically explored the evolution of physicochemical properties of nanoparticle slurry and their hydrogen production under concentrated solar light irradiation over TiO_2 of different dimensions, i.e., nanosphere, nanorod, and nanosheet. Interestingly, monotonously enhanced hydrogen production activities versus increasing light intensity up to 11 suns (1 sun = 1 $kW \cdot m^{-2}$) were observed for nanorods and nanosheets. However, hydrogen production exhibited an initial rapid increase and then an obvious falling tendency for nanospheres once the light intensity beyond 8 suns. It was revealed that nanospheres slurry with higher thermal conductivity and lower viscosity under higher light intensity resulted in heavier particle agglomeration due to the stronger collision tendency among particles, hence, decreased light absorption and lowered reaction temperature. Consequently, fewer photo-induced charge carriers and slower reaction kinetics resulted in the falling tendency of hydrogen production under high light intensities over nanosphere TiO_2. We believe that this work could provide a useful guidance for designing optimal photocatalytic slurry reaction system under concentrated solar light.

MOF 衍生的一维多孔碳纤维纳米限域氢化镁及吸放氢机理研究

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摘要：较高的放氢温度和较慢的吸放氢速率严重限制了氢化镁的实际应用。本文通过模板法热解 MOF 材料，合成了一种具有高比表面积的一维多孔碳纤维（pCNF），并将其作为框架材料对氢化镁进行纳米限域。该复合材料具有优异的吸放氢性能和循环稳定性，在 200°C 就可实现可逆吸放氢，甚至在 100°C 的低温便可以吸氢，放氢活化能降低到了 96KJ/mol H_2。研究表明，该复合材料性能的改善得益于三方的协同效应：多孔碳纤维限域氢化镁纳米颗粒，从而有效抑制氢化镁吸放氢过程中的长大和团聚；N 掺杂的碳纤维具有优良的给电子性能，加速了循环过程中的电子转移；原位形成的 Mg_2Ni/Mg_2NiH_4 起到“氢泵”的作用，促进了氢气分子的解离和扩散。该研究不仅拓宽了 MOF 材料的应用领域，同时为其他氢化物的纳米限域提供了更多的框架材料的选择范围。

关键词：氢化镁；金属有机框架材料；镍；纳米限域；储氢

Rational design of MOF derived 1D N-doped hierarchically porous carbon nanofibers to confine MgH_2 for enhanced hydrogen storage performances

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Abstract: The widespread application of MgH_2 is restricted by the high desorption temperature and sluggish kinetics. 1D N-doped hierarchically porous carbon nanofibers (pCNF) with high specific surface area are synthesized by pyrolysis of MOF, and then MgH_2 nanoparticles decorated by Ni are self-assembled on pCNF. The formed nanocomposites show faster desorption kinetics ($E_a = 96$ kJ/mol H_2) along with high hydrogen capacity (up to 4 wt.% at 275 °C) over long-term cycling. The composites start to release hydrogen at 200 °C, which is 150 °C lower than that of the commercial MgH_2, and rehydrogenation could be achieved even at 100 °C. The synergetic effects of nanoconfinement of pCNF, electron-donating ability of N atoms and “hydrogen pump” mechanism derived from Mg_2Ni/Mg_2NiH_4 are contributed to the optimized hydrogen storage performances. It is believed that the well-controlled 1D N-doped hierarchically porous carbon nanofibers not only extend the application scope of MOF derived carbon materials, but also provide guidance in designing efficient scaffolds for the self-assembling of other metal hydrides nanoparticles.

中空 ZIF-67@ZIF-8 核壳结构衍生物对 MgH_2 储氢性能的改性研究

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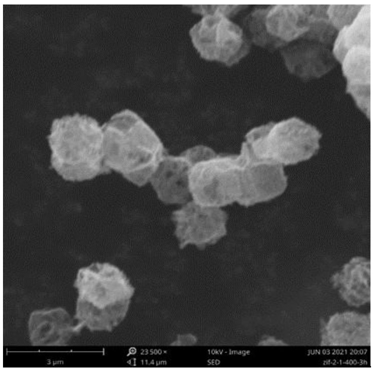
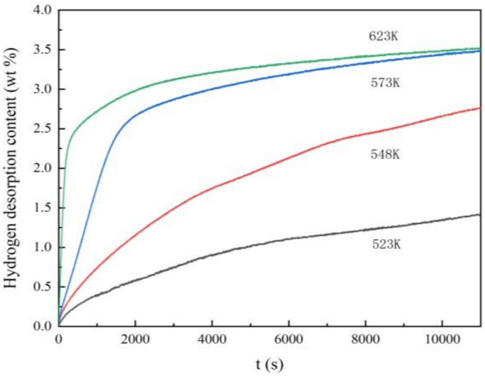
摘要：氢化镁（MgH_2）凭借其较高的储氢容量（7.6 wt%）和良好的循环性能等优点，被认为是极具应用前景的固态储氢材料。但是，稳定的热力学性能和缓慢的动力学性能严重阻碍了其大规模商业化应用。因此，该工作通过溶剂热及后续的热处理工艺，成功制备了一种中空 ZIF-67@ZIF-8 核壳结构衍生物，并将其作为框架材料，促进 MgH_2 纳米颗粒的形核。在纳米限域和原位形成的金属 Co 催化的协同作用下，MgH_2 的放氢活化能降至 127.47 kJ/mol，放氢速率显著提升，起始放氢温度降至 250 ℃以下。该工作为制备高性能的储氢材料提供了新思路。并且，该衍生物的多孔性有利于其他协同催化金属粒子的掺杂。





关键词：氢化镁；纳米限域；储氢性能

Improving hydrogen storage performances of MgH_2 through nanoconfinement in hollow ZIF-67@ZIF-8 core-shell structure derivant

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Abstract: Magnesium hydride (MgH_2) has been regarded as one of the most promising solid-state hydrogen storage materials, due to high hydrogen capacity (7.6 wt%) and good cycling performance. However, high dehydrogenation temperature and poor kinetic restrict its widespread application. Herein, hollow Zn/Co metal-organic framework derivant, synthesized by solvothermal method and subsequent heat treatment, was used as scaffold to support MgH_2 nanoparticles. Benefitting from the nanoconfinement effect and in-situ catalysis of Co, the desorption activation energy of MgH_2 for decreases to 127.47 kJ/mol and the onset temperature of dehydrogenation reduce to 250 ℃. Our work gives lights to the fabrication of hydrogen storage materials with remarkable performances. Moreover, the intrinsic porosity of the framework allows introduction of other co-catalytic metal particles, which may further improve the hydrogen storage performance of MgH_2.

考虑碳沉积效应的阳极支撑合成气燃料电池基本反应动力学模型

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摘要：固体氧化物燃料电池（SOFC）可以在 600-800℃的高温下将燃料的化学能直接转化为电能，SOFC 的高温运行使其不仅可以使用氢气，还可以使用含碳燃料，如合成气、天然气和沼气等。当使用碳氢化合物燃料时，尽管使用外部重整器可以在一定程度上避免碳沉积，但合成气中的 CO、CO2 和 CH4 的存在仍可能导致阳极处的碳沉积。因此建立了考虑碳沉积效应的阳极支撑固体氧化物燃料电池（SOFC）一维瞬态基本反应动力学模型。该模型考虑了非均相元素化学和电化学反应、电极微观结构以及电荷和质量传输过程的耦合效应。通过实验中的 I-V 曲线和电化学阻抗谱对模型进行了验证。模拟结果与实验数据吻合较好。进一步研究了操作条件对表面碳沉积的影响。

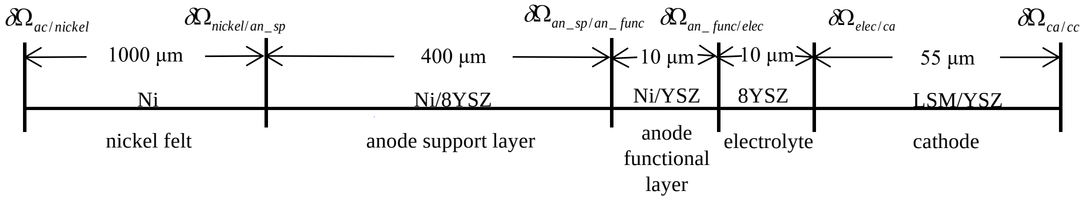

图 1 阳极支撑 SOFC 的一维几何模型和计算域

Fig. 1 Model Geometry and Calculation Domain of The Anode-supported SOFC.

关键词：固体氧化物燃料电池；积碳；一维瞬态模型；电化学阻抗谱

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Elementary Reaction Kinetic Model of An Anode-supported Syngas Fueled Solid Oxide Fuel Cell Considering The Carbon Deposition Effect

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Abstract: Solid oxide fuel cells (SOFC) can convert the chemical energy of the fuel into electricity directly at high temperatures between 600-800ºC, the high temperature operation of the SOFCs enables it to use not only hydrogen but also carbon-contained fuels, such as syngas, natural gas, and biogas, etc. When using hydrocarbon fuels, although the carbon deposition can be avoided to an extend by using an external reformer, the existence of CO, CO_2 and CH_4 in the syngas may still lead to carbon deposition at the anode. A one-dimensional transient elementary reaction kinetic model of an anode supported solid oxide fuel cell (SOFC) fueled with syngas is developed considering the carbon deposition effect. This model incorporates the coupling effect of heterogeneous elementary chemical and electrochemical reactions, the electrode microstructure and the charge and mass transport processes. The model is validated by both experimental I-V curves and electrochemical impedance spectra. The simulation results agree reasonably well with the experimental data. The effects of the operation conditions on surface carbon deposition were further studied.

无人机固体氧化物燃料电池推进系统的尺寸设计与仿真

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摘要：续航时间短是无人机应用的关键障碍之一。与储能电池相比，用燃料电池的推进系统可以提高动力系统的能量密度，进一步延长巡航时间。固体氧化物燃料电池（SOFC）相比其他的燃料电池具有能够使用碳氢燃料的优势，碳氢燃料的储能密度比氢气高得多。设计了无人机应用背景下的 SOFC 推进系统。进一步研究了 SOFC 和储能元件之间的功率分配问题。开发了一个系统模型，包括 SOFC 电堆、催化部分氧化（CPOx）重整器、尾气燃烧器、热交换器、能量管理模块等。为满足无人机的功率和能量需求，合理选择了 SOFC 电堆和其他部件的设计参数，并制定了基于规则的能量管理策略。该系统的额定功率 265.5W，具备启动和正常工作两种模式。该模型为无人机-固体氧化物燃料电池系统的设计和仿真提供了有用的工具。

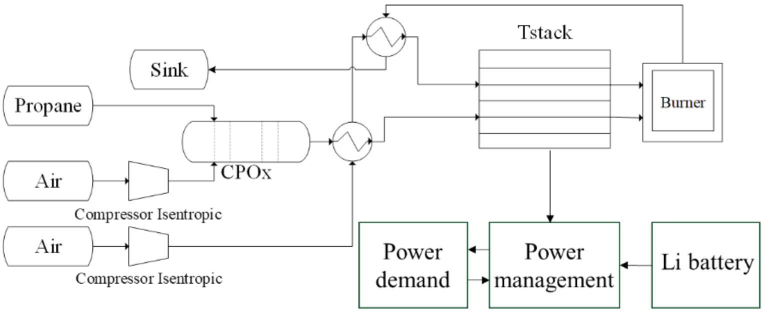

图 1 基于无人机的 SOFC 推进系统示意图

Fig. 1 Schematic of the SOFC-Based UAV Propulsion System

关键词：固体氧化物燃料电池；无人机推进系统；尺寸设计；能量管理

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Sizing Design and Simulation of An SOFC Propulsion System for Unmanned Aerial Vehicles

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Abstract: The short flight endurance is one of the key obstacles for the application of unmanned aerial vehicles (UAVs). Applying the fuel cells as the propulsion system of UAVs instead of batteries can increase the energy density and further lead to a longer cruise duration. Compared to other kinds of fuel cells, the solid oxide fuel cell (SOFC) is advantageous for its ability to use hydrocarbon fuels with a much higher energy storage density than hydrogen. In this paper, a SOFC propulsion system is sized and designed for UAV applications. The power allocation between the SOFC and energy storage components was further studied. A system model was developed, including an SOFC stack, a catalytic partial oxidation (CPOx) reformer, an after burner, heat exchangers, and energy management model, etc. The design parameters of the SOFC stack and other components were selected to meet the power and energy demand of the UAV. A rule-based energy management strategy is formulated. The rated power of the system is 265.5w and has two modes of start-up and normal operation. The model is proved to be a useful tool for the design and simulation of the UAV-SOFC systems.

阳极厚度对直接 NH_3 固体氧化物燃料电池性能影响探究

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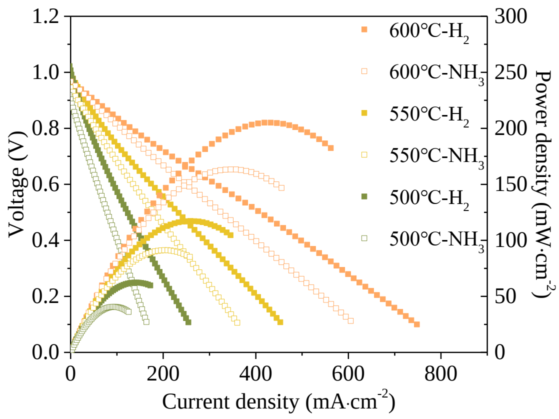
摘要：氨作为一种良好的氢载体，无碳，氢容量大于液氢。它作为燃料电池的一种很有前途的燃料，相对便宜，易于储存和运输，而且任何泄漏都很容易被其刺鼻的气味所检测到，因此相对安全[1]。固体氧化物直接 NH_3 燃料电池(DA-SOFC)能够高效地将 NH_3 转化为电能，是最有望商业化的直接氨发电技术。本研究基于直接氨固体氧化物燃料电池(DA-SOFC)在较低工作温度下的氨分解不完全问题，详细探索了质子导体 Ni-BCZY/BCZY/BSCF 燃料电池的制备工艺，确定了燃料电池的工艺参数;以 H_2、NH_3 为燃料，在 500~600°C下，测试其在不同阳极厚度燃料电池上的性能，表征其微观结构和性能。

关键词：质子导体；固体氧化物燃料电池；NH_3 催化分解



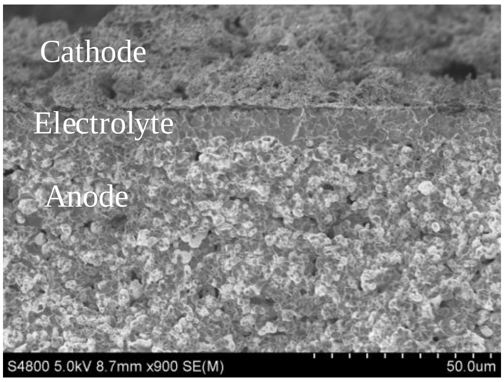


图 1. 500~600°C下质子导体 NH_3-SOFC 及 H_2-SOFC 电化学性能 图 2.阳极支撑单电池截面扫描电镜图

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燃料电池用超薄非标密封材料压缩率的研究

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摘要：燃料电池密封件厚度<1 mm，不能根据传统机械静密封进行设计。通过研究质子交换膜燃料电池密封件的压缩率问题，考察了双极板表面粗糙度、平面度以及热膨胀对密封件压缩率的影响。结果表明，双极板的表面粗糙度与平面度对燃料电池密封有重要影响，而且平面度的影响较大，这对双极板的加工和电堆装配精度有更高要求。热膨胀因素对密封件压缩率的影响可以忽略。实际燃料电池密封件的压缩率范围须达到 34.7 %~49.7 %。

关键词：燃料电池；压缩率；表面粗糙度；平面度

Compressibility of ultra-thin non-standard sealing materials for fuel cells

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Abstract: The thickness of fuel cell seal is less than 1 mm, so it cannot be designed according to the traditional mechanical static seal. The compressibility of seals for proton exchange membrane fuel cells was studied. And the effects of surface roughness, flatness and thermal expansion of bipolar plates on the compressibility of seals were investigated. The results showed that the surface roughness and flatness of the bipolar plate had an important impact on the seal for fuel cell. And the flatness had a greater impact, which required higher machining accuracy of the bipolar plate and stack assembly. The influence of thermal expansion on the compressibility of seals could be ignored. The compression ratio of seal for the actual fuel cell should reach 34.7% - 49.7%.

燃料电池金属双极板极端状况下的电化学腐蚀

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摘要：燃料电池在实际运行过程中，会出现不良的运行状态，如不良的水热管理、反应气体的饥饿等，会影响燃料电池的正常运行，严重时会造成燃料电池的损坏，如电池的金属板和膜电极的表面腐蚀，甚至发生穿孔现象。为了探究燃料电池金属板腐蚀穿孔的机理以及腐蚀影响规律，本文研究金属双极板（316L 和 304 不锈钢）在 20℃-90℃下的电化学腐蚀行为以及带镀层的 316 不锈钢金属板在高电位下的腐蚀行为。采用开路电位法（OCP）、Tafel 曲线法对金属双极板在频繁的启动/停机周期内的耐蚀性进行了分析。OCP 法试验和 Tafel 曲线法试验表明，两种不锈钢的自腐蚀电流密度的对数与温度呈线性关系，自腐蚀电流密度增加了两个数量级。316L 和 304 的点蚀电位与温度呈线性关系，而 316L 的斜率略高于 304。不同坡度下，316L 的低温点蚀电位较高，304 的高温点蚀电位较低。同时，这两种不锈钢在 90℃时均具有相同的点蚀电位 1.11V，突破了 DOE 提出的用于评价 PEMFC 金属双极板电化学腐蚀行为的温度限制。此外，采用恒电位测试方法对带镀层的 316 不锈钢金属板进行了分析，研究表明在高电位下的腐蚀速率显著提高，并得出双极板在高电位下的穿孔寿命曲线。

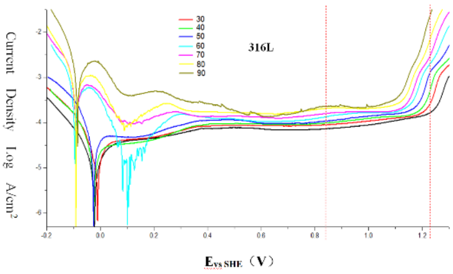

图 1 不同温度下 316L 不锈钢在不断通入空气的 $0.5MH_2SO_4+5ppmF^-$溶液的 TAFEL 曲线
Fig. 1 TAFEL curves of 316L stainless steel in $0.5MH_2SO_4+$ 5PpMF-solution continuously injected into air at different temperatures (20°C~90°C)

关键词：质子交换膜燃料电池；双极板；腐蚀

Electrochemical corrosion of metal bipolar plates in fuel cells under extreme conditions

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Abstract: In the actual operation process of fuel cell, there will be bad operation status, such as poor hydrothermal management, reaction gas starvation, will affect the normal operation of fuel cell, serious damage to fuel cell, such as the surface corrosion of the metal plate and membrane electrode of the battery, and even perforation phenomenon. In order to explore the mechanism of corrosion and perforation of fuel cell metal plate and the law of corrosion effect, the electrochemical corrosion behavior of metal bipolar plate (316L and 304 stainless steel) at 20℃-90℃ and the corrosion behavior of 316 stainless steel plate with coating at high potential were studied in this paper. Open-circuit potential (OCP) and Tafel curve method were used to analyze the corrosion resistance of metal bipolar plates during frequent start-up/shutdown cycles. OCP test and Tafel curve test show that the logarithm of the self-corrosion current density of the two kinds of stainless steel is linear with temperature, and the self-corrosion current density increases by two orders of magnitude. The pitting potential of 316L and 304 has a linear relationship with temperature, while the slope of 316L is slightly higher than that of 304.Under different slopes, the pitting potential of 316L at low temperature is higher than that of 304 at high temperature. At the same time, both stainless steels have the same pitting potential of 1.11V at 90℃, breaking the temperature limit proposed by DOE for evaluating the electrochemical corrosion behavior of PEMFC metal bipolar plates. In addition, using potentiostatic test method to analyze the 316 stainless steel plate with coating, the study shows that the corrosion rate is significantly increased at high potential, and the perforation life curve of bipolar plate at high potential is obtained.

热处理制备双壳层 Pt-Ni 合金催化剂用于质子交换膜燃料电池

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摘要：形貌可控的Pt-Ni合金在氧还原反应（ORR）中总能表现出优异的催化活性，但制备其常用的湿化学方法总不可避免地向结构中引入氧化物和多晶问题。本文通过热处理湿化学方法合成的多晶缺陷 Pt-Ni 合金，获得了具有 NiO-Pt 双层外壳和单晶 Pt-Ni 合金核的稳定结构合金，并首次观察到了伴随热处理 Pt-Ni 合金中 PtOx 和 NiO 的表面聚集现象。形成的 NiO 外壳可以方便地被去除而不影响催化剂形貌特征，被认为是一种新型的去合金化手段。以去合金化后的Pt-Ni合金催化剂制作的膜电极（MEA），最高输出功率密度达到679.8 mW/cm^2，较以商业 Pt/C 催化剂制作的 MEA 最高输出功率密度提升达 138.4 mW/cm^2。

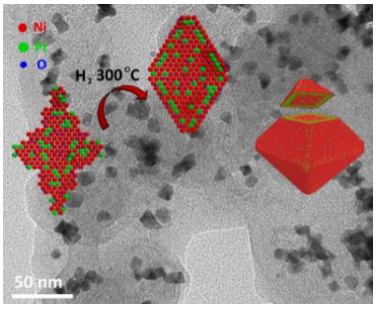

图 1 双壳层结构演化机理示意图

Fig.1 Schematic diagram of double-shell structure formed mechanism

关键词：质子交换膜燃料电池；氧还原反应；热处理；去合金化

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Thermal annealing synthesis of double-shell Pt-Ni alloy catalysts for polymer electrolyte membrane fuel cells

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Abstract: Shape-controlled Pt-Ni alloys offer an exceptional activity towards the oxygen reduction reaction (ORR). Their special structures, however, are usually fabricated by wet-chemical method which can introduce oxides and heterogeneous structures. In this paper, a novel synthesis of Pt-Ni alloys that consist of homogeneous Pt-Ni cores enclosed by NiO-Pt double shells through thermally annealing defective heterogeneous alloys obtained by wet-chemical method is reported. The outward segregation of both PtOx and NiO during annealing are first observed. The removal of NiO outer-shell could be considered as a novel dealloying method without morphological changes. The de-alloyed core-shell Pt-Ni based membrane electrolyte assembly (MEA) with 0.1 mg$_{Pt}$/cm^2 Pt loading performs a high peak power density of 679.8 mW/cm^2 under H$_2$/air, increased by 138.4 mW/cm^2 comparing with that of commercial Pt/C catalyst.

一种去合金化的高活性 $RuNiO_x$ 酸性电解水催化剂

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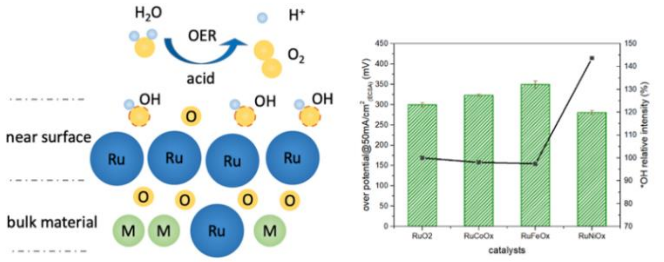
摘要：电化学电解水被广泛认为是一种可持续产生氢气的方式。我们报道了一种采用去合金化处理的 $RuNiO_x$ 催化剂，从而提高在酸性环境中的氧析出性能。经过去合金处理的 RuNiOx 能够在过电位 280 mV 的电压下达到 50 mA cm^{-2} 的电流密度，经过 10,000 次循环伏安扫描加速衰减后，仍然表现出卓越的稳定性。经过去合金处理，催化剂近表面层的镍氧化物将在酸性环境中析出，从而实现催化剂表面重构，使催化剂表面有更多的活性羟基位点，显著提升在酸性环境中的氧析出活性。



With surface MO_x leaching, lager ECSA and strengthened hydroxyl adsorption will boost OER activity.

图 1 去合金化 RuNiOx 表面重整过程

Fig. 1 Surface reconstruction schematic diagram of the dealloyed-RuNiOx

关键词：酸性电解水；氧析出；去合金

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Dealloyed RuNiOx as a robust electrocatalyst for oxygen evolution reaction in acidic media

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Abstract: Electrochemical water splitting is widely recognized as a way for the sustainable production of hydrogen. We report here the dealloying treatment on RuNiOx catalyst for enhanced acidic oxygen evolution reaction (OER) performance. Specifically, the dealloyed RuNiOx is capable to deliver a current density of 50 mA cm^{-2} at a low overpotenital of 280 mV and demonstrates a supurior stability after 10,000 potential cycles. Nickel oxides in the near surface region will be leached with surface reconstructurtion in acidic electrolyte, together with the adsorption of more reactive surface oxygenate species. A strengthened hydroxyl adsorption will promote the OER activity.

掺氢天然气对低碳钢氢脆增强作用研究

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摘要：本文采用疲劳裂纹扩展速率（FCGR）试验研究了低碳钢 20 号钢在实际天然气/氢气混合物和二氧化碳/氢气/氮气混合物中的疲劳性能。首次发现材料在掺氢天然气中的疲劳裂纹扩展速率比在氢气或天然气中要快得多。天然气/氢气混合物使材料疲劳断裂方式由延性疲劳条纹转变为脆性解理断裂，并限制了裂纹周围的塑性变形活动。天然气中的二氧化碳和氢气的协同作用有可能是导致材料在掺氢天然气中性能异常的主要原因。

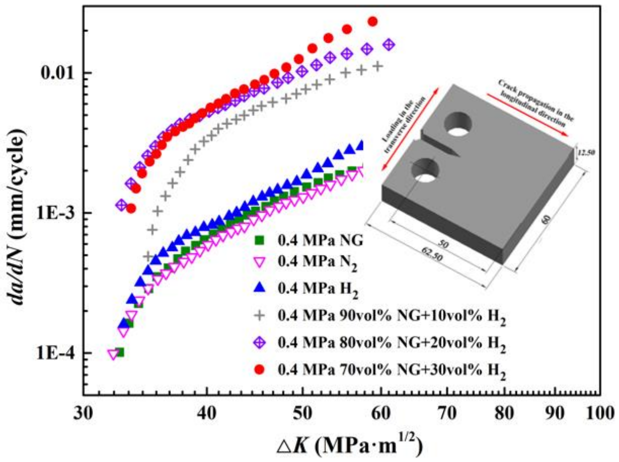

图 1 20 号钢在多种环境下疲劳裂纹扩展速率试验结果

Fig. 1 Results of FCGR tests on GB 20 grade steel in various environments

关键词：氢脆；低碳钢；EBSD；疲劳性能；掺氢天然气

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Enhanced hydrogen embrittlement of low-carbon steel to natural gas/hydrogen mixtures

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Abstract: Fatigue crack growth rate (FCGR) tests were used to investigate the fatigue property of low-carbon steel in actual natural gas/hydrogen mixtures and carbon dioxide/hydrogen/nitrogen mixtures. It is found for the first time that the acceleration of FCGRs in the mixtures are much faster than that in hydrogen or natural gas. Natural gas/hydrogen mixtures changed the fracture mode from ductile fatigue striation to brittle cleavage fracture, and restricted the deformation activities around the crack. Synergy effect of carbon dioxide and hydrogen on the material is proposed to be the major reason for the abnormal performance of steel in the mixtures.

基于压力波和中间产物对氢气内燃机爆震机理的研究

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摘要：中国作为汽车保有量大国，在能源安全与环境的全球大环境和我国的“双碳”战略下，寻求可再生清洁能源作为内燃机的替代燃料具有重要意义。氢气具有高热值、燃烧速度快、可燃极限宽以及零碳排放等优势，是一种理想的替代燃料。本文利用 CFD 数值分析的方法从压力波与火焰的耦合以及中间产物的角度研究了爆震的机理。结果表明氢气自燃位置往往是火焰锋面前距离很近的位置，并且迅速和主火焰面融合，产生压力波。压力波会促进 H、O 和 H_2O_2 等中间产物的产生，这些物质的聚集会加快 H_2O 的生成，释放大量的热量，进而增加压力波的强度，最后导致爆震的发生。因此氢气爆震是压力波和主火焰面互相增强的过程。

关键字：氢气；爆震；压力波；中间产物

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Based on the study of the detonation mechanism of hydrogen internal combustion engine based on pressure wave and intermediate product

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Abstract: As a country with a large automobile ownership, it is of great significance to seek renewable clean energy as an alternative fuel for internal combustion engine under the global background of energy security and environment and China's "double carbon" strategy. Hydrogen is an ideal alternative fuel with high heat value, fast combustion speed, wide flammable limit and zero carbon emissions. In the paper, the mechanism of knock is studied by CFD numerical analysis from the perspective of coupling of pressure wave and flame and intermediate products. The results show that hydrogen spontaneous ignition occurs on the position close to the flame front, and quickly merges with the main flame, which results in pressure wave. Pressure wave promotes the production of intermediate products such as H, O, and H_2O_2, which accelerate the generation of H_2O, releasing large amounts of heat. Finally, pressure wave is enhanced leading to knock. Therefore, knock is the process in which pressure waves and the flame reinforce each other in hydrogen engine.

掺氢体积分数对 GDI 发动机燃烧性能的影响

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摘要：氢气因其单位热值高、燃烧速度快、点火能量低、燃烧产物清洁的特点，是一种比较理想的内燃机掺混燃料。为了探究氢气对 GDI 发动机燃烧的影响，本文建立了发动机的三维模型，研究了不同掺氢体积分数对发动机性能参数的影响。结果表明，随着掺氢比例的增加，OH生成量增加，燃烧速率加快，气缸压力峰值和指示热效率增加；点火延迟、燃烧持续时间缩短；CA50 提前。HCHO 的消耗和 OH 的生成是自燃点出现的重要标志，随着点火正时提前，自燃点出现的时刻也会提前，掺氢工况爆震强度比纯汽油工况更加剧烈。

关键词：掺氢；氢气体积分数；自燃

Effect of hydrogen volume fraction on combustion performance of a GDI Engine

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Abstract： Hydrogen is an ideal blending fuel for the engine because of its high calorific value, fast combustion speed, lower ignition energy and clean products. In order to explore the effect of hydrogen on GDI engine combustion, a three-dimensional model of the engine was built and the effects of different hydrogen volume fractions on the engine performance were studied. The results show that with the increase of hydrogen blending ratio, the amount of OH increases, the combustion rate accelerates, the peak cylinder pressure and the indicated thermal efficiency increase; the delay in ignition and combustion duration decrease, the CA50 advances. The consumption of HCHO and generation of OH are important signs of the occurrence of auto-ignition. With the advance of ignition timing, the occurrence time of auto-ignition will also be advanced, the knock is more severe than that under gasoline condition.

富硒无定形 $NiSe_{1+x}$ 助剂增强光催化制氢性能与机理研究

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摘要：由于过渡金属硒化物的 Se-H_{ads} (273 kJ mol^{-1}) 与 Pt-H_{ads} (273 kJ mol^{-1}) 键能相似，因而广泛认为硒化物是最有希望取代贵金属的制氢助剂，然而它们的析氢活性仍然受到活性 Se 原子暴露不足的限制。在此，我们提出了本征活性位富集和无定形化的协同思想，进而通过温和的一步光诱导沉积法构建了富硒无定形 $NiSe_{1+x}$ 纳米点助剂，最终实现了活性 Se 位点的最大限度地暴露。光催化实验结果表明，与纯 TiO_2 和 c-NiSe/TiO_2 相比，a-$NiSe_{1+x}$/TiO_2 具有更高的光催化制氢性能。DFT 理论计算和原位辐照 XPS 测试表明：a-$NiSe_{1+x}$/TiO_2 优异的制氢活性来源于 a-$NiSe_{1+x}$ 对 TiO_2 光生电子转移的有效促进作用及大量活性 Se 可充当有效的析氢活性位点。事实上，除了 TiO_2，a-$NiSe_{1+x}$ 还可作为通用型助剂；同时，本研究中的光诱导沉积法还可用于合成其它硒化物助剂(如 a-$FeSe_{1+x}$, a-$CoSe_{1+x}$ 和 a-$CuSe_{1+x}$)。这项工作可能为构建及合成活性位富集型助剂提供新的研究思路。

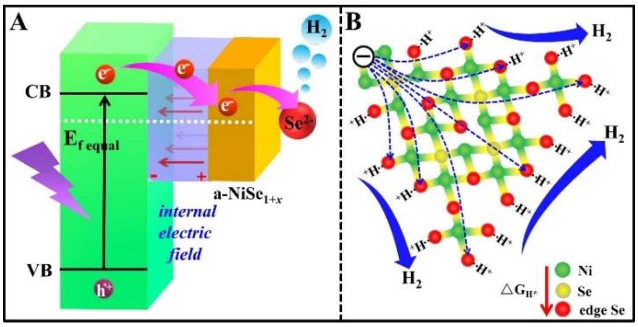

图 1 富硒无定形 $NiSe_{1+x}$ 助剂促进光生电子分离及界面析氢反应机理图
Fig. 1 Proposed photocatalytic H_2-generation mechanism of a-$NiSe_{1+x}$/TiO_2

关键词：光催化制氢；助剂；富硒；无定形

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Selenium-enriched amorphous $NiSe_{1+x}$ nanoclusters as a highly efficient cocatalyst for photocatalytic H_2 evolution

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Abstract: Transition-metal selenides have been evidenced to be the promising candidates for efficient H_2-evolution cocatalyst due to the similar Se-H_{ads} (273 KJ/mol) bond energy to Pt-H (251 KJ/mol), while their H_2-evolution activity is still limited by the insufficient exposure of active Se atoms. Herein, a synergic idea of selenium-rich configuration and amorphization was developed to construct selenium-rich amorphous $NiSe_{1+x}$ nanodots for maximumly exposing more active selenium sites. For this purpose, the selenium-rich amorphous $NiSe_{1+x}$ nanodots can be resourcefully grafted with the TiO_2 via the facile photoinduced electron-reduction way. Photocatalytic results manifeste that the selenium-rich a-$NiSe_{1+x}$/TiO_2(0.5wt%) attains a maximal H_2-production activity, which can be ascribed to the cooperation of accelerated photoinduced electron migration from TiO_2 to a-$NiSe_{1+x}$ and rapid H_2 evolution on the enriched active Se sites.

表面原位硒化构建新型核壳 Ag@AgSe$_x$ 纳米粒子实现高效光催化产氢

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摘要：尽管金属银（Ag）具有比铂（Pt）更好的导电性，但是其作为光催化产氢助剂的活性仍然十分有限。本研究通过原位表面硒化过程在金属 Ag 表面构建无定形 AgSe$_x$ 作为产氢活性中心，以提升 Ag 修饰 TiO$_2$ 材料的光催化产氢活性。这种核壳 Ag@AgSe$_x$ 结构主要通过两步实现，包括光沉积金属 Ag 助剂及金属 Ag 选择性表面硒化过程。合成的 Ag@AgSe$_x$/TiO$_2$(20μL)光催化材料具有最高的光催化产氢速率（853.0 μmol h^{-1} g^{-1}），性能分别是 TiO$_2$ 和 Ag/TiO$_2$ 样品的 11.6 和 2.4 倍。进一步通过实验及 DFT 理论计算发现，Ag@AgSe$_x$/TiO$_2$ 性能增强可以归因于核壳结构 Ag@AgSe$_x$ 助剂的协同机理，即金属 Ag 核结构可以快速分离并转移光生电子，而 AgSe$_x$ 壳可以提供丰富的产氢活性位点实现快速的界面催化反应，两者协同作用提升 TiO$_2$ 的光催化产氢活性。

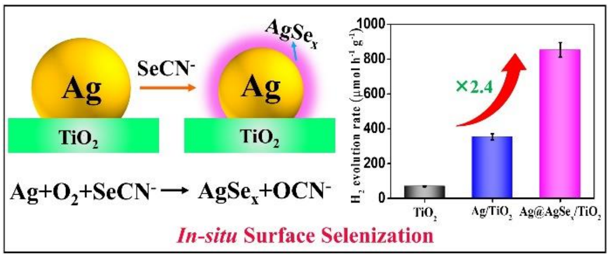

图 1 原位表面硒化及其光催化产氢性能提升示意图

Fig. 1 Schematic diagram of in-situ surface selenization and efficient photocatalytic H$_2$ production

关键词：光催化产氢；助剂；表面硒化；Ag@AgSe$_x$

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Novel core-shell Ag@AgSe$_x$ nanoparticles: In-situ surface selenization for efficient photocatalytic H$_2$ production

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Abstract: In this research, the amorphous AgSe$_x$ as a novel and excellent H$_2$-evolution active site has been in-situ fabricated on the metallic Ag surface, with the aim of promoting the interfacial H-generation rate of metallic Ag nanoparticles in Ag/TiO$_2$ system. The core-shell Ag@AgSe$_x$ nanoparticle modified TiO$_2$ photocatalysts were prepared by a two-step pathway, including the photodeposition of metallic Ag and the selective surface selenization of metallic Ag to amorphous AgSe$_x$ shell. The as-prepared Ag@AgSe$_x$/TiO$_2$(20μL) photocatalyst possesses the highest H$_2$-evolution performance of 853.0 μmol h^{-1} g^{-1}, prominently outperforming the TiO$_2$ and Ag/TiO$_2$ samples by a factor of 11.6 and 2.4 times, respectively. The promoted H$_2$-evolution rate of the Ag@AgSe$_x$/TiO$_2$ photocatalyst can be accounted by a synergistic mechanism of the Ag@AgSe$_x$ cocatalyst, namely, the metallic Ag core can quickly capture and transport the photoinduced electrons from TiO$_2$ to the amorphous AgSe$_x$ shell, while the amorphous AgSe$_x$ shell provides massive active sites for boosting interfacial H$_2$ evolution.

Dynamic current cycles effect on the degradation characteristic of a H_2/O_2proton exchange membrane fuel cell

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Abstract: The durability and reliability of H_2/O_2 proton exchange membrane fuel cell (PEMFC) is a key factor that prevents its wide application in the civil field. PEMFC inevitably experience different dynamic loading cycles according to different power switching requirements during practical operation. To explore the degradation behavior under different dynamic cycles, a single H_2/O_2 PEMFC with 50 cm^2 active area was operated under the circulating current density from 100 mAcm^2 to 600 mAcm^2, 100 mAcm^2 to 800 mAcm^2, and 100 mAcm^2 to 1000 mAcm^2, respectively. The change of polarization curve, performance degradation at different current density, Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS) were characterized to investigate the performance degradation over dynamic current cycles. Besides, the Scanning Electron Microscopy (SEM) was used to evaluate the degradation of catalyst layer. The results indicated that the degradation rate of the fuel cell performance increased corresponding to the cycle number, at 1200 mA/cm^2, it with a total performance degradation rate of 1 1.83% after 2000 dynamic loading cycles with the circulating current density from 100 mAcm^2 to 600 mAcm^2. The degradation of electrochemical performance such as CV and EIS was consistent with that of fuel cell performance. The degradation rate is accelerated with the increase of loading cycle number and load step amplitude. What' more, EIS provides additional sensitivity to differentiate catalyst layer degradation within PEMFC. Moreover, the degradation of the catalyst layer became much more severe under a larger load step amplitude.

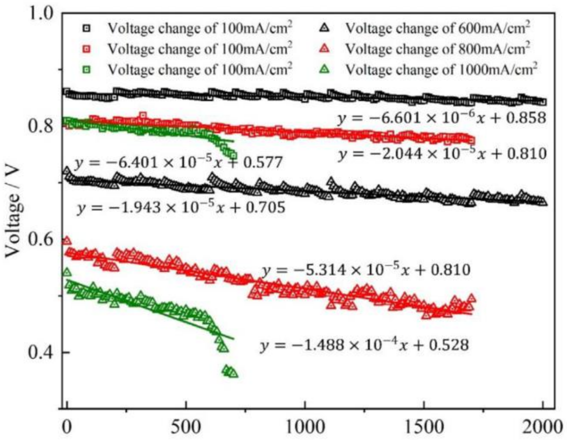

Fig. 1 Voltage decay with different dynamic loading cycles

Keywords: Proton exchange membrane fuel cell; Dynamic current cycles; Loading rate; Performance degradation

闭口质子交换膜燃料电池性能研究

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摘要：本文设计了一种阴阳极全闭口质子交换膜燃料电池，研究了不同操作条件下电池性能。结果显示，在不同工况下，设计燃料电池能保持氢氧全闭口稳定运行；电池工作温度越高，其输出性能越好；提高电池工作压力对闭口燃料电池性能提升明显，且未影响闭口电池运行的稳定性；对闭口质子交换膜燃料电池尾气进行冷凝可提高闭口电池的输出性能及稳定性。尾气冷凝装置与电池内部工作温度之间的温差增大，电池性能提升越明显。

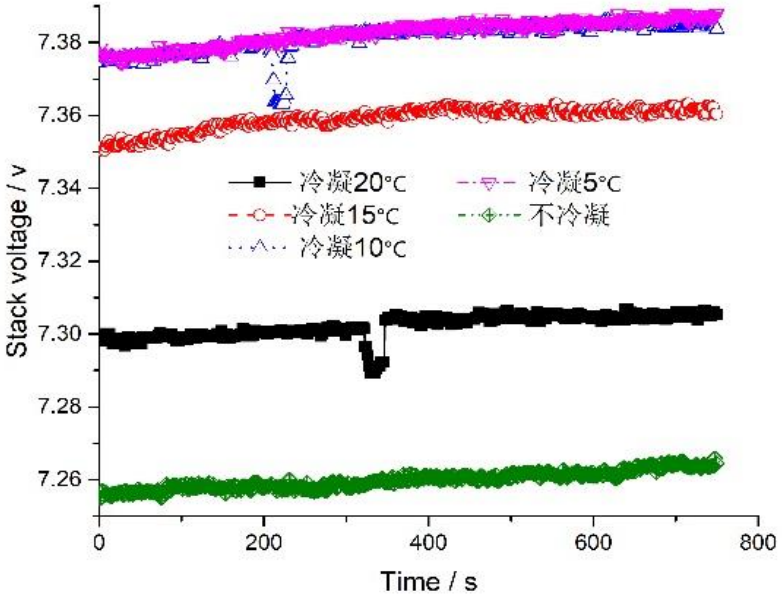

图 1 不同冷凝温度下电池电压变化曲线

Fig. 1 Effect of different condensing temperature on stack voltage

关键词：质子交换膜燃料电池；水管理；尾气冷凝；性能研究

不同装配扭矩下 PEM 燃料电池性能实验研究

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摘要：质子交换膜（PEM）燃料电池设计和装配最重要的目标是获得合理、均匀的压力分布；装配扭矩不合适，会对燃料电池性能造成影响，甚至会损坏电池。本文根据仿真所采用的 PEM 燃料电池参数，加工合适的燃料电池各部件，通过适当的顺序通过螺栓装配起来，通过设置 PEM 燃料电池工作温度为 75℃，燃料电池堆工作温度为 65℃，保证每次实验仅有螺栓扭矩单一变量，通过实验研究得到在不同螺栓装配扭矩下 PEM 燃料电池与 PEM 燃料电池堆的极化曲线，通过曲线我们可知随着装配扭矩的增加，曲线整体呈先抬升、后下降的趋势，电池的性能先提高、后降低；当装配扭矩分别为 7N·m 与 12N·m 时，燃料电池与电池堆性能达到最佳。合适的装配扭矩可以较好的平衡 PEM 燃料电池工作中的损失与欧姆损耗，使其性能达到最佳。

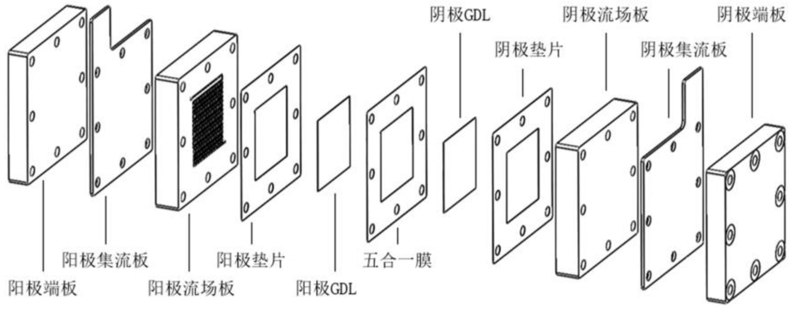

图 1 PEM 燃料电池装配顺序

Fig. 1 PEM fuel cell assembly torque

关键词：质子交换膜（PEM）燃料电池；装配扭矩；性能；实验研究

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Experimental study on the performance of PEM fuel cell under different assembly torque

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Abstract: The most important goal of Proton Exchange Membrane (PEM) fuel cell design and assembly is to obtain reasonable and uniform pressure distribution; Improper assembly torque would affect the performance of fuel cell and even damage the battery. According to the PEM fuel cell parameters used in the simulation, the appropriate fuel cell components are processed in this paper. By setting the working temperature of PEM fuel cell to 75℃ and the working temperature of fuel cell stack to 65℃, only a single variable of bolt torque was guaranteed in each experiment. The polarization curves of PEM fuel cell and PEM fuel cell stack under different bolt assembly torques were obtained. Through the curve, we can see that with the increase of assembly torque, the whole curve rises first and then decreases, and the performance of the fuel cell improves first and then decreases. When the assembly torque was 7N·m and 12N·m, the performance of fuel cell and stack were the best. Appropriate assembly torque can balance the loss and ohmic loss of PEM fuel cell in operation, and make its performance reach the best.

球磨法引起的原子碳掺杂对镁吸氢性能的增强

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摘要：镁具有很高的储氢密度，被认为是极具应用前景的储氢材料。然而迟缓的吸放氢动力学性能限制了其在储氢方面的应用[1]。过去的数十年中，为改善镁的储氢性能，很多碳材料被用作球磨添加剂。但是原子 C 的催化机理以及其的迁移路径依然需要进一步探索。本文研究了 Mg-C 复合材料的结构及吸氢性能，并且利用第一性原理模拟了材料的吸氢机理。从图 1（a）中可以看到，球磨过程中有大量六方形片状 Mg 被剥落，原子 C 可以不断的掺杂在新晶面上。经过热处理后，原子 C 进入镁晶格，形成 Mg_2C_3，如图 1（a）的内插图所示，XRD 中出现 Mg_2C_3 的衍射峰。这意味着镁中生成了 C 掺杂结构。图 1（b）为球磨过程中原子碳掺杂示意图。在图 1（b）的内插图中可以看出，随着球磨时间增加，Mg 沿着(0001)晶面发生定向滑移。与此同时，C 原子从碳材料上脱落，吸附于新形成的 Mg(0001)晶面。理论研究表明，C 掺杂能使 H_2 在 Mg(0001)晶面的解离能垒降低。此外，H 可以与掺杂的 C 原子共享电子，并与之结合形成 CH_4，从晶格中逸出。因此，吸氢后的 Mg-C 复合材料中没有检测到 Mg_2C_3。

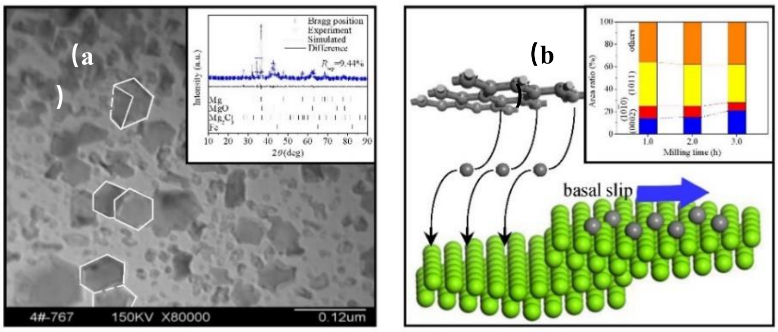

图 1（a）镁碳复合材料 TEM 图，内插图为材料热处理后的 XRD 图；（b）球磨过程中原子碳掺杂示意图，内插图为不同球磨时间制备镁碳复合材料 XRD 图中镁衍射峰的面积比。

关键词：金属镁；石墨烯；球磨；滑移；氢化机理

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Enhancement in hydriding performance of C-doped magnesium by ball milling

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Abstract: Magnesium exhibits high hydrogen storage density and is considered as a promising candidate for hydrogen storage, while the poor kinetics performance hinders its practical usage. Various carbon materials are used as additives during ball milling to enhance the hydrogen storage property of magnesium in the last decades, but the migration path and catalytic mechanism of atomic carbon are still indistinct. In this present paper, structural change and hydriding mechanism of Mg with C doping are characterized and simulated by first-principles calculation. The TEM image of Mg-C composite (Fig.1a) shows that many hexagonal Mg flakes peel off from particles continually during ball milling so that atomic C can dope on new crystal surface ceaselessly. With the heat treatment, C can infiltrate into Mg crystal to form Mg_2C_3, as shown in the inset of Fig.1(a). The diffraction peaks of Mg_2C_3 is appeared in the XRD pattern which means C-doping structure is formed in Mg crystal. Fig.2 (b) is the schematic of C doping on Mg(0001) plane during milling. With the increase of milling time, the basal slip of Mg(0001) become more obvious. Meanwhile, C atoms fall off and then are absorbed by new Mg(0001) plane. Theoretical studies suggest that C-doping can reduce the energy barrier of H_2 dissociation on Mg(0001) plane. In addition, H can share its electron with C atom and form C-H bond. The C atom can combine with four H atoms and form CH_4. Then, the CH_4 escapes from Mg crystal. Therefore, the Mg_2C_3 disappeared after the hydrogenation of Mg-C composite.

$Mg_{95}Ni_5$ 对 $Mg(BH_4)_2•2NH_3$ 抑氨促氢的双重调节作用

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摘要：抑制 $Mg(BH_4)_2•2NH_3$ 氨释放的研究引起了众多研究者的关注。本文采用一种简便的方法，将经过氢化燃烧合成处理的 $Mg_{95}Ni_5$ 引入 $Mg(BH_4)_2•2NH_3$ 体系，成功地抑制了氨的释放。当 $Mg(BH_4)_2•2NH_3$ 和 $Mg_{95}Ni_5$ 以 2:1 的质量比混合时，复合材料表现出最佳的氢脱附动力学。复合材料的初始脱氢温度低至 75°C，比 $Mg(BH_4)_2•2NH_3$ 低 70°C。在热脱附试验中，当温度升高到 500°C 时，氢释放量为 11.66 wt%，达到氢释放总量的 98.4%。MgH_2 和镍的双重调节作用使其具有良好的抑氨释氢性能。氢化镁能有效抑制氨的释放，镍的高分散性提高了 MgH_2 在体系中的动力学性能。本研究进一步证实了 MgH_2 对 $Mg(BH_4)_2•2NH_3$ 的氨抑制作用，为改善复合体系的动力学性能提供了思路。

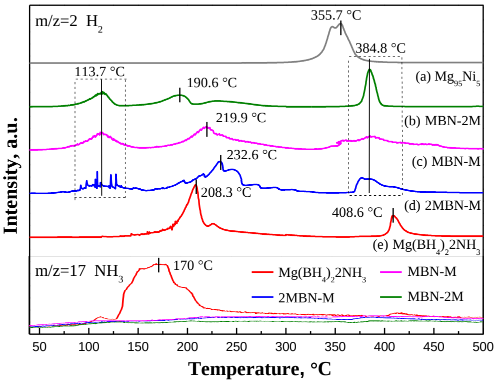

图 1 MBN-M（x=0.5,1,2）复合材料的 TPD-MS 曲线，加热速率为 5°C/min。

Fig. 1 TPD-MS curves for the MBN-M (x=0.5, 1, 2) composites at a heating rate of 5 °C/min.

Double regulation of $Mg_{95}Ni_5$ in suppressing ammonia and promoting hydrogen evolution for $Mg(BH_4)_2·2NH_3$

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Abstract: The study on inhibiting the release of ammonia from $Mg(BH_4)_2·2NH_3$ has attracted the attention of many researchers. In this paper, a facile method was used to introduce HCS (hydriding combustion synthesis) processed $Mg_{95}Ni_5$ into the $Mg(BH_4)_2·2NH_3$ system, which successfully suppressed the release of ammonia completely. The composite shows the best hydrogen desorption kinetics when $Mg(BH_4)_2·2NH_3$ and $Mg_{95}Ni_5$ are mixed in a mass ratio of 2:1. The initial dehydrogenation temperature of the composite is as low as 75 °C, which is 70 °C lower than that of $Mg(BH_4)_2·2NH_3$. In the thermal desorption test, when the temperature is raised to 500 °C, the amount of hydrogen released is 11.66 wt%, reaching 98.4% of the total amount of hydrogen released. The excellent performance of inhibiting ammonia and releasing hydrogen is attributed to the dual regulation effects of MgH_2 and nickel. Magnesium hydride can effectively inhibit the release of ammonia and the high dispersibility of nickel improves the kinetic performance of MgH_2 in the system. This study further confirms the ammonia suppression effect of MgH_2 on $Mg(BH_4)_2·2NH_3$, and provides ideas for the improvement of the kinetic performance of the composite system.

添加 NbF_5 对 $Mg(BH_4)_2·2NH_3$ 放氢性能的影响及其催化机理

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摘要：$Mg(BH_4)_2·2NH_3$ 具有较高的储氢容量(16.02 wt.%)和较低的放氢温度(150 ℃左右)，是一种很有前景的储氢材料。但其实际应用受到放氢温度高、放氢动力学性能差、有副产物氨气释放等不利因素的限制。采用球磨法将不同含量(2.5，5，10 和 15 mol%)的 NbF_5 引入 $Mg(BH_4)_2·2NH_3$ 中，研究了 $Mg(BH_4)_2·2NH_3$- $xNbF_5$ 复合材料的热解放氢性能。NbF_5 的加入显著提高了 $Mg(BH_4)_2·2NH_3$ 的放氢动力学性能，抑制了氨的释放。$Mg(BH_4)_2·2NH_3$- $xNbF_5$ 复合体系在 50~60 ℃时开始放氢，与纯 $Mg(BH_4)_2·2NH_3$ 相比，其放氢量下降了近 70 ℃。当加热到 150 ℃和 200 ℃时，$Mg(BH_4)_2·2NH_3$- 5 mol%NbF_5 材料的放氢量分别为 3.61 wt.%和 8.15 wt.%，是相同条件下纯 $Mg(BH_4)_2·2NH_3$ 的 6.7 倍和 3.5 倍。分析发现，NbF_5 与 $Mg(BH_4)_2·2NH_3$ 在加热过程中发生反应，生成稳定的 MgF_2 和 NbB_2 异相形核剂，两者都有利于 $Mg(BH_4)_2·2NH_3$- $xNbF_5$ 体系的放氢。

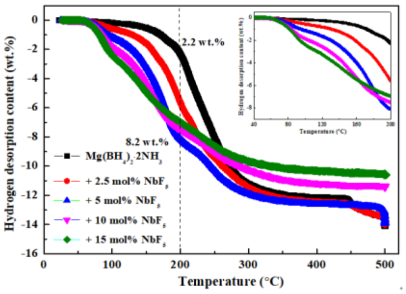

图 1·$Mg(BH_4)_2·2NH_3 – x NbF_5$ (x= 2.5, 5, 10 and 15 mol%) 的随温放氢曲线
Fig. 1 Volumetric release curves of the as-prepared $Mg(BH_4)_2·2NH_3$ and $Mg(BH_4)_2·2NH_3 – x NbF_5$ (x= 2.5, 5, 10 and 15 mol%) composites,

关键词：储氢；硼氢化镁；氨合物；NbF_5；催化

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Introduction of NbF_5 into $Mg(BH_4)_2·2NH_3$ for Improved Dehydrogenation Properties

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Abstract: $Mg(BH_4)_2·2NH_3$ is a promising hydrogen storage material for its high gravimetric hydrogen capacity of 16.02 wt.% and a lower dehydrogenation temperature starting at around 150 ℃. However, its practical applications are limited by the still higher dehydrogenation temperature, slower kinetics, and the hydrogen released suffering from contamination by ammonia. In the present work, different amounts (2.5, 5, 10, 15 mol%) of NbF_5 were introduced to $Mg(BH_4)_2·2NH_3$ by ball milling, and the dehydrogenation properties of the $Mg(BH_4)_2·2NH_3$- $xNbF_5$ composites were investigated. The addition of NbF_5 significantly enhanced the dehydrogenation kinetics properties and greatly depressed ammonia release. $Mg(BH_4)_2·2NH_3$ with NbF_5 begins to release hydrogen at 50- 60 ℃, which is sharply decreased by almost 70 ℃bwith respect to the pristine $Mg(BH_4)_2·2NH_3$. The hydrogen yields of $Mg(BH_4)_2·2NH_3$- 5 mol%NbF_5 were 3.61 and 8.15 wt.% when heated to 150 and 200 ℃ respectively, almost 6.7 and 3.5 times that of the pristine $Mg(BH_4)_2·2NH_3$ under the same conditions. NbF_5 reacts with $Mg(BH_4)_2·2NH_3$ upon heating, generating stable MgF_2 and NbB_2 heterogeneous nucleation agent, both of which can facilitate the dehydrogenation of the $Mg(BH_4)_2·2NH_3$- NbF_5 system.

典型 MOFs 储氢系统充放气与强化传热仿真实验研究

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摘要：航运业每年排放了全球约三分之一的温室气体，高效船用储氢技术的研发日益受到重视。本文针对氢在 MIL-101（Cr）和 MEI-01 两种材料吸脱附过程中的特性及储氢系统的强化传热技术，采用平台实验，结合 comsol 软件建立吸附床仿真模型展开研究。结果表明，氢在 MIL-101（Cr）和 MEI-01 上低压区域吸附平衡满足 Henry 定律，Toth 势函数确定的等量吸附热分别为 2.248-3.673kJ/mol 和 2.240-3.673kJ/mol，最大绝对吸附量为 22.029mmol/g 和 15.613mmol/g。在 77.15K 液氮浴脱附过程中，有效放气时间 306s 内添加蜂巢传热翅片吸附床累计放气量为 3.669g，比添加 ENG 的增加了 12%，脱附效率（DR）也提高了 0.6%；仿真结果显示蜂巢传热翅片和 ENG 吸附床平均温升分别为 214.7℃、210.5℃，在 310s 有效放气时间内，累积放气量分别为 3.688g、3.284g，DR 前者比后者提高了 2.16%；添加 ENG 对累计充放气量影响较大，布置传热翅片可兼顾吸附床强化传热和循环吸脱附性能。

关键词：MOFs 储氢；充放气；强化传热；comsol 仿真

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Simulation and experimental study on charging and venting and enhanced heat transfer of typical MOFs hydrogen storage system

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Abstract: The shipping industry emits about one third of the global greenhouse gases every year. The research and development of efficient marine hydrogen storage technology has attracted more and more attention. In this paper, the characteristics of hydrogen in the adsorption and desorption process of MIL-101 (Cr) and MEI-01 materials and the enhanced heat transfer technology of hydrogen storage system are studied by using platform experiment and COMSOL software. The results show that the adsorption equilibrium of hydrogen in the low pressure region on MIL-101 (Cr) and MEI-01 satisfies Henry's law. The equivalent adsorption heat determined by Toth potential function is 2.248-3.673kJ/mol and 2.240-3.673kJ/mol respectively, and the maximum absolute adsorption capacity is 22.029mmol/g and 15.613mmol/g. In the desorption process of 77.15K liquid nitrogen bath, the cumulative outgassing amount of honeycomb heat transfer finned adsorption bed is 3.669g within 306s, which is 12% higher than that of ENG, and the desorption efficiency (DR) is also increased by 0.6%; The simulation results show that the average temperature rise of honeycomb heat transfer fin and ENG adsorption bed are 214.7 ºC and 210.5 ℃ respectively. Within 310s effective venting time, the cumulative venting gas is 3.688g and 3.284g respectively. The former is 2.16% higher than the latter; The addition of ENG has a great impact on the cumulative gas charge and discharge. The arrangement of heat transfer fins can take into account the enhanced heat transfer of adsorption bed and the performance of cyclic adsorption and desorption.

核壳结构 NiCu@C 对 MgH_2 储氢性能的催化改性

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摘要：本工作以双金属络合物为前驱体，制备了具有核壳结构的双金属纳米催化剂 NiCu@C（~15 nm）。MgH_2-11wt.% NiCu@C 复合体系的起始脱氢温度为 175 ℃，峰值脱氢温度为 282 ℃。根据基辛格方程计算得到 MgH_2-11wt.% NiCu@C 复合样品表观脱氢活化能为 68.0 kJ/mol，远低于仅做球磨处理的 MgH_2（156.4 kJ/mol）。此外，MgH_2-11 wt.%NiCu@C 具有优异的循环稳定性。MgH_2 储氢性能的显著改善主要归因于复合样品在吸放氢反应过程中 Mg_2Ni（Cu）/Mg_2Ni（Cu）H_4 之间可逆的相转变反应，以及催化剂中碳壳优异的导热性能和纳米限域作用。同时，这项工作为设计具有特殊微观形貌的双金属纳米催化剂来改善金属氢化物的储氢性能扩展了视野。

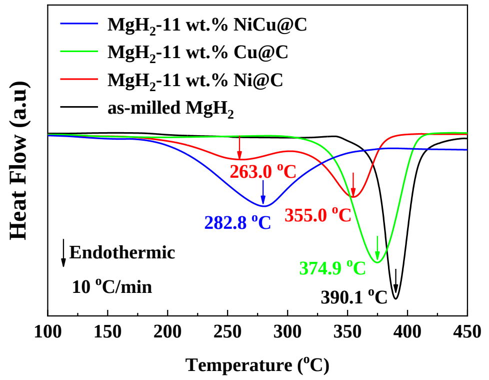

图 1 MgH_2-11wt.% NiCu@C 和三个对比样的 DSC 曲线
Fig. 1 DSC curves of MgH_2-11wt.% NiCu@C and three contrast samples

关键词：双金属催化剂；核壳结构；MgH_2；协同效应

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Catalytic Effect of Core-shell NiCu@C on Hydrogen Storage Performance of MgH_2

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Abstract: In this work, a bimetallic complex is used as a precursor to prepare a bimetallic nanocatalyst NiCu@C (~15 nm) with a core-shell structure. We reveal the internal mechanism of the catalyst in improving the hydrogen storage kinetic performance of MgH_2. The onset and peak dehydrogenation temperatures of MgH_2-11 wt.%NiCu@C are 175 ℃ and 282 ℃, respectively. The E_a value of dehydrogenated reaction was calculated to be 68.0 kJ/mol, which is significantly lower than as-milled MgH_2 (156.4 kJ/mol). Moreover, MgH_2-11 wt.%NiCu@C owns great cyclic stability. The notable improvement of hydrogen storage properties of MgH_2 is attributed to the reversible phase transitions of Mg_2Ni(Cu)/Mg_2Ni(Cu)H_4, and the excellent thermal conductivity and confinement effect of the carbon shell. This work extends the horizon of bimetallic nanoparticles with especial microstructure for enhancing the hydrogen storage properties of metal hydrides.

氮缺陷氮化碳载体助力氧化铱提升 PEM 电解水析氧动力学

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摘要：为解决 PEM 电解水阳极低铱下低活性和稳定性特性,[1] 本文通过缺陷工程引入 N 缺陷，实现了石墨氮化碳（g-C_3N_4，简称 CN）的高比表面积、丰富的孔隙和良好的导电性。结合 N 缺陷 g-C_3N_4（N-CN）作为 IrO_2 载体的整合，在 PEM 单电池中 IrO_2/N-CN 的质量活性和比活性分别是 IrO_2 的 7.86 倍和 1.75 倍。此外，IrO_2/N-CN 在 1.6 A cm^{-2} 的 1.778 V 下表现出最佳 OER 活性，其显著小于 IrO_2/CN（1.824 V）和 IrO_2（1.846 V）。这可能是由于在 IrO_2 和 N-CN 界面上存在协同电子相互作用，使得复合催化剂加速了动力学并提高了 Ir 利用率。此外，通过电压损失分析，证实了 IrO_2/N-CN 比 IrO_2 和 IrO_2/N-CN 的动力学损失和质量传输损失更低。最后，在 1.6 A cm^{-2} 下运行 300 h 的稳定性试验中，证明 IrO_2/N-CN 具有良好的稳定性。这项工作为设计和优化高效电催化催化剂提供了可行的策略。

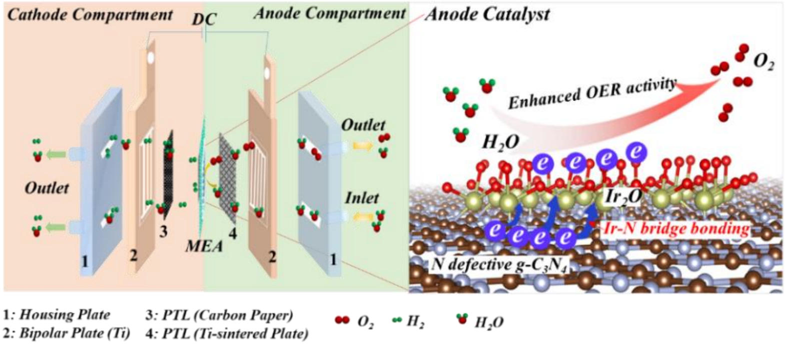

图 1 抗反极膜电极水电解平台失效示意图

Fig. 1 Schematic diagram of the failure of WEP for RTA

关键词：质子交换膜电解槽；阳极催化剂；析氧；氧化铱

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Defect engineering assisted support effect: IrO_2/N defective g-C_3N_4 composite as highly efficient anode catalyst in PEM water electrolysis

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Abstract: To address the low activity and stability of PEM electrolytic water under low iridium, high specific surface area, rich pore, and good electronic conductivity of graphite carbon nitride (g-C_3N_4, noted as CN) are conducted with the introduction of N defects via defect engineering. Together with the integration of N defective g-C_3N_4 (N-CN) as support of IrO_2, 7.86 times of mass activity and 1.75 times of specific activity for IrO_2/N-CN are obtained than that of IrO_2 in PEM single-cell. Also, IrO_2/N-CN exhibits the optimal OER activity at 1.6 A cm^{-2} of 1.778 V, which is substantially smaller than that of IrO_2/CN (1.824 V) and IrO_2 (1.846 V). This could be due to the existence of synergistic electronic interaction at the interface of IrO_2 and N-CN endows the composite catalyst accelerated kinetic and augmented Ir utilization. Moreover, the feeble kinetic loss and mass transport loss of IrO_2/N-CN lower than that of IrO_2 and IrO_2/N-CN are verified by the break-down of voltage loss analyses. Finally, the good stability of IrO_2/N-CN is demonstrated during the stability test operated for 300 h at 1.6 A cm^{-2}. This work provides a feasible strategy for designing and optimizing highly efficient catalysts in electrocatalytic.

$Zr_{0.4}Ti_{0.6}Co$ 纳米片与碳纳米管协同催化增强 MgH_2 储氢性能

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摘要：过渡金属纳米颗粒对 MgH_2 有着良好的催化作用，碳纳米管的加入使其具有良好的循环稳定性。本文设计了 MgH_2 + 10 wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% 碳纳米管(CNTs)复合材料，研究 $Zr_{0.4}Ti_{0.6}Co$ 纳米片和碳纳米管的协同催化作用对 MgH_2 储氢性能的影响。与纯 MgH_2 相比，MgH_2 + 10 wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% CNTs 复合材料的初始放氢温度降至 180℃，在 300℃下，复合材料在 10 min 内即可快速释放 90%的 H_2。完全脱氢的样品在 125℃、3 Mpa 氢气压力下，20 min 内可吸收 3.51 wt% H_2。进一步研究指出，在 10% wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% CNTs 的作用下，MgH_2 脱氢和再加氢的活化能分别降至 70.5±7.8 kJ/mol 和 35.8±3.8 kJ/mol,并合理解释了氢吸附温度的显著减少。此外，MgH_2 + 10 wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% CNTs 复合材料表现出良好的循环性能，预示着在不久的将来，该体系在实际储氢中具有潜在的应用价值。

关键词：储氢；MgH_2；协同催化；可逆性

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Enhanced hydrogen storage properties of MgH_2 by the synergetic catalysis of $Zr_{0.4}Ti_{0.6}Co$ nanosheets and carbon nanotubes

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Abstract: Transition metal nanoparticles have shown great catalytic effect on MgH_2, yet excellent cyclic stability can be attached due to the addition of carbon nanotubes. In this paper, MgH_2 + 10 wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% Carbon nanotubes (CNTs) composite is designed to investigate the synergistic modification of $Zr_{0.4}Ti_{0.6}Co$ nanosheets and carbon nanotubes on the hydrogen storage performance of MgH_2. Compared with pure MgH_2, the initial hydrogen release temperature of MgH_2 + 10 wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% CNTs composite decreases to 180 °C and the composite can quickly release 90% H_2 within 10 min at 300 °C. In addition, the completely dehydrogenated sample can absorb 3.51 wt% H_2 within 20 min under 3 Mpa hydrogen pressure at 125 °C. Ulteriorly, the activation energy values of dehydrogenation and rehydrogenation of MgH_2 decrease to 70.5 ± 7.8 kJ/mol and 35.8 ± 3.8 kJ/mol on account of the presence of 10 wt% $Zr_{0.4}Ti_{0.6}Co$/5 wt% CNTs, which reasonably explains the remarkable reduction of the temperature for hydrogen sorption. Furthermore, the MgH_2 + 10 wt% $Zr_{0.4}Ti_{0.6}Co$ /5 wt% CNTs composite shows excellent cycling performance, indicative of potential application in practical hydrogen storage in the nearest future.

金属有机骨架负载的 Ni_2O_5 纳米颗粒对 MgH_2 的储氢性能具有高效的催化作用

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摘要：为了解决高储氢容量的 MgH_2 热力学稳定和动力学缓慢的问题。本文通过简单的水热反应和煅烧，成功地合成了以菱形十二面体金属有机骨架（MOF）为载体的平均粒径为 10 nm 的 Nb_2O_5 纳米颗粒。实验结果表明，所制备的催化剂显著改善了 MgH_2 的储氢性能。7 wt.% Nb_2O_5@MOF 掺杂 MgH_2 在 181 ℃时开始放氢。在 275℃和 250℃下，2.6 min 和 6.3 min 内的放氢量均达到 6.2 wt. %。完全脱氢的复合材料也表现出良好的吸氢性能，在 25℃的室温下就可以吸氢，在 175℃下，6 分钟内可以吸收 6.5 wt.%的氢气。此外，计算出放氢的活化能为 75.57±4.16 kJ mol^{-1}，解氢反应的活化能为 51.38±1.09 kJ mol^{-1}。20 次循环后，MgH_2-7 wt.% Nb_2O_5@MOF 损失了 0.5 wt.%的氢容量。微观结构分析表明，Nb_2O_5 颗粒均匀分布在 MgH_2 基体表面，并与 MOF 协同改善 MgH_2 的储氢性能。

关键词：储氢；氢化镁；Nb_2O_5@MOF；催化机理。

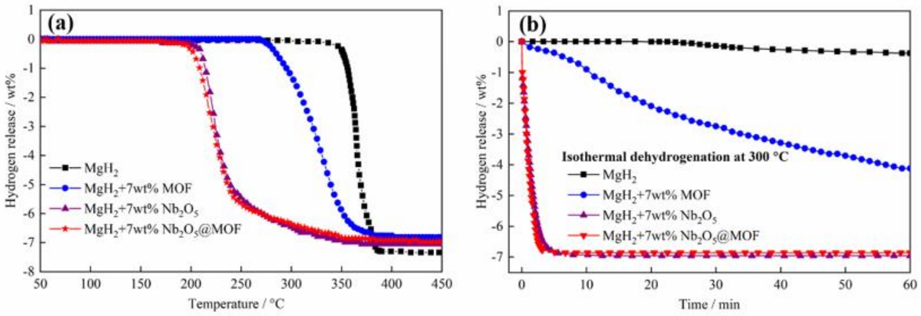

Fig. 1. Non-isothermal dehydrogenation (a) and isothermal dehydrogenation curves (b) for MgH_2 with and without additives.

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Metal organic framework supported niobium pentoxide nanoparticles with exceptional catalytic effect on hydrogen storage behavior of MgH_2.

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Abstract: Nb_2O_5 nanoparticles with an average particle size of 10 nm supported on a rhombic dodecahedral metal organic framework (MOF) were successfully synthesized by a facile one-pot hydrothermal reaction and subsequent calcination process. Experimental results demonstrated that the prepared catalyst drastically improved the hydrogen storage behaviors of MgH_2. 7 wt.% Nb_2O_5@MOF doped MgH_2 started to desorb hydrogen at 181.9 ℃ and 6.2 wt.% hydrogen could be released within 2.6 min and 6.3 min at 275 ℃ and 250 ℃, respectively. The fully dehydrogenated composite also displayed excellent hydrogenation by decreasing the onset absorption temperature to 25 ℃ and taking up 4.9 wt.% and 6.5 wt.% hydrogen within 6 min at 150 ℃ and 175 ℃, respectively. Moreover, the corresponding activation energy was calculated to be 75.57±4.16 kJ mol^{-1} for desorption reaction and 51.38±1.09 kJ mol^{-1} for absorption reaction. After 20 cycles, 0.5 wt.% hydrogen capacity was lost for the MgH_2+7 wt.% Nb_2O_5@MOF composite, much lower than 1.5 wt.% of the MgH_2+7 wt.% Nb_2O_5 composite. However, the addition of Nb_2O_5@MOF had limited effect on reducing the dehydrogenation enthalpy of MgH_2. Microstructure analysis revealed that Nb_2O_5 particles were uniformly distributed on surface of the MgH_2 matrix and synergistically improved the hydrogen storage property of MgH_2 with MOF.

核壳结构 NiCu@C 对 MgH$_2$ 储氢性能的催化改性

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摘要：本工作以双金属络合物为前驱体，制备了具有核壳结构的双金属纳米催化剂 NiCu@C（~15 nm）。MgH$_2$-11wt.% NiCu@C 复合体系的起始脱氢温度为 175 °C，峰值脱氢温度为 282 °C。根据基辛格方程计算得到 MgH$_2$-11wt.% NiCu@C 复合样品表观脱氢活化能为 68.0 kJ/mol，远低于仅做球磨处理的 MgH$_2$（156.4 kJ/mol）。此外，MgH$_2$-11 wt.%NiCu@C 具有优异的循环稳定性。MgH$_2$ 储氢性能的显著改善主要归因于复合样品在吸放氢反应过程中 Mg$_2$Ni（Cu）/Mg$_2$Ni（Cu）H$_4$ 之间可逆的相转变反应，以及催化剂中碳壳优异的导热性能和纳米限域作用。同时，这项工作为设计具有特殊微观形貌的双金属纳米催化剂来改善金属氢化物的储氢性能扩展了视野。

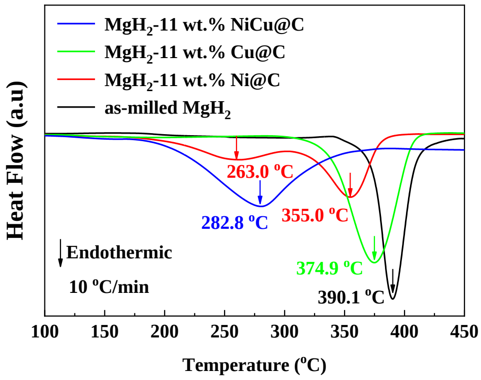

图 1 MgH$_2$-11wt.% NiCu@C 和三个对比样的 DSC 曲线

Fig. 1 DSC curves of MgH$_2$-11wt.% NiCu@C and three contrast samples

关键词：双金属催化剂；核壳结构；MgH$_2$；协同效应

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Catalytic Effect of Core-shell NiCu@C on Hydrogen Storage Performance of MgH$_2$

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Abstract: In this work, a bimetallic complex is used as a precursor to prepare a bimetallic nanocatalyst NiCu@C (~15 nm) with a core-shell structure. We reveal the internal mechanism of the catalyst in improving the hydrogen storage kinetic performance of MgH$_2$. The onset and peak dehydrogenation temperatures of MgH$_2$-11 wt.%NiCu@C are 175 °C and 282 °C, respectively. The E$_a$ value of dehydrogenated reaction was calculated to be 68.0 kJ/mol, which is significantly lower than as-milled MgH$_2$ (156.4 kJ/mol). Moreover, MgH$_2$-11 wt.%NiCu@C owns great cyclic stability. The notable improvement of hydrogen storage properties of MgH$_2$ is attributed to the reversible phase transitions of Mg$_2$Ni(Cu)/Mg$_2$Ni(Cu)H$_4$, and the excellent thermal conductivity and confinement effect of the carbon shell. This work extends the horizon of bimetallic nanoparticles with especial microstructure for enhancing the hydrogen storage properties of metal hydrides.

碳包覆异质结微纳米阵列电解水催化剂

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摘要：开发大电流密度下具有超高活性和超高稳定性的催化材料对于电解水制氢意义重大[1]。我们将结合碳包覆，金属耦合金属氧化物及自支撑微纳米阵列的优势，从催化剂的合成及表征等方面入手，开展一系列过渡金属异质结微纳米阵列大电流密度电解水催化剂的研究。通过调控催化剂的微观形貌及物质组成等，提升催化剂的本征活性及稳定性；结合理论计算阐明催化剂的反应机理和构效关系；揭示催化剂在大电流密度下的活性及稳定性增强机制，为制备新型非贵金属大电流密度电解水催化材料提供新的思路。

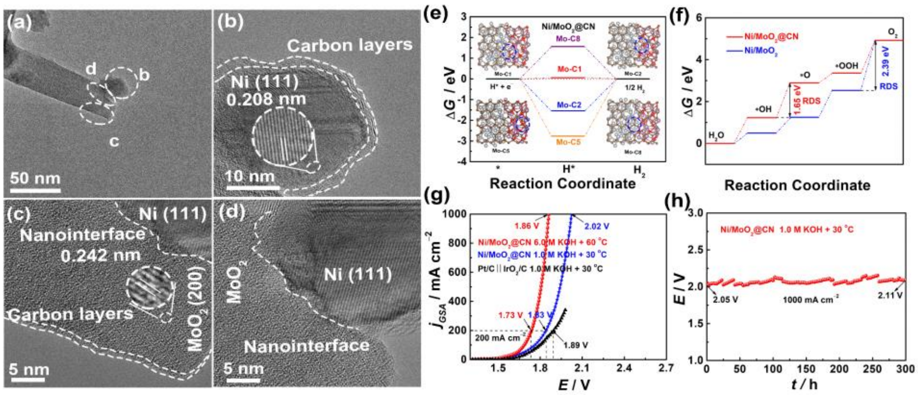

图 1 (a-d) 碳包覆镍/二氧化钼纳米针的 TEM；(e) 不同吸附位点的ΔG_{H*}; (f) OER 的吉布斯自由能图；(g-h) 全水解极化曲线和稳定性曲线

Fig. 1 (a-d) TEM of N-doped-carbon encapsulated Ni/MoO_2 nano-needle; (e) Corresponding ΔG_{H*} calculated at different adsorb sites; (f) The ΔG value during OER; (g-h) The LSV and CP curves of water electrolysis

关键词：异质结；碳包覆；微纳米阵列；大电流密度；电解水

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Carbon-encapsulated heterojunction micro-nano array catalysts for water electrolysis

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Abstract: Developing ultra-high activity and stability catalytic materials with large current density for water electrolysis is of great significance for hydrogen production [1]. Starting from the synthesis and characterization of catalysts, we combine the advantages of carbon-encapsulated, metal-coupled metal oxides and self-supporting micro-nano arrays to carry out a series of transition metal heterojunction micro-nano arrays catalysts for water electrolysis. By adjusting the microscopic morphology and material composition of catalysts, the intrinsic activity and stability of catalysts are improved. Theoretical calculations are combined to clarify the reaction mechanism and structure-activity relationship of catalysts. The activity and stability enhancement mechanism of catalysts are revealed; this work provide a new idea to prepare novel non-precious metal catalytic materials for water electrolysis at large current density.

电子耦合的 PtCo-PtSn/C 异质结催化剂用于提高氧还原和析氢反应性能

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摘要：开发用于氧还原反应（ORR）和析氢反应（HER）的高效催化剂对于质子膜交换燃料电池(PEMFC)和电解水制氢反应至关重要。[1]在此，我们采用溶剂热和热处理相结合的策略成功制备了 PtCo-PtSn/C 异质结构催化剂。得益于其独特的电子结构，PtCo-PtSn/C 对 ORR 和 HER 表现出高活性和高稳定性，其 ORR 半电位为 0.93 V（质量活性为 1158 mA $mgPt^{-1}$）；对于 HER，-10 mA cm^{-2} 对应的过电位仅为 18 mV，且能稳定循环 100,000 圈。理论计算表明，PtCo-PtSn/C 催化活性和稳定性的增强源于 PtCo 与 PtSn 之间的强电子耦合作用导致 Pt 的 d 能带中心下降。这削弱了催化剂表面与*H 和含氧中间体的键合强度，从而降低 ORR 过电位和 HER 水分子的活化能垒，提高 ORR 和 HER 性能。这项工作为设计和制备用于 PEMFC 和 HER 的铂基催化剂开辟了一条新途径。

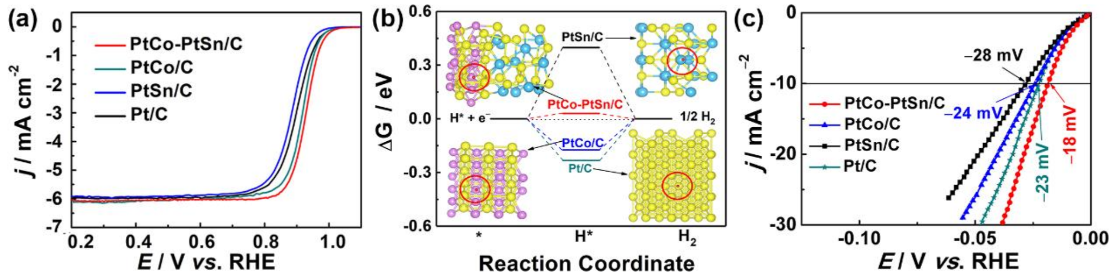

图 1 (a)氧还原极化曲线；(b)不同催化剂的吉布斯自由能值；(c)析氢极化曲线

Fig. 1 (a) ORR LSV curves; (b) The ΔG_{H*} of different catalysts; (c) HER LSV curves

关键词：氧还原反应；析氢反应；异质结；催化剂；全 pH

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Electronically coupled PtCo-PtSn/C heterostructure for enhancing oxygen reduction and hydrogen evolution reaction performance

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Abstract: Developing efficient catalysts for both oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER) is crucial for proton membrane exchange fuel cells (PEMFCs) and producing hydrogen. [1] Herein, PtCo-PtSn/C heterostructure catalyst is successfully synthesized by solvothermal and thermal treatment. Benefitting from unique electronic-properties, PtCo-PtSn/C exhibits highly active and durable electrocatalytic performance for ORR and HER. It achieves an ORR half-potential of 0.93 V (mass activity: 1158 mA mg_{Pt}^{-1}). For HER, the overpotential at 10 mA cm^{-2} is only 18 mV, and it can steadily work for 100,000 cycles. Theoretical calculation indicates that the significantly enhanced ORR/ HER activity originates from the downshift of d-band center for Pt induced by strong electronic interaction between PtCo and PtSn，which weakens the binding strength of *H and oxygenated intermediates. Thus, the ORR overpotential and the activation energy barrier of water molecules are reduced to improve ORR and HER activity. This work opens a new strategy to design and prepare the highly efficient Pt-based alloy catalysts for PEMFCs and HER.

Pt 电极中 EIS 测试不稳定的现象

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摘要：电化学阻抗谱(EIS)是一种广泛应用于电池、电解电池等电化学系统的诊断工具。EIS 数据有效性的四个条件中，稳定性在实际测量的电化学体系中很难满足。本文研究了 Pt 在 EIS 测试中的不稳定现象，发现 Pt 电极在 EIS 测试过程中的不稳定现象主要由 R_{ct} 的变化导致，并且这种不稳定现象与测试电压有关，0.8 V 以上测试时，R_{ct} 值会随着测试次数的增加越来越大，并且稳定性随着电压的升高变差，这可能与 Pt 表面氧化物的覆盖有关。我们进一步探究了单电池中的稳定性，发现 Pt 电极在单电池中的 EIS 稳定性高于电解池。

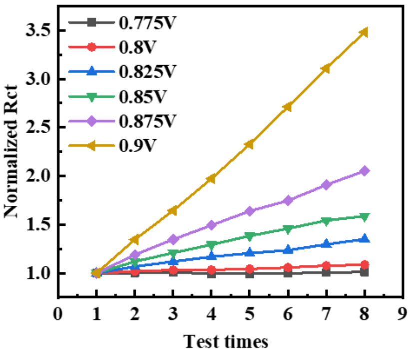

图 1 不同电压下Pt电极的归一化R_{ct}值随测试次数变化图
Fig. 1 Normalized Charge-transfer resistances of Pt electrode as a function of test times at different potentials

关键词：质子交换膜燃料电池；电荷转移阻抗；稳定性

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The unstable phenomenon of EIS test in Pt electrode

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Abstract: Electrochemical impedance spectroscopy (EIS) is a diagnostic tool widely used in electrochemical systems such as batteries and electrolysis cells. Among the four conditions for the validity of EIS data, stability is difficult to meet in the actual measured electrochemical system. This paper studies the instability of Pt in the EIS test and finds that the instability of the Pt electrode during the EIS test is mainly caused by the change of R_{ct}, and this instability is related to the test voltage. When tested above 0.8 V, R_{ct} will increase with the increase of the number of tests, and the stability will become worse with the increase of the voltage, which may be related to the coverage of Pt surface oxide. We further explored the stability of the single cell and found that the EIS stability of the Pt electrode in the single cell is higher than that of the electrolytic cell.

武汉理工大学简介

武汉理工大学是教育部直属全国重点大学，是首批列入国家“211 工程”和“双一流”武汉理工大学是教育部直属全国重点大学，是首批列入国家“211 工程”和“双一流”建设高校，是教育部和交通运输部等部委共建高校。学校办学历史起源于 1898 年建立的湖北工艺学堂，办学 123 年特别是近 70 年来，学校共培养了 60 余万名高级专门人才，是教育部直属高校中为建材建工、交通、汽车三大行业培养人才规模最大的学校，已成为我国“三大行业”高层次人才培养和科技创新的重要基地。目前学校在校普通本科生 36000 余人，博士、硕士生 18000 余人，留学生 1700 余人。

学校经过长期的育人实践，形成了特色鲜明的办学思想体系：构筑了“建设让人民满意、让世人仰慕的优秀大学”的大学理想，铸就了“厚德博学、追求卓越”的大学精神，确立了“育人为本、学术至上”的办学理念，树立了“实施卓越教育、培养卓越人才、创造卓越人生”的卓越教育观。学校致力于为社会培养一代又一代以智慧引领人生、具有卓越追求和卓越能力的卓越人才。

学校现有马房山校区、余家头校区和南湖校区，占地 4000 余亩，校舍总建筑面积 186.1 万平方米，4 座现代化图书馆藏书 329.53 万册。设有 25 个学院（部），建有 6 个独立建制的科研院所。现有教职工 5419 人，其中中国科学院院士 1 人，中国工程院院士 4 人，比利时皇家科学院院士 1 人，澳大利亚工程院院士 1 人，欧洲科学院院士 3 人，俄罗斯工程院外籍院士 1 人，世界陶瓷科学院院士 1 人；获中组部、科技部、国家自然科学基金委员会、教育部和湖北省政府人才计划支持的高端人才 125 人。

学校已形成以工学为主，理、工、经、管、艺术、文、法等多学科相互渗透、协调发展的学科专业体系。现有一级学科博士学位授权点 19 个，一级学科硕士学位授权点 45 个，博士后科研流动站 17 个；有 22 个硕士专业学位授权类别，39 个硕士专业学位授权领域。在国家第四轮学科评估中，材料科学与工程获 A+，机械工程、交通运输工程、设计学、马克思主义理论等学科获 B+。现有本科专业 96 个，其中国家一流本科专业建设点 37 个、国家特色专业 15 个、卓越工程师教育培养计划试点专业 28 个、国家综合改革试点专业 4 个、国家战略性新兴产业专业 2 个。现有国家级一流本科课程 40 门、国家级精品资源共享课 17 门、国家级精品视频公开课 8 门。拥有国家级教学团队 5 个、教育部人才培养模式实验区 4 个、国家级实验教学示范中心 5 个、国家级工程实践教育中心 13 个、国际化示范学院 1 个、全国高校实践育人创新创业基地与全国创业孵化示范基地各 1 个。

学校建有材料复合新技术国家重点实验室、硅酸盐建筑材料国家重点实验室、光纤传感技术国家工程实验室、国家水运安全工程技术研究中心等 40 个国家级和省部级科研基地，建有内河智能航运交通运输部协同创新中心、汽车零部件技术湖北省协同创新中心、安全预警与应急联动技术湖北省协同创新中心等 3 个省部级协同创新中心。学校获批交通强国建设试点单位，入选首批国家知识产权示范高校、第二批高等学校科技成果转化和技术转移基地，与地方政府和行业企业共建产教融合示范区、科教创新园、工业技术研究院等科教合作与成果转化机构 257 个。2010 年以来，学校以第一完成单位获国家自然科学奖 2 项、技术发明奖和科技进步奖 16 项、省部级一等奖及以上奖励 66 项；作为参加单位获国家科技进步特等奖 1 项、一等奖 2 项；获授权发明专利 5524 项；在世界顶尖学术期刊 Science 发表论文 1 篇、Nature 发表论文 4 篇。

百廿余年，风雨兼程，武汉理工大学将以习近平新时代中国特色社会主义思想为指导，以立德树人为根本，围绕建设“让人民满意、让世人仰慕的优秀大学”的崇高大学理想，坚持以特色创优势的发展道路，努力建设成为特色鲜明的世界一流大学。

武汉理工大学材料科学与工程学院简介

武汉理工大学材料科学与工程学院是我国材料科学与工程学科人才培养、科学研究的重要基地之一。武汉理工大学材料科学与工程学科创建于1958年，1988年被列为首批国家重点学科，1996年被列为国家“211工程”重点建设学科，2007年被列为一级学科国家重点学科，2016年获首批国家“双一流”建设学科和国防特色学科，在国家第四轮学科评估中与清华大学、北京航空航天大学并列排名A+，进入世界ESI学科排名前1‰。过去60多年中，学院为国家建材、汽车与交通行业培养了4万多名高层次人才，提供了近100项重大科技成果，特别是为建材工业从无到有、从小到大、走向世界并引领世界建材工业发展作出了重大贡献，为国防、现代工业、新兴产业、国家和区域经济提供了关键新材料技术支撑。

学科建设了一支以院士、国家重大科技计划首席科学家、全球高被引科学家等为学术带头人，整体科研能力强、结构合理、富于创新的学术队伍，拥有国家自然科学基金委创新群体、教育部创新团队、科技部重点领域创新团队、国防科技创新团队、湖北省创新群体等省部级团队20余支，2010年以来获得国家自然科学奖、国家科技进步奖、国家技术发明奖共17项。材料科学与工程学科现有教职员工440名，教授167人，副教授128人，其中中国科学院院士1人、中国工程院院士2人、发达国家院士6人，国家教学名师2人，国家级教学团队2支以及湖北省级教师/教学团队称号5个，国家级人才23名和国家级青年人才14名，同时10人当选英国皇家化学会会士、美国物理学会会士。

学科依靠党建引领，重视师德师风建设，坚守文化传承，形成了以“团结、合作、专注、创新”为核心的独特学科文化，培育出首批全国高校黄大年式教师团队、首批全国高校“双带头人”教师党支部书记工作室、全国党建工作样板支部，获全国师德先进个人2人、国家级教学名师奖3人、全国优秀教师2人、全国先进工作者2人、全国优秀科技工作者3人、全国创新争先奖2人、万人计划教学名师1人、全国杰出工程师奖1人。

学科瞄准国际一流，推行国际化发展战略，先后与牛津、密歇根、日本东北大学等国际著名大学开展实质合作，建立了“材料复合新技术国际联合实验室”和“环境友好建筑材料国际联合实验室”2个国家级国际联合实验室，“材料复合新技术与先进功能材料”（2007年）和“功能薄膜新材料的先进制备技术及工程应用”（2013年）2个“111”学科创新引智基地（国家外国专家局和教育部）。2009年以来，与世界多所著名大学建立了联合实验室，联合承担重大国际合作项目22项，总经费5600万元；联合培养研究生40余名，联合发表SCI论文300余篇。主办有影响的国际会议20余次，包括第35届国际热电会议、第13届国际非晶态固体物理会议、《Nature》能源材料国际会议、世界大学材料科学与工程领导论坛和2019《自然》太阳能燃料国际会议等。

学科将国际先进的教学理念融入特色班本科教学，为学生提供多层次国际化培养途径。与美国密歇根大学、澳大利亚蒙纳士大学、英国玛丽皇后大学等世界知名大学建立了“2+2”“3+2”“4+1”等人才联合培养模式，近100名学生参与。2015年国家外专局和教育部依托本学科建立了全国首个“材料科学与工程国际化示范学院”。

近五年，学科面向世界科技前沿及国家重大需求，承担国家“973”、国家基金重大研究计划、国家重点研发计划、武器装备重点型号项目等国家重点科研项目330余项，其他各类各级项目300余项，总经费12.5亿元，发表高水平学术论文4200余篇，获得国家科技奖励4项，取得的一批应用技术成果对国家和区域经济建设及社会、行业发展做出重大贡献。