陕西师范大学 SHAANXI NORMAL UNIVERSITY

化学化工学院 School of Chemistry & Chemical Engineering

新概念传感器与分子材料研究院 INSTITUTE OF NEW CONCEPT SENSORS AND MOLECULAR MATERIALS

新概念传感器与分子材料研究院 简报 11 2024

Institute of New Concept Sensors and Molecular Materials Newsletter

目 录 Contents

房喻院士出席《物理化学学报》创刊 40 周年学术研讨会并作报告

Fang Yu speaks at 40th Anniversary Symposium of Acta Physico-Chimica Sinica

2024 年 11 月 1 日至 4 日，《物理化学学报》创刊 40 周年学术研讨会暨能源催化科学与技术论坛在河北石家庄正定举行，房喻院士出席会议，主持了 2 日上午的大会报告，并于 3 日下午作了题为《创新驱动发展需要更加重视长周期的基础研究》的报告。

此次会议由《物理化学学报》编辑部和河北师范大学主办，河北师范大学化学与材料科学学院承办，聚焦国际研究前沿，满足国家需求，鼓励积极探索，以期突破技术瓶颈，进一步推进我国能源催化与环境催化领域的科学与技术发展及成果推广。

From 1 to 4 November 2024, the 40th Anniversary Symposium of the Journal of Acta Physico-Chimica Sinica and the Energy Catalysis Science and Technology Forum was held in Zhengding, Shijiazhuang, Hebei Province, and Prof. Fang Yu attended the meeting, presided over the plenary report session in the morning of 2 November, and gave a report titled “Innovation-driven development needs to place more emphasis on long-cycle basic research” in the afternoon of 3 November.

Sponsored by the Editorial Board of the Journal of Acta Physico-Chimica Sinica and Hebei Normal University, and hosted by HNU’s College of Chemistry and Materials Science, the conference focuses on the international research frontiers, meet national needs and encourage active exploration in order to break through technical bottlenecks and further promote the scientific and technological development and achievements in the fields of energy catalysis and environmental catalysis in China.

薄鑫参加 2024 第二十二次全国电化学大会并作报告

Bo Xin presents at 22nd National Electrochemical Congress

2024 年 11 月 5 至 8 日，2024 第二十二次全国电化学大会在海口举行，新概念传感器与分子材料研究院薄鑫副研究员参加会议并于 6 日下午作了题为“绿色宏量制备非均相析氢催化剂”的学术报告。

本次会议由中国化学会电化学专业委员会主办，海南大学和海南师范大学联合承办。

From November 5 to 8, 2024, the 22nd National Electrochemical Congress in 2024 was held in Haikou, and Associate Researcher Dr. Bo Xin of Institute of New Concept Sensors and Molecular Materials attended the conference and presented a report titled “Green & Scalable Synthesis of the Heterogeneous Catalysts for Hydrogen Evolution Reaction” on November 6.

The conference was sponsored by the Electrochemistry Committee of the Chinese Chemical Society and jointly hosted by Hainan University and Hainan Normal University.

张荷兰为曲江第二中学学生作科普报告

Zhang Helan presents science popularization report for Qujiang No. 2 Middle School students

2024 年 11 月 8 日，张荷兰高级工程师参加在曲江第二中学举行的“乐学科技 畅思未来”科普进校园活动，为高中部 200 多名学生作题为“基于马兰戈尼效应的多孔材料制备策略”的科普报告，通过一系列生动有趣的视频案例，介绍了马兰戈尼效应的基本原理及其在多孔材料制备中的创新应用。

此次活动由赛迪思教育科技研究院联合曲江街道关工委、曲江街道团委、曲江街道万科城市之光社区、曲江第二中学、陕西师范大学化学 + 科学教育研究中心共同开展。

On November 8, 2024, Senior Engineer Zhang Helan presebted a science popularization report titled “Preparation Strategy of Marangoni Effect-based Porous Materials” for more than 200 high school students of Qujiang No. 2 Middle School, in the science popularization activity of “Happy Learning Technology and Thinking the Future”, introducing the basic principle of Marangoni effect and its innovative application in the preparation of porous materials.

The activity was jointly carried out by Cedsie Education Technology Research Institute, Qujiang Sub-district Next Generation Committee, Qujiang Sub-district Youth League Committee, Qujiang Sub-district Vanke City Light Community, Qujiang No. 2 Middle School, and Shaanxi Normal University Chemistry + Science Education Research Center.

研究院参展第 26 届中国国际高新技术成果交易会

INCSMM participates in 26th China High-tech Fair

2024 年 11 月 14 日至 16 日，第二十六届中国国际高新技术成果交易会在深圳举行，新概念传感器与分子材料研究院科研助理罗艳彦、王佩和何怡楠携新概念便携式苯系物检测仪、透气不透水内相结构可调高分子膜材料和宽频低损耗介电梯度材料及制备技术参加了此次展会，并进行现场技术讲解与宣传推广工作。

From November 14 to 16, 2024, research assistants Luo Yanyan, Wang Pei and He Yinan of the Institute of New Concept Sensors and Molecular Materials participated in the 26th China High-tech Fair held in Shenzhen with new concept portable benzene series detector, breathable and impermeable inner phase structure adjustable polymer membrane material and broadband low loss dielectric gradient material and preparation technologies, and carried out on-site technical explanation and promotion.

研究院老师参加第七届胶体与界面化学青年学者论坛

INCSMM teachers attend 7th Colloids and Interface Chemistry Young Scholars Forum

2024 年 11 月 15 至 17 日，房喻院士、丁立平教授、刘静教授、彭军霞教授、刘凯强教授、边红涛教授、刘小燕副研究员、苗荣副教授和刘忠山副教授等 9 人赴北京参加了第七届胶体与界面化学青年学者论坛。

房喻院士应邀作为论坛专家对青年学者进行了指导。刘忠山副教授做了题为“基于整体材料的吸附分离和荧光传感”的口头报告。

本次论坛由中国化学会胶体与界面化学专业委员会主办，中国地质大学（北京）承办。

From November 15 to 17, 2024, Prof. Fang Yu, Prof. Ding Liping, Prof. Liu Jing, Prof. Peng Junxia, Prof. Liu Kaiqiang, Prof. Bian Hongtao, Associate Researcher Liu Xiaoyan, Assoc. Prof. Miao Rong and Assoc. Prof. Liu Zhongshan attended the 7th Colloids and Interface Chemistry Young Scholars Forum in Beijing.

Prof. Fang Yu was invited to provide guidance to the young scholars as an expert of the forum. Assoc. Prof. Liu Zhongshan gave an oral presentation titled “Integral Material Based Adsorption Separation and Fluorescence Sensing”.

The forum was sponsored by the Colloidal and Interfacial Chemistry Committee of the Chinese Chemical Society and hosted by China University of Geosciences (Beijing).

彭浩南教授赴新加坡参加第二届国际教育会议

Peng Haonan attends SUSS SoTL Symposium 2024

2024 年 11 月 26 日至 27 日，新概念传感器与分子材料研究院彭浩南教授在新加坡参加了由新加坡社会科学大学主办的主题为“教育中的可持续学习：传承与变革”的第二届国际教育会议。

本次会议汇聚了全球教育领域的专家、政策制定者和学者，围绕当今社会快速变化的背景下，教育如何实现可持续发展展开深入探讨，包括如何在后疫情时代巩固在线学习的优势、如何应对生成式人工智能工具的冲击，以及如何确保教育的普适性和公平性。

From 26 to 27 November 2024, Prof. Pang Haonan of the Institute of New Concepts Sensors and Molecular Materials participated in the SUSS SoTL Symposium 2024 hosted by the Singapore University of Social Sciences in Singapore, which was themed “Sustainable Learning in Education: What Should Remain and What Should Change” .

The Scholarship of Teaching and Learning Symposium brought together global education experts, policymakers and scholars to discuss how education can be sustainable in today’s rapidly changing society, including how to consolidate the benefits of online learning in the post-pandemic era, how to cope with the impact of generative AI tools, and how to ensure universal and equitable education.

研究院教师参加国家重点研发计划“纳米前沿”重点专项项目2024年度总结暨2025年度工作计划会议

INCSMM faculty participate in 2024 Summary and 2025 Work Plan Meeting of National Key R&D Plan “Nano Frontier” Key Project

2024年11月23日，新概念传感器与分子材料研究院房喻院士、丁立平教授、薛东旭教授、刘太宏副教授和刘忠山副研究员参加了在深圳召开的国家重点研发计划“纳米前沿”重点专项项目“超高灵敏检测痕量危险有害化学物质的纳米材料与技术”2024年度总结暨2025年度工作计划会议。

丁立平教授汇报了课题研究进展，并与项目组成员一起与其他项目组就课题研究进展、考核指标完成情况、现存问题及解决方法、下一年度研究计划等情况进行了讨论。

最后房喻院士总结发言，指出国家重点研发计划旨在解决国家重大需求和社会经济发展中的关键问题，需要学术和实践两个方面把重点成果突出展示出来，希望项目成员继续努力，争取在下次会议上展示出能打动人的成果。

会议由中国科学院新疆理化技术研究所牵头，联合陕西师范大学、中国人民解放军军事科学院防化研究院、中国科学院化学研究所、公安部禁毒情报技术中心、深圳砺剑防卫技术有限公司等单位共同举办，项目各承担单位负责人、部分科研骨干和新疆理化所科技处负责人等近30人参加了会议。

On November 23, 2024, Prof. Fang Yu, Prof. Ding Liping, Prof. Xue Dongxu, Assoc. Prof. Liu Taihong and Associate Researcher Liu Zhongshan of the Institute of New Concept Sensors and Molecular Materials participated in the 2024 Summary and 2025 Work Plan meeting of the “Nano Frontier” Special Key Project “Ultra-sensitive Nanomaterials and Technologies for Detecting Trace Hazardous and Harmful Chemicals” of the National Key Research and Development Plan held in Shenzhen.

Prof. Ding Liping reported the research progress of her project, and together with her team members, discussed with other project teams the research progress of the project, the completion of assessment indicators, existing problems and solutions, and the research plan for the next year.

In the end, Prof. Fang Yu summed up the meeting, pointing out that the national key R&D plan aims to solve the major needs of the country and the key problems in social and economic development, and it needs both academic and practical aspects to highlight the key achievements, and he

hoped that the members of the projects would continue to work hard and strive to show impressive results at the next meeting.

The meeting was led by Xinjiang Technical Institute of Physics and Chemistry of the Chinese Academy of Sciences and co-organized by Shaanxi Normal University, Chemical Defense Research Institute of the PLA Academy of Military Sciences, Chemical Research Institute of the Chinese Academy of Sciences, Anti-Drug Information Technology Center of the Ministry of Public Security, and Shenzhen SRED Security and Surveillance Technology Co., Ltd. Nearly 30 people attended the meeting, including the heads of the project undertaking units, key researchers and the heads of the Science and Technology Department of Xinjiang Institute of Physics and Chemistry.

房喻院士获聘滁州市人才工作顾问

Fang Yu appointed Chuzhou Talent Work Consultant

2024 年 11 月 27 日，房喻院士应邀出席安徽省来安县第四届“星耀来安·人才科技节”暨产才融合·赋能新质生产力发展大会开幕式。

开幕式上，房喻院士接受了滁州市委书记吴劲颁发的滁州市人才工作顾问荣聘证书并致辞。

当天，房喻院士还赴滁州市釉美生物技术有限公司参加了国家重点研发计划项目《新型生物组装自愈合牙修复材料的制备与性能研究》项目年度总结会暨子课题2成果产品发布会，并出席了“生物组装高分子脱敏剂”产品发布仪式。

On November 27, 2024, Prof. Fang Yu was invited to attend the opening ceremony of the fourth “Stars Shining on Lai’an • Talent and Technology Festival” and the Conference on Production and Talent Integration Enabling New Quality Productivity Development held in Lai’an County, Anhui Province.

At the ceremony, Fang Yu was awarded the honorary appointment certificate of Chuzhou City Talent Work Consultant by Chuzhou Municipal Party Committee secretary Wu Jin, and delivered a speech.

On the same day, Fang Yu also went to Chuzhou Youmei Biotechnology Co., Ltd. to participate in the annual summary meeting and sub-project 2 product launch of the national key research and development plan “Preparation and Performance Research of New Biological Assembly Self-healing Dental Restoration Materials”, and attended the product launch ceremony of “Biological Assembly Polymer Desensitization Agent”.

Chemical Engineering Journal 500 (2024) 156764

Contents lists available at ScienceDirect

Chemical Engineering Journal

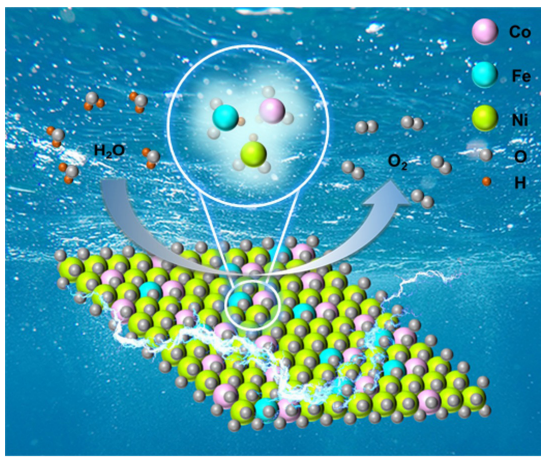
journal homepage: www.elsevier.com/locate/cej

Valence electronic engineering of hollow-nanocube-structured CoFeNi-layered double hydroxides for highly efficient oxygen evolution

Lu Liu [a,1], Lingxing Zan [a,1,*], Yunchuan Tu [b,*], Hongling Zhang [a], Dan Zhu [a], Zhe Li [a], Jiawen Zheng [a], Zhuangzhuang Zhang [a], Yu Sun [c], Qiang Weng [c], Jian Li [d], Qingbo Wei [a], Huicong Xia [e], Xin Bo [c,*], Feng Fu [a,*]

高价电子结构优化层状氢氧化钴铁镍中空立方体提升析氧催化效率

Lu Liu#, Lingxing Zan#, Yunchuan Tu*, Hongling Zhang, Dan Zhu, Zhe Li, Jiawen Zheng, Zhuangzhuang Zhang, Yu Sun, Qiang Weng, Jian Li, Qingbo Wei, Huicong Xia, Xin Bo*, Feng Fu*, Chemical Engineering Journal, 2024, 500, 156764. DOI:/10.1016/j.cej.2024.156764



基于金属有机骨架的衍生层状氢氧化物是构建高效催化剂的策略之一。通过调节优化活性金属位点配位环境和价电子结构达到协同催化效果，可有效提高其内在电化学析氧活性。本文采用了一种简单的溶剂法，合成了具有高价态电子结构的中空钴铁镍层状氢氧化物纳米立方体催化剂，表现出强烈的协同催化效应和优异的电化学活性及稳定性。在 100 mA cm^{-2} 的输出电流下，其过电位低至 294 mV；在高电流密度 1 A cm^{-2} 时，也具有良好的稳定性，超越了商用贵金属铱、钌基催化剂的性能。原位谱学研究表明，材料的金属配位环境和金属位点的价态电子结构可以充当活性中心。本研究为高效析氧催化剂的设计以及电解水的发展提供了理论基础和物。

共同第一作者：延安大学硕士研究生刘璐、延安大学昝灵兴副教授
通讯作者：重庆大学涂云川副教授、陕西师范大学薄鑫副研究员、延安大学付峰教授
全文链接：https://doi.org/10.1016/j.cej.2024.156764

The layered double hydroxides (LDH) derived from metal-organic framework (MOF) is one of the strategies for constructing efficient catalysts. It has been widely studied that adjusting and optimizing the coordination environment and valence electronic structure of active metal sites can achieve the synergistic effect and improve the intrinsic activity. We employed a facile solvent method to synthesize a well-defined hollow nanocube-structured CoFeNi-LDH with an optimized valence electronic structure of metal sites as an efficient electrocatalyst. The catalyst exhibites a strong synergistic catalytic effect and an excellent activity and stability. It achieved a lower overpotential of 294 mV at 100 mA cm^{-2}, and high durability at the current density of 1 A cm^{-2}, outperforming the commercial Ir-/Ru-based catalysts. The optimized the coordination environment and valence electronic structure of metal sites can definitely serve as active centers for triggering OER, thereby improving the intrinsic electrocatalytic performance. This study provides theoretical basis and material guarantee for the design of excellent OER catalyst and the development of electrolytic water.

Co-first Authors: Master's candidate Liu Lu, Yan'an University; A/Prof. Zan Lingxing, Yan'an University
Correspondence Authors: A/Prof. Tu Yunchuan, Chongqing University, A/Prof. Bo Xin, Shaanxi Normal University, and Prof. Fu Feng, Yan'an University
Full Text Link: https://doi.org/10.1016/j.cej.2024.156764

molecules

MDPI

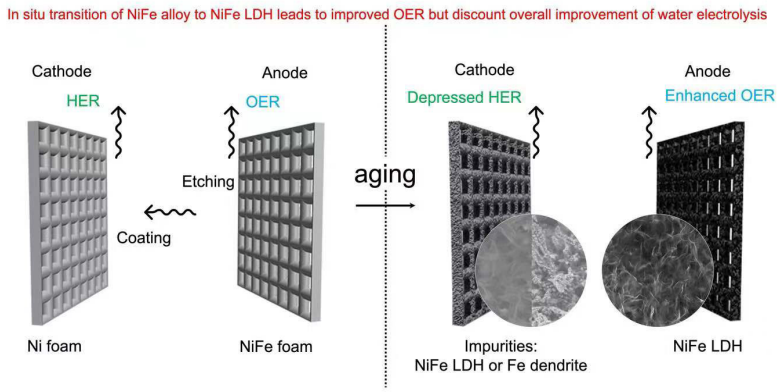
Article

In Situ Anodic Transition and Cathodic Contamination Affect the Overall Voltage of Alkaline Water Electrolysis

Zheng Liu [1,†], Zhaoyu Liu [2,†], Lingxing Zan [3], Yu Sun [2], Huizhen Han [2], Zhe Li [3], Han Wang [1], Ting Cao [1], Yao Zhu [1], Haiyang Lv [1], Yuxuan Liu [4], Juzhe Liu [4,*] and Xin Bo [2,*]

原位阳极转变和阴极污染对碱性水解制氢总电压的影响

Zheng Liu#, Zhaoyu Liu#, Lingxing Zan, Yu Sun, Huizhen Han, Zhe Li, Han Wang, Ting Cao, Yao Zhu, Haiyang Lv, Yuxuan Liu, Juzhe Liu*, Xin Bo*, Molecules, 2024, 29, 5298. DOI:/10.3390/molecules29225298



镍铁氢氧化物作为一种高效的碱性电解水制氢阳极析氧催化剂已被广泛应用于制氢设备中，且该类催化材料可由镍铁合金整体式电极原位老化获得。因此，工业上可将镍铁合金电极直接安装于电解槽中，随着设备运转，其析氧效率会自行提升。本研究通过模拟工业这一过程，指出电解槽的总体节能效率是来自于阳极析氧和阴极析氢反应两者的共同贡献。我们观察到虽然从镍铁合金电极原位生成的镍铁氢氧化物具有催化促进作用，但其耦合的镍阴极受到污染，导致析氢活性损失和整体效率提升大打折扣。Ni^{2+} 和 Fe^{3+} 阳离子在长期工业模拟过程中不可避免地从阳极溶解到电解液中，并在镍阴极上电沉积。该研究强调了催化应用不应局限于孤立的半反应，合理的耦合电极匹配以去除电解液中的污染物，对于充分展现真实应用中的内在催化能力也具有重要意义。

第一作者：中国环境科学院刘铮副教授，陕西师范大学硕士研究生刘兆宇
通讯作者：华北电力大学刘聚哲副教授，陕西师范大学薄鑫副研究员
全文链接：https://doi.org/10.3390/molecules29225298

NiFe (oxy)hydroxide has been widely used as a benchmark anodic catalyst for oxygen evolution reaction (OER) in alkaline water electrolysis devices and can be achieved via in situ aging from the NiFe alloy, therefore, NiFe alloy monolithic electrodes can be directly installed in the industrial electrolyzer and the OER efficiency will spontaneously improve by aging. We simulated the industrial scenario and pointed out the energy saving actually takes contributions from both the anodic OER and cathodic HER (hydrogen evolution reaction). The coupled nickel cathode is contaminated, leading to the loss of HER activity and a reduction in overall efficiency. Ni^{2+} and Fe^{3+} cations are inevitably detached from the anode into the electrolyte and electrodeposited on the nickel cathode after the long-term industrial simulation. This research emphasizes that the catalytic application should not only be isolated on the half reaction, but a reasonable coupled electrode match to get rid of the contamination from the electrolyte is also of great significance to sufficiently present the intrinsic catalytic yielding for the real application.

First Authors: A/Prof. Liu Zheng, Chinese Research Academy of Environmental Sciences; Master's candidate Liu Zhaoyu, Shaanxi Normal University
Correspondence Authors: A/Prof. Liu Juzhe, North China Electric Power University; A/Prof. Bo Xin, Shaanxi Normal University
Full Text Link: https://doi.org/10.3390/molecules29225298

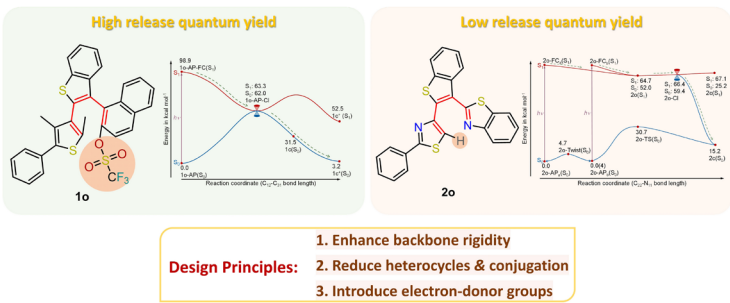
From the journal:
Chemical Science

Gaining the Molecular Design Principles for Efficient Diarylethene Photoacid and Photohydride Generators Based on Photochemical Reaction Mechanism

Yifan Su, Dexin Zheng, Lingfeng Ge, Le Yu, David Lee Phillips, Jiani Ma and Yu Fang

基于机理研究获得高效二芳基乙烯光酸和光氢化物发生剂的分子设计原则

Yifan Su, Dexin Zheng, Lingfeng Ge, Le Yu,* David Lee Phillips, Jiani Ma,* and Yu Fang. Chem. Sci., 2024, DOI: 10.1039/D4SC06202G



光致产酸剂（PAGs）和光氢化物发生剂（PHGs）分别是释放酸和氢化物的特定光敏保护基。在过去的十年里，研究者致力于开发高效的新型 PAGs 和 PHGs。基于二芳基乙烯开发的 PAGs 和 PHGs 具有优异的光敏性，可在光致变色环化过程中释放酸或氢化物（图 1）。研究表明：PAGs 的释放量子产率可以达到 50%，而 PHGs 即使在分子结构修饰后也仅有 4.2%。为了提供分子设计的理性指导思想，我们分别选取化合物 1o 和 2o 作为 PAGs 和 PHGs 的模型分子，利用飞秒 / 纳秒时间分辨光谱以及 DFT/TD-DFT 计算，阐明了 PAGs 和 PHGs 的光化学反应机制，并基于此总结了高效二芳基乙烯光酸和光氢化物发生剂的分子设计原则。

近日，马佳妮教授课题组在 Chemical Science 上发表了基于二芳基乙烯的光酸和光氢化物发生剂的分子设计。利用超快时间分辨光谱技术辅以理论计算，研究了光致产酸剂（1o）和光氢化物发生剂（2o）的光化学反应机制（图 2 和图 3）。基于机理研究揭示了 1o 和 2o 释放量子产率差异的关键。对于 1o 而言，在室温下，其反平面构型（1o–AP，即活性构型）为稳定构型，所以 1o–AP 占多数。并且 1o–AP → 1o–P（非活性构型）的势垒为 3.0 kcal mol^{-1}。此外，1o–AP 的光化学反应是无势垒的（图 2），从而抑制了系间窜越过程的竞争。实验结果表明可以自发生成产物 1c^{+}。然而，对于 2o 而言，2o–AP 并非室温下的优势构型，并且光化学反应存在势垒（图 3）。并且在只有加入氢化物受体才能生成 2c^{+}。

基于实验和理论结果，我们提出了高效二芳基乙烯光酸和光氢化物发生剂的分子设计的核心原则。第一，可通过增强骨架的刚性来稳定分子基态的活性反应构型。如通过引入空间位阻或分子内氢键来抑制苯基噻唑和苯并噻唑基团的单键旋转；第二，由于三重态反应通道是与单线态环化反应途径的竞争过程，因此可通过降低系间窜越效率提高 PHGs 的光释放量子产率。通常，含氮和硫的杂环分子通常会增加旋轨耦合常数，提供系间窜越的效率；而扩展分子共轭程度可降低三线态的能量，并为低单线态提供了更多可能的系间窜越通道。因此，在未来分子设计中可通过调控取代基及母体的共轭程度来优化分子设计，获得高效光酸和光氢化物发生剂；第三，可通过引入供电子基团来提高 2c 的脱氢负离子活性，从而提高其生成终产物的效率。

第一作者：陕西师范大学博士研究生苏怡帆
通讯作者：陕西师范大学马佳妮教授，西北大学于乐副教授
全文链接：https://doi.org/10.1039/d4sc06202g

Photoacid generators (PAGs) and photohydride generators (PHGs) are specific photolabile protecting groups that release acid and hydride, respectively. Over the past decade, great efforts have been devoted to developing novel PAGs and PHGs with advanced efficiency, among which, two of the promising candidates are the diarylethene (DAE)-based PAGs and PHGs, which release acids/hydrides during photochromic electrocyclization. The release quantum yields of PAGs can up to 50%, while PHGs are only 4.2% even after molecular structure modification. In this work, we reveal the photochemical reaction mechanisms of PAG (1o) and PHG (2o) using femtosecond/nanosecond time-resolved spectroscopy and DFT/TD-DFT calculations (Fig. 1).

The different photochemical mechanisms are the key that leads to distinctive release quantum yields between 1o and 2o. For 1o, at room temperature, 1o-AP (reactive conformation) is the stable conformation, so 1o-AP is in majority. And the potential barrier of 1o-AP → 1o-P (non-reactive conformation) is 3 kcal mol^{-1}. In addition, according to the potential energy curve, the photochemical reaction of 1o-AP is barrierless (Fig. 2), which suppresses intersystem crossing (ISC). And the experimental results showed that the product $1c^+$ could be generated spontaneously. However, for 2o, 2o-AP is minority among all 2o conformers at room temperature and there is a potential barrier for the photochemical reaction (Fig. 3). In addition, experimental results indicated that $2c^+$ can only be observed in the presence of a hydride acceptor.

Based on the experimental and DFT/TD-DFT results, we propose the following ideas to improve the quantum yield of 2o. First, in order to stabilize 2o-AP(S0), enhancing the rigidity of the skeleton is a possible strategy. For example, the single bond rotation of the phenylthiazole and benzothiazole groups could be suppressed by introducing steric hindrance or an intramolecular hydrogen bond. Second, ISC competes with cyclization pathways in the singlet state, so decreasing the ISC efficiency is a feasible way to increase the quantum yield. The N and S-containing heterocycles usually give rise to enhanced spin orbit coupling strength and are beneficial for promoted ISC efficiency. The extended conjugating system lowers the energy of triplet states and offers more possible ISC channels for low-lying singlet states. In addition, it is expected that increasing the dehydrogenate capability of 2c by incorporating electron-donating groups would promote the 2c → $2c^+$ efficiency.

First Author: Su Yifan, doctoral candidate, Shaanxi Normal University
Correspondence Authors: Prof. Ma Jiani, Shaanxi Normal University; Assoc. Prof. Yu Le, Northwest University
Full Text Link: https://doi.org/10.1039/d4sc06202g

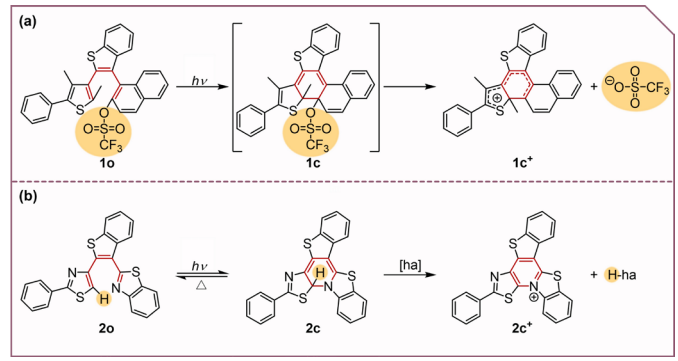


图 1. (a) 1o 和 (b) 2o 的光释放反应。“ha”是指“氢化物受体”。
Figure 1. Photochemical reactions of (a) 1o and (b) 2o. “ha” refers to the “hydride acceptor”.

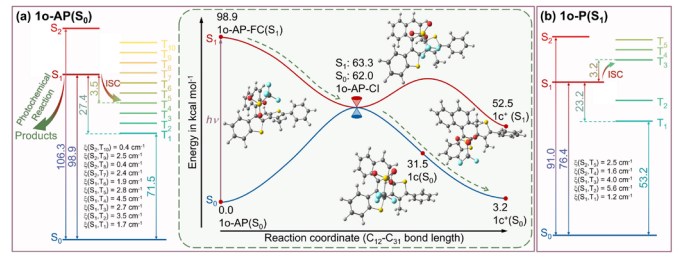


图 2. (a) 1o−AP(S0) 和 (b) 1o−P(S1) 的计算单线态和三线态能级图。插图：1o−AP 的势能曲线。(1o−AP(S0) 的基态能量作为零点以获得相对能量。) [(TD)M062X/6−311G★★/SMD(ACN)]
Figure 2. The calculated singlet and triplet states energy level diagram for (a) 1o-AP(S0) and (b) 1o-P(S1). Inset: PEC of 1o-AP. (the ground state energy of 1o-AP(S0) is used as zero for obtaining relative energies). [(TD)M062X/6-311G**/SMD (ACN)].

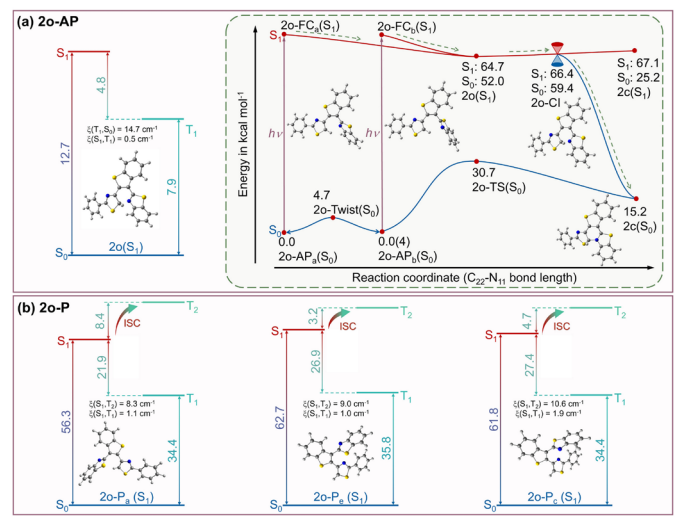


图 3. (a) 2o−AP 和 (b) 2o−P 的计算单线态和三线态能级图。插图：2o−AP 的势能曲线。(2o−APa(S0) 的基态能量作为零点以获得相对能量。) [(TD)M062X/6−311G★★/SMD(THF)]
Figure 3. The calculated singlet and triplet states energy level diagram for (a) 2o-AP and (b) 2o-P. Inset: PEC of 2o-AP. (the ground state energy of 2o-APa(S0) is used as zero for obtaining relative energies). [(TD)M062X/6-311G**/SMD (THF)].

浙江大学吴子良教授应邀作报告

Prof. Wu Ziliang of Zhejiang University invited to give a report

2024 年 11 月 1 日下午，国家杰出青年基金获得者、浙江大学吴子良教授应邀访问新概念传感器与分子材料研究院，并作题为“高性能水凝胶材料与器件”的学术报告。

报告重点阐述了吴子良教授课题组近年来在高性能水凝胶设计制备、变形驱动功能调控等方面的重要进展，特别是水凝胶玻璃态分子形成机制与多稳态变形控制方法的突破。

报告会由刘凯强教授主持，研究院师生及西北大学于游教授等 60 余人参加了报告会，并与吴子良教授在凝胶设计与软物质驱动策略方面进行了讨论。

On Nov 1, 2024, Prof. Wu Ziliang from Zhejiang University, recipient of the National Outstanding Youth Fund, was invited to visit Institute of New Concept Sensors and Molecular Materials and give a report titled “High Performance Hydrogel Materials and Devices”.

The report focuses on the important progress made by Prof. Wu’s group in recent years in the design and preparation of high-performance hydrogels, deformation-driven functional regulation, especially the breakthroughs in the molecular formation mechanism of the glassy state of hydrogels and the method of multi-stable deformation control.

The report was moderated by Prof. Liu Kaiqiang, and attended by more than 60 people, including faculty and students of the Institute and Prof. Yu You of Northwestern University, who discussed with Prof. Wu in issues of gel design and soft-matter driving strategies.

深圳晶泰科技有限公司来院技术交流

Shenzhen XtalPi Technology guests received for technological exchange visit

2024 年 11 月 5 日上午，深圳晶泰科技有限公司自动化负责人刘卫东等一行六人到访新概念传感器与分子材料研究院进行技术交流。

在研究院一层报告厅举行的报告会上，晶泰科技自动化团队介绍了公司在人工智能领域的前沿技术、典型应用场景以及相关解决方案，内容覆盖人工智能在催化剂、药物筛选、高分子合成自动化等多个领域的创新应用，展现了人工智能如何推动各学科智能化转型。

晶泰科技自动化团队产品总监张晨曦、技术负责人欧阳力、商务总监李敬芝、产品经理江豪及商务经理冯晓龙参加了交流，并特别针对研究院的相关研究方向、科研需求和技术发展趋势提出多项技术方案，涵盖了高效数据处理、智能化实验系统、精准预测模型等方面。

研究院多位师生参与了此次交流，结合各自的研究方向对技术方案进行了讨论，并就技术方案提出了意见和建议，提出了具体的技术需求与期望。

最后，房喻院士表达了对人工智能技术的应用前景的期望，希望能够进一步深化人工智能与科研的融合，推动智能技术在科研领域的创新应用，以提升研究效率，促进科研成果的转化和实际落地。

On November 5, 2024, six guests from Shenzhen XtalPi Technology Co., Ltd., headed by its chief of automation department Mr. Liu Weidong, visited the Institute of New Concept Sensors and Molecular Materials in a technological exchange visit.

At the presentation held in the lecture hall of the Institute, XtalPi automation

team briefed about the company's cutting-edge technologies in the field of artificial intelligence, typical application scenarios and related solutions, covering the innovative AI applications in fields such as catalysts, drug screening, and polymer synthesis automation, showing how AI promotes the intelligent transformation of various disciplines.

XtalPi automation team product director Zhang Chenxi, technical director Ouyang Li, commercial director Li Jingzhi, product manager Jiang Hao and business manager Feng Xiaolong participated in the exchange, and presented a number of technical solutions for the relevant research direction, research needs and technical development trends of the Institute, covering efficient data processing, intelligent experimental system, accurate prediction model and other aspects.

Some teachers and students of the Institute participated in the exchange, discussing the technical solutions according to their respective research directions, and putting forward opinions and suggestions and specific technical needs and expectations.

Finally, Prof. Fang Yu expressed his expectations for the application prospects of AI technology, hoping to further deepen the integration of AI and research, promote the innovative application of AI technology in the field of research, in order to improve research efficiency, and promote the transformation and actual commercialization of research results.

中国空间技术研究院西安分院一行来访

China Academy of Space Technology Xi'an Branch visitors received

2024 年 11 月 8 日下午，中国空间技术研究院西安分院副院长马小飞研究员一行 6 人来访新概念传感器与分子材料研究院，参观了研究院展厅，并与房喻院士等进行了座谈交流。

座谈会上，中国空间技术研究院西安分院朱忠博研究员、岳震震高级工程师分别作了题为《太赫兹空间通信技术及其发展》和《3D 打印球透镜技术及应用》的报告。随后，双方就后续科研合作进行了讨论交流。

西安分院副主任崔万照研究员、研发处沈俊处长、周卫来研究员，研究院副院长丁立平教授、彭浩南教授、彭军霞教授、办公室主任杨小刚、秘书左振男、专职科研人员何怡楠、马剑飞、罗艳彦及物理与信息技术学院辛云宏教授参加了座谈交流。

On November 8, 2024, a delegation of six people from Xi'an Branch of China Academy of Space Technology headed by vice dean Mr. Ma Xiaofei visited the Institute of New Concept Sensors and Molecular Materials, touring the INCSMM exhibition hall and meeting with Prof. Fang Yu.

At the meeting, CAST Xi'an Branch researcher Zhu Zhongbo and senior engineer Yue Zhenzhen presented reports titled "Taihertz Space Communication Technology and Its Development" and "3D Printing Globe Lens Technology and Application" respectively. Subsequently, the two sides discussed and exchanged views on follow-up research cooperation.

CAST Xi'an Branch vice director Cui Wanzhao, R&D Department deputy director Shen Jun, researcher Zhou Weilai; INCSMM vice dean Prof. Ding Liping, Prof. Peng Haonan, Prof. Peng Junxia, Administrative Office director Yang Xiaogang, secretary Zuo Zhenan; research assistants He Yinan, Ma Jianfei, Luo Yanyan, and Prof. Xin Yunhong of the School of Physics and Information Technology participated in the meeting.

总策划：房喻教授
Producer & Editor-in-Chief: Prof. Fang Yu
责任编辑：马佳妮 冯伟
Executive Editors: Ma Jiani, Feng Wei
翻译：冯伟
Translator: Feng Wei
校对：团队全体老师
Proofreading: Fang Group teachers

地址：陕西省西安市长安区西长安街 620 号陕西师范大学长安校区
Chang'an Campus, Shaanxi Normal University, 620 West Chang'an Avenue, Chang'an District, Xi'an, Shaanxi, P. R. China
联系电话 (Tel)：86-29-81530726
电子邮箱 (Email)：incsmm@snnu.edu.cn

装帧设计：泛象艺术空间
Designed by FanForm Art Space