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 08 2024

Institute of New Concept Sensors and Molecular Materials Newsletter

目 录 Contents

房喻院士在第 6 期教材建设和管理国家级培训班上作报告

Fang Yu speaks at 6th National Training Course on Textbook Construction and Management

2024 年 7 月 31 日至 8 月 2 日，教育部贵州省贵阳市举办第 6 期教材建设和管理国家级培训班，房喻院士应邀为培训班学员作报告。

普通高中数学、物理、化学、生物学、地理、信息技术和通用技术教材的主要编写人员和出版单位责任编辑等共约 280 人参加培训。

From July 31 to August 2, 2024, the Ministry of Education held the 6th National Training Course on Textbook Construction and Management in Guiyang, Guizhou Province, and Prof. Fang Yu was invited to deliver a report for the participants.

About 280 people, including the main writers of mathematics, physics, chemistry, biology, geography, information technology and general technology textbooks and the responsible editors of publishing units, participated in the training.

科研助理王佩参加 2024 年突发环境卫生事件应急处置技术培训班

Wang Pei attends 2024 training course on Response Techniques for Environmental Health Emergencies

2024 年 8 月 6 日至 8 日，新概念传感器与分子材料研究院科研助理王佩与陕西中造立成环保科技有限公司张晓丽总经理一行携带合作研发的二氧化氯消毒除菌系列产品参加中华预防医学会环境卫生分会在沈阳举办的 2024 年突发环境卫生事件应急处置技术培训班。

在此次培训班，王佩学习了突发环境卫生事件的应急准备、现场处置、自然灾害卫生防病要点、预防性消毒和大型活动卫生保障消毒技术等专业知识，并参加了国家级继续医学教育培训考试。

普立瑞 ® 产品基于研究院开发的透气不透水专利膜材料实现高效除菌消毒剂二氧化氯气体的可控、高效、长期释放，致力于为基层医务工作人员提供职业安全防护，产品的精准消毒和科学消毒特性符合未来全球生态环境绿色发展的理念，获得了参会专家及学者的广泛关注。

From August 6 to 8, 2024, Wang Pei, a research assistant of the Institute of New Concept Sensors and Molecular Materials, and Zhang Xiaoli, general manager of Shaanxi Zhongzao Licheng Environmental Protection Technology Co., Ltd. participated in the 2024 Training Course on Emergency Response Techniques for Emergency Response to Environmental Health Incidents held by the Environmental Health Branch of Chinese Preventive Medical Association in Shenyang, bringing with them the chlorine dioxide disinfection and sterilization series products jointly developed by the two parties.

During the course, Wang Pei learned professional knowledge of emergency preparedness for environmental health emergencies, on-site disposal, key points of natural disaster hygiene and disease prevention, preventive disinfection and disinfection techniques for hygiene protection of large-scale events, and participated in the national-level continuing medical education training examination.

The POLIPOROUS® products are based on the breathable and impermeable patented membrane material developed by the Institute to realize the controlled, efficient and long-term release of chlorine dioxide gas, which is a highly effective sterilizing agent, providing occupational safety protection for grass-roots medical staff, and the precise and scientific disinfection characteristics of the products are in line with the concept of green development of the global ecological environment in the future, which has gained wide attention from the participating experts and scholars.

彭灵雅老师参加第 15 届全国理论与计算化学会议

Peng Lingya attends 15th National Conference on Theoretical and Computational Chemistry

2024 年 8 月 6 日至 9 日，新概念传感器与分子材料研究院彭灵老师雅参加了在吉林省长春市举行的中国化学会第 15 届全国理论与计算化学会议，并获最佳墙报奖。

此次会议由中国化学会理论化学专业委员会主办、吉林大学共同主办，吉林大学化学学院、理论化学研究所、超分子结构与材料国家重点实验室共同承办。

From August 6th to 9th, 2024, Dr. Peng Lingya of the Institute of New Concept Sensors and Molecular Materials participated in the 15th National Conference of Theoretical and Computational Chemistry of Chinese Chemical Society and was awarded the Best Poster Award.

The conference was co-sponsored by the Theoretical Chemistry Committee of the Chinese Chemical Society and Jilin University, and co-organized by the College of Chemistry, the Institute of Theoretical Chemistry and the State Key Laboratory of Supramolecular Structures and Materials of Jilin University.

刘静教授参加“六盘山论坛 2024”并作学术报告

Liu Jing presents at Liupan Mountain Forum 2024

2024 年 8 月 10 日至 13 日，新概念传感器与分子材料研究院刘静教授参加了在宁夏固原召开的“六盘山论坛 2024”，并作了题为“铂配合物 (II) 自组装与发光性质调控研究”的学术报告。

“六盘山论坛 2024”由中共固原市委、固原市政府、宁夏师范大学主办，宁夏绿色催化材料与技术重点实验室承办，旨在为促进新能源材料与纳米材料领域的创新发展，加强 AI 与新材料的融合。

From August 10 to 13, 2024, Prof. Liu Jing of the Institute of New Concept Sensors and Molecular Materials participated in the “Liupan Mountain Forum 2024” held in Guyuan, Ningxia Autonomous Region, and presented a report titled “Self-assembly of Platinum Complex (II) and regulation of luminous Properties”.

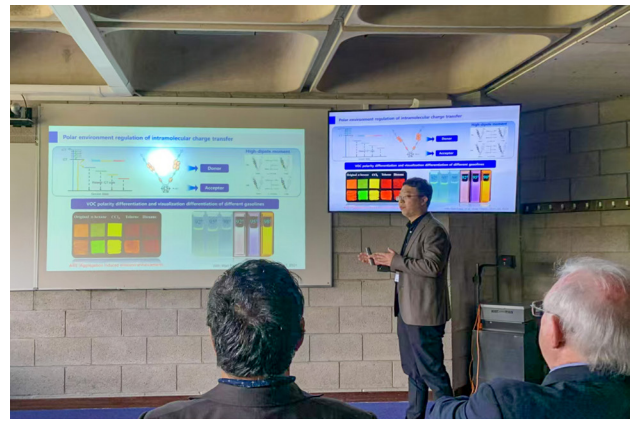
The forum, sponsored by the CPC Guyuan Municipal Committee, Guyuan Municipal Government and Ningxia Normal University, and hosted by Ningxia Key Laboratory of Green Catalytic Materials and Technology, aims to promote the innovative development of new energy materials and nanomaterials, and strengthen the integration of AI and new materials.

房喻院士、彭浩南教授赴爱尔兰参加第 20 届传感器及应用大会

Fang Yu and Peng Haonan attend 20th Sensors and their Applications Conference in Ireland

2024 年 8 月 11 日至 14 日，新概念传感器与分子材料研究院房喻院士和彭浩南教授受邀参加在爱尔兰利莫瑞克大学举办的第 20 届传感器及应用大会暨第 5 届光纤和光子传感技术产业与安全应用国际会议。

房喻院士做了题为 Adlayer Structure Innovation and Film-BASED Fluorescent Sensors 的特邀报告，详细



介绍了团队在薄膜荧光传感器领域的最新研究进展，得到了与会专家的高度评价。彭浩南教授在分会场做了题为 Construction of fluorescent compounds exhibiting strong luminescence and high photochemical stability for VOC sensing 的邀请报告。

本次会议由英国皇家特许计量及测试学会主办，得到了中国仪器仪表学会、英国物理学会、爱尔兰利莫瑞克大学及中国光学工程学会光纤传感器分会等多方支持。

作为国际传感技术领域的重要学术盛会，本次会议吸引了来自全球的众多专家学者及企业界人士参会，共同探讨传感技术的最新研究成果和未来发展方向。

会议期间，房喻院士和彭浩南教授与众多国际同行开展了深入交流，探讨了未来的合作方向。此外，团队的研究成果，特别是薄膜荧光传感技术以及气体传感器隔膜材料的应用，也引起了企业界同行的浓厚兴趣。

From August 11 to 14, 2024, Prof. Fang Yu and Prof. Peng Haonan of the Institute of New Concept Sensors and Molecular Materials attended the 20th Sensors and their Application Conference and the 5th International Conference of Fibre Optic and Photonic Sensors for Industrial and Safety Application held at the University of Limerick, Ireland.

Fang Yu made an invited report titled "Adlayer Structure Innovation and Film-based Fluorescent Sensors", detailing the latest research progress of his group in the field of Film-based fluorescent sensors, which was highly praised by the experts attending the meeting. Peng Haonan presented an invited report titled "Construction of fluorescent compounds exhibiting strong luminescence and high photochemical stability for VOC sensing" at the parallel session.

The conference was sponsored by the Institute of Measurement & Control, and was supported by the China Instrument and Control Society, the Institute of Physics, the University of Limerick in Ireland and the Fiber Optic Sensor Branch of the Chinese Society of Optical Engineering.

As an important academic event in the field of sensing technology, this conference attracted many experts, scholars and business people from around the world to discuss the latest research results and future development direction of sensing technology.

During the conference, Fang Yu and Peng Haonan conducted in-depth exchanges with international counterparts and discussed the future direction of cooperation. In addition, Fang group's research results, especially the application of film-based fluorescence sensing technology and gas sensor diaphragm materials, have also aroused strong interest in the industry.

薄鑫参加“武创源”国际光化学及绿色制造技术创新大赛预赛

Bo Xin participates in preliminary of “WuChuangyuan” Int’l Photochemistry and Green Manufacturing Technology Innovation Competition

2024 年 8 月 14 至 17 日，薄鑫副研究员参加了在武汉举行的“武创源”国际光化学及绿色制造技术创新大赛预赛，并作了题为“高效非贵金属析氢催化剂的绿色宏量制备”的路演汇报。

本次大赛由武汉市科技创新局、武汉市青山区人民政府、华中师范大学主办，涵盖光化学合成、光化学减污降碳、光电磁功能材料、光响应合成生物学、人工智能光化学、光化学绿色制造技术、电化学绿色制造技术、热化学绿色制造技术及其他成熟度高、可落地转化绿色制造技术领域。

From August 14 to 17, 2024, Dr. Bo Xin participated in the preliminary competition of “WuChuangyuan” International Photochemistry and Green Manufacturing Technology Innovation Competition held in Wuhan, and presented a roadshow report titled “Green scaled production of non-precious-metal catalyst for efficient hydrogen evolution”.

The competition was organized by Wuhan Science and Technology Innovation Bureau, Wuhan Qingshan District People’s Government and Central China Normal University and covers the fields of photochemical synthesis, photochemical pollution reduction and carbon reduction, photoelectromagnetic functional materials, photoresponsive synthetic biology, artificial intelligence photochemistry, photochemical green manufacturing technology, electrochemical green manufacturing technology, thermochemical green manufacturing technology and other green manufacturing technologies with high maturity for industrialization.

房喻院士为“全国科学教育暑期学校”中小学教师培训作报告

Fang Yu speaks to primary and secondary school teachers at National Science Education Summer School

2024 年 8 月 20 日，2024 年“全国科学教育暑期学校”中小学教师培训（西安会场）开班，房喻院士以“从基础研究的重要性看科学教育与人才培养”为题作了首场报告。

此次培训由教育部教师工作司、中国科学院学部工作局主办，陕西师范大学、中国科学院西安分院共同承办，来自陕西、安徽、甘肃、宁夏、新疆的 52 位小学科学教师参加了培训。

On August 20, 2024, Prof. Fang Yu presented the first report on the topic of “Science Education and Talent Training from the Perspective of the Importance of Basic research” at the 2024 “National Science Education Summer School” Primary and Secondary School Teacher Training (Xi’an Camp).

Fifty-two primary school science teachers from Shaanxi, Anhui, Gansu, Ningxia and Xinjiang participated in the training, which was sponsored by the Department of Teachers’ Work of the Ministry of Education and the Work Bureau of the Faculty of Sciences of the Chinese Academy of Sciences, and co-organized by Shaanxi Normal University and Xi’an Branch of the Chinese Academy of Sciences.

房喻院士出席首届西部有机高分子材料科学与工程高质量发展高端论坛

Fang Yu attends first Forum on High-quality Development of Organic Polymer Materials in Western China

2024 年 8 月 21 日，房喻院士出席在西安举办的首届西部有机高分子材料科学与工程高质量发展高端论坛并作交流发言。

在论坛的战略研讨环节，房喻院士发言表示，西安高校和产业密集，亟需建立并进一步完善高分子新材料合作发展机制。

此次论坛由西安交通大学主办，陕西延长石油西北橡胶有限责任公司、中化西北橡胶塑料研究设计院有限公司协办，为西部地区有机高分子材料科学与工程领域的首届论坛，包括 12 位两院院士在内的 40 余位有机高分子材料科学与工程领域知名专家学者出席论坛。

On August 21, 2024, Prof. Fang Yu attended and spoke at the first High-end Forum on High-quality Development of Organic Polymer Materials Science and Engineering in Western China held in Xi'an.

At the strategic discussion session, Fang Yu said that with the numerous universities and industries in Xi'an, it is urgent to establish and further improve the cooperative development mechanism of polymer new materials.

The forum, sponsored by Xi'an Jiaotong University and co-organized by Shaanxi Yanchang Petroleum Northwest Rubber Co., Ltd., and Sinochem Northwest Rubber and Plastics Research and Design Institute Co., Ltd., was the first forum in the field of organic polymer materials science and engineering in western China. More than 40 well-known experts and scholars in the field of organic polymer materials science and engineering, including 12 academicians of the Chinese Academy of Sciences and Chinese Academy of Engineering, attended the forum.

房喻院士出席能源材料与化学战略研讨会并讲话

Fang Yu speaks at Seminar on Energy Materials and Chemical Strategy

2024 年 8 月 22 日，房喻院士出席在西安召开的“能源材料与化学战略研讨会”，并作了题为《基础科学与基础研究的重要作用》的大会邀请报告。

在报告中，房喻院士强调了基础研究在国家科技事业发展中的重要作用及创新驱动发展的必然性。他指出，我国发展进入新的阶段，创新驱动发展成为必然选择。他号召广大科技工作者要充分认识到基础科学和基础研究对国家、民族和人类社会的重要性，要从源头上解决真问题，为夯实科技自立自强根基贡献自己的力量。

此次会议主题为“聚焦新能源，携手向未来”，由陕西省化学会和西安理工大学共同主办，省内外知名高校院所的国家级人才及省内 7 所高校的化学和材料学院院长出席大会。

On August 22, 2024, Prof. Fang Yu attended the Seminar on Energy Materials and Chemical Strategy held in Xi'an, and gave an invited report titled “The Important Role of Basic Science and Basic Research”.

In the report, Fang Yu stressed the important role of basic research in the development of national science and technology and the inevitability of innovation-driven development in China. He said that China's development has entered a new stage, and innovation-driven development has become an inevitable choice. He called on scientific and technological workers to fully realize the importance of basic science and basic research to the country, the nation and human society, to solve the real problems at the source, and to contribute their own strength to consolidate the foundation of scientific and technological self-reliance.

Themed “Focus on new energy, Join hands for

the future" and co-sponsored by Shaanxi Chemical Society and Xi'an University of Technology, the seminar was attended by state-level talents from well-known universities and institutes inside and outside the province and deans of chemistry and materials schools of seven universities in the province.

研究院在 2024 年中国大学生机械工程创新创意大赛上获奖

INCSMM teams win awards at 2024 China Collegiate Mechanical Engineering Innovation and Creativity Competition

2024 年 8 月 24 日，新概念传感器与分子材料研究院两支参赛队伍在烟台黄渤海新区举行的"2024 年中国大学生机械工程创新创意大赛'明石杯'微纳传感技术与智能应用赛总决赛"上获得 1 项二等奖和 1 项三等奖。

其中，《界面聚合共价有机框架膜用于检测 ppm 级湿度》项目（团队学生：刘向泉、张驰、邢文龙、付耀；指导教师：刘小燕、马剑飞）获二等奖；《基于无缺陷纳米膜的表面增强拉曼散射衬底的可控制备》项目（团队学生：翟宾宾、闫珍、赵天宇、李宏涛、孙瑞洁，指导教师：丁立平、马剑飞）获三等奖。

本届大赛以"感联世界 智创未来"为主题，由中国机械工程学会主办，共有 109 所高校和研究所的 309 支参赛队伍进入决赛，最终评选出一等奖 24 个，二等奖 96 个，三等奖 63 个。

On August 24, 2024, two teams from the Institute of New Concept Sensors and Molecular Materials won one second prize and one third prize at the "2024 China Collegiate Mechanical Engineering Innovation and Creativity Competition 'Mingshi Cup' Micro and Nano Sensing Technology and Intelligent Application Finals" held in Yantai HuangBohai New Area.

Among them, the project "Interfacial polymerized covalent organic frame film for detection of ppm level humidity" (Team students: Liu Xiangquan, Zhang Chi, Xing Wenlong, Fu Yao; Instructors: Liu Xiaoyan, Ma Jianfei) won the second prize; The project "Controlled preparation of surface enhanced Raman scattering substrate based on defact-free nanofilms" (Team students: Zhai Binbin, Yan Zhen, Zhao Tianyu, Li Hongtao, Sun Ruijie, Instructors: Ding Liping, Ma Jianfei) won the third prize.

In the competition, which was themed "Connect the world through sensing, create the future with intelligence" and sponsored by the Chinese Society of Mechanical Engineering, 24 first prizes, 96 second prizes, and 63 third prizes were awarded to teams from 309 teams from 109 universities and institutes entering the finals.

房喻院士应邀加入 RSC Appl. Interfaces 顾问编委会

Fang Yu joins Advisory Editorial Board of RSC Appl. Interfaces

近日，房喻院士应邀加入英国皇家化学会 RSC Applied Interfaces 顾问编委会。

RSC Applied Interfaces 是一本金色开放获取新刊，专注于表面和界面应用前沿研究的跨学科期刊。

据英国皇家化学会微信公众号介绍，房喻院士致力于设计创新传感荧光分子和激发态过程调控，以开发基于薄膜的荧光传感器。此外，房喻院士的研究还包括开发具有多样化内部结构的智能分子材料，并重点研究相关系统表面、界面和叠加层的物理化学。

Recently, Prof. Fang Yu was invited to join the Advisory Editorial Board of the Royal Society of Chemistry's RSC Applied Interfaces.

RSC Applied Interfaces is a new gold open access interdisciplinary journal, focusing on cutting-edge research in surface and interface applications.

According to the RSC WeChat public account, Prof. Fang Yu is dedicated to designing innovative sensing fluorescence molecules and excited state process regulation to develop film-based fluorescence sensors. In addition, his research also includes the development of intelligent molecular materials with diverse internal structures, and focuses on the physical chemistry of the surfaces, interfaces and adlayers of related systems.

薄鑫副研究员获聘《碳中和》青年编委

Bo Xin appointed Young Editorial Board Member of Carbon Neutralization

近日，薄鑫副研究员被《碳中和》（Carbon Neutralization）期刊聘任为青年编委，聘任期为 2024 年 8 月至 2026 年 8 月。

《碳中和》为国际性跨学科开放期刊，截至目前共上线了 3 卷 13 期，收录高质量论文 100 篇。作为 ESCI 期刊 Carbon Energy 的姊妹刊，聚焦未来“碳时代”，面向材料、化学、环境、物理及经济等交叉学科，重点关注碳利用、碳减排、清洁能源相关的基础研究及实际应用。

Recently, Dr. Bo Xin was appointed as a Young Editorial Board Member of the journal Carbon Neutralization for the period from August 2024 to August 2026.

Carbon Neutralization is an international interdisciplinary open journal. Up to now, it has been published 100 high-quality papers in 3 volumes and 13 issues. As a sister journal of ESCI journal Carbon Energy, it focuses on the future “Carbon Age” and the basic research and practical applications related to carbon utilization, carbon emission reduction and clean energy for interdisciplinary subjects such as materials, chemistry, environment, physics and economics.

研究院教师获 5 项国家自然科学基金项目资助

Five INCSMM teachers funded by National Natural Science Foundation of China

近日，国家自然科学基金委公布了 2024 年度国家自然科学基金项目资助结果，新概念传感器与分子材料研究院 5 位教师获得资助。

刘静教授、薛东旭教授、刘小燕副研究员获批国家自然科学基金面上项目，分别获资助经费 50 万元；薄鑫副研究员、彭灵雅博士获批国家自然科学基金青年项目，分别获资助经费 30 万元。

负责人	项目名称	经费	项目类别
刘 静	熵驱动自组装提升手性材料的圆偏振发光不对称性、发光效率和抗热淬性能研究	50 万	面上项目
薛东旭	高连接三基元 MOF 形成机制与甲烷存储性能调控	50 万	面上项目
刘小燕	软物质纳米颗粒胞吞作用和液 – 液界面自组装行为的机制研究	50 万	面上项目
薄 鑫	非均相电解水析氢催化剂可控与放大制备中的凝胶限域效应	30 万	青年项目
彭灵雅	有机铜配合物光催化反应中非绝热过程的理论研究	30 万	青年项目

Recently, the National Natural Science Foundation of China announced the 2024 list of projects to be funded, and five teachers from the Institute of New Concept Sensors and Molecular Materials were funded.

Prof. Liu Jing, Prof. Xue Dongxu and Assoc. Researcher Liu Xiaoyan have been granted general projects with a funding of CNY 500,000 yuan each; Assoc. Researcher Bo Xin and Dr. Peng Lingya have been granted youth projects with a funding of CNY 300,000 yuan respectively.

PI	Project Name
Liu Jing	Study on circular polarization luminescence asymmetry, luminescence efficiency and thermal quenching resistance of chiral materials improved through entropy-driven self-assembly
Xue Dongxu	Formation mechanism of highly connected trielemental MOF and regulation of methane storage performance
Liu Xiaoyan	Mechanism study of endocytosis and liquid-liquid interface self-assembly behavior of soft matter nanoparticles
Bo Xin	Gel limiting effect in controllable and scale-up preparation of heterogeneous electrolytic water hydrogen evolution catalysts
Peng Lingya	Theoretical study of non-adiabatic process in photocatalytic reactions of organocupric complexes

研究院举行 2024 年半年汇报总结会

INCSMM 2024 Mid-year Report and Summary Meeting held

2024 年 8 月 30 日下午，新概念传感器与分子材料研究院在报告厅举行 2024 年半年汇报总结会，研究院科研团队教师、专职科研人员、行政人员及研究生等 30 余人参加了汇报总结会，会议由副院长丁立平教授主持。

科研团队教师 14 人和专职科研人员 5 人分别作 2024 年半年工作汇报，汇报了各自的工作进展、取得成绩和下半年工作计划。

房喻院士发表总结讲话，鼓励大家再接再厉，在即将开始的新学期努力做出更大成绩。

On August 30, 2024, the Institute of New Concept Sensors and Molecular Materials held the 2024 Mid-year Report and Summary Meeting in the lecture hall. About 30 research faculty members, full-time research assistants, administrative staff members and postgraduate students of the Institute attended the meeting, which was chaired by vice dean Prof. Ding Liping.

Fifteen research faculty members and five research assistants presented the summaries of their work, progress they made during the spring semester of 2024 and their plans for the following fall semester respectively.

In his concluding speech, Prof. Fang Yu encouraged everyone to work together to make greater achievements in the upcoming semester.

analytical chemistry

pubs.acs.org/ac Article

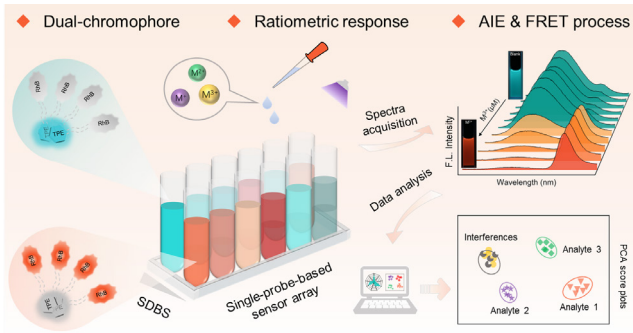
Single-Probe-Based Sensor Array for Fingerprint Recognition of Trivalent Metal Ions and Application in Water Identification

Zhen Yan, Rongrong Zhang, Min Qiao, Miao Ma, Taihong Liu,* Liping Ding,* and Yu Fang

Cite This: *Anal. Chem.* 2024, 96, 13801−13810 Read Online

基于单一探针的三价金属离子指纹识别传感器阵列及其在水区分中的应用

Zhen Yan, Rongrong Zhang, Min Qiao, Miao Ma, Taihong Liu,* Liping Ding,* and Yu Fang. Anal. Chem. 2024, 96, 13801−13810 DOI: 10.1021/acs.analchem.4c01287



重金属离子的痕量测定和毒性评价在水质监测、医疗诊断、食品安全控制等领域得到了广泛关注，其在特定条件下的最大污染水平应严格遵循世界卫生组织（WHO）指南。在多种三价金属离子（M^{3+}）中，Fe^{3+}、Al^{3+}、Cr^{3+} 等广泛参与生物生理活动或存在于我们的生活中。另一方面，异常浓度的 M3+ 可能阻碍其在生理过程中的正常活动，对健康造成严重危害。因此，跟踪环境和生物系统中的 M^{3+} 离子具有重要意义。荧光传感器因其操作简单、灵敏度高、实时检测等优点而引起持续的关注。已有大量基于特定波长荧光变化的研究报道，但选择性和区分识别能力的问题可能会限制其实际应用。单组分荧光传感器阵列和双发色团探针凭借其多发射带、比率型变化和交互响应的优势，近年来成为具有吸引力的工具，在一定程度上有利于解决上述问题。

罗丹明单元（Rhodamine, RhB）具有从无色闭环的螺内酯结构到强橙色开环结构的显著转变，其刺激响应开关特性被广泛应用到各种分析物的传感体系构建。四苯乙烯（TPE）类似物在单分子状态下无荧光或弱发射，但在聚集态下由于分子内旋转（RIR）的限制而强发射。TPE 作为天然的自组装结构单元，其光物理性质可以通过分子聚集行为进行调节。本工作开发了一种双发色团探针（RhB-TPE），通过分析 RhB 与 TPE 单元的双发色团强度比、RhB 单元的刺激开关、TPE 单元的聚集程度，以及集成两个功能单元之间的 FRET 效率，构建一个多信号传感平台（图 1）。探针自身在 ACN/H_2O 中呈球形聚集体，进而表现出显著的聚集诱导发光性能。通过与两种不同浓度的阴离子表面活性剂 SDBS 共组装，进一步构建了基于单一探针的传感器阵列。遵循表面活性剂调控策略，该阵列对水介质中的三种 M^{3+} 离子（Fe^{3+}，Al^{3+} 和 Cr^{3+}）表现出交互响应和区分识别能力。这种交互响应差异归因于 M^{3+} 对从 TPE 到开环型 RhB 的有效 FRET 过程的影响。在特异性 Al^{3+} 共存所形成的阵列进一步可用于区分不同类型的品牌水（图 2）。

第一作者：陕西师范大学博士研究生闫珍
通讯作者：陕西师范大学丁立平教授，刘太宏副教授

全文链接：https://doi.org/10.1021/acs.analchem.4c01287

Trace determination and toxicity evaluation of heavy metal ions have been extensively considered in the fields of water quality monitoring, medical

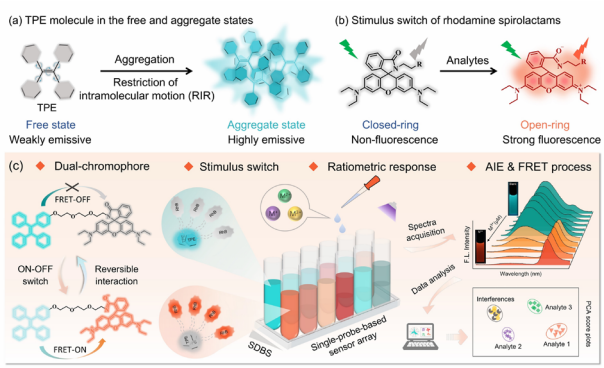


图 1.（a）TPE 单分子态呈现弱发射，由于 RIR 聚集态呈现强发射；（b）罗丹明螺内酰胺单元在分析物刺激下从无荧光闭环形态向荧光开环形态的转变；（c）基于单一探针的二元传感器阵列鉴别 M^{3+} 的示意图。

Figure 1. (a) Non-fluorescent TPE in free states but strongly emissive in aggregates due to RIR. (b) Stimulus switch of rhodamine spirolactam unit from the non-fluorescent closed-ring form to fluorescent open-ring form. (c) Representative scheme of the single-probe-based two-element sensor array for discriminating M^{3+} analytes.

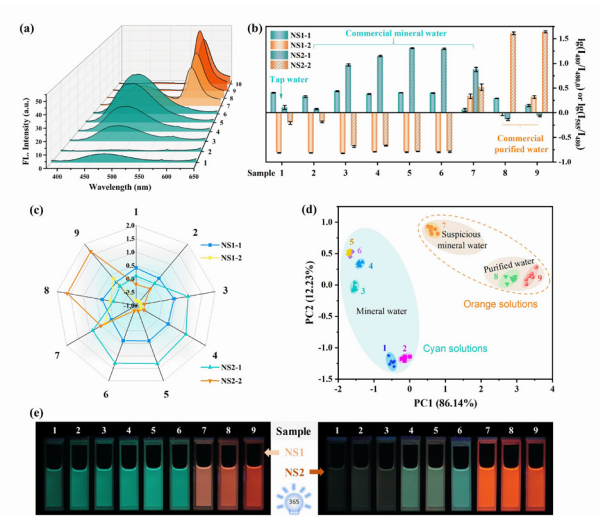


图 2.（a）传感器元件 NS2 在不同品牌水中的荧光发射光谱；传感器阵列 2 对 9 种不同的饮用水样品（1–9）通过收集在 480 和 585 nm 的荧光变化的响应图：（b）四信号指纹图谱，（c）雷达图，（d）PCA 图；NS1−1 和 NS1−2 分别是从传感器单元 NS1 获得的 $\lg(I_{480}/I_{480,0})$ 和 $\lg(I_{585}/I_{480})$；NS2−1 和 NS2−2 由传感器单元 NS2 获得；（e）传感器阵列 2 在不同水样中的可视化照片（1–9），左：NS1; 右：NS2。

Figure 2 (a) Fluorescence emission spectra of sensor element NS2 in different types of water. Fluorescence responses of Sensor Array 2 to nine different drinking water samples (1-9) by collecting fluorescence variations at 480 and 585 nm: (b) four-signal recognition patterns, (c) radar plots, and (d) PCA plots. NS1-1 and NS1-2 represent $\lg(I_{480}/I_{480,0})$ and $\lg(I_{585}/I_{480})$ acquired from sensor element NS1, respectively. NS2-1 and NS2-2 acquired from sensor element NS2. (e) Photographs of Sensor Array 2 in different water samples (1-9). Left: NS1; Right: NS2.

diagnosis, food safety control, etc. Their maximum contaminant levels under specific conditions are strictly limited following the World Health Organization (WHO) guidelines. Among various trivalent metal ions (M^{3+}), Fe^{3+}, Al^{3+}, and Cr^{3+} act either significantly in many physiological and pathological processes or exist widely in our lives. On the other hand, abnormal concentration levels of M3+ might hinder their natural biological activities in physiological processes and cause severe health hazards. Consequently, tracking the M^{3+} ions in the environment and biological systems is of great significance. fluorescent sensors have evoked continuous attention because of their merits of easy operation, high sensitivity, real-time detection, etc. Numerous studies based on fluorescence changes at a specific wavelength have been reported, but selectivity and discrimination concerns may limit their practical utilizations. With the advantages of multiple emission bands, ratiometric characteristics, and cross-reactive response, single-component fluorescence sensor arrays and dual-chromophore probes have emerged as attractive tools for favorably solving the aforementioned problems to a certain extent in recent years.

Rhodamine (RhB) units are known to possess marked transformations from the colorless closed-ring form of the spirolactam structure to the strong orange ring-opened structure, and are widely used as sensing platforms for a variety of analytes due to its stimulus-response switching properties. Tetraphenylethene (TPE) analogues are found to be nonfluorescent or weakly emissive in molecular states but emit intensely in aggregate states due to the restriction of intramolecular rotation (RIR). The photophysical properties of TPE as natural self-assembling building blocks can be easily modulated by molecular aggregation behavior. Therefore, a multiple-signal sensing platform could be built through RhB-TPE as a dual chromophore provides AIE properties accompanied by the analyte switching response of RhB emission and further integrated FRET process (Figure 1). In this contribution, a dual-chromophore probe (RhB-TPE) composed of conjugated TPE and RhB units linked via a long alkyl-oxygen chain was developed. The probe RhB-TPE intrinsically aggregated into sphere-shape in ACN/H_2O and exhibited special AIE properties. Single-probe-based sensor array was further constructed by co-assembling with the anionic surfactant SDBS at two different concentrations. Following the surfactant modulation strategy, the two-element array showed cross-reactive and discriminative responses to three M^{3+} ions (Fe^{3+}, Al^{3+}, and Cr^{3+}) in aqueous media. The cross-reactive sensing mechanism was attributed to M^{3+} influences on an efficient FRET process from TPE to open-ring form RhB. With the coexistence of specific Al^{3+}, the obtained ensemble array was further applied to discriminate different types of brand water (Figure 2).

First Author: Yan Zhen, doctoral candidate, Shaanxi Normal University
Corresponding Authors: Prof. Ding Liping, Assoc. Prof. Liu Taihong, Shaanxi Normal University
Full Text Link: https://doi.org/10.1021/acs.analchem.4c01287

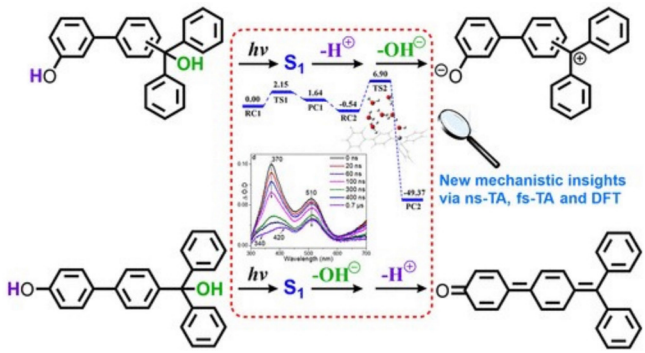
THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
pubs.acs.org/JPCL
Letter

Different Reaction Mechanisms Triggered by the Meta Effect: Photoinduced Generation of Quinone Methides from Hydroxybiphenyl Derivatives

Yan Guo, Lingfeng Ge, David Lee Phillips, Jiani Ma,* and Yu Fang

间位效应引发的不同反应机制：羟基联苯衍生物光致生成醌甲基中间体

Yan Guo, Lingfeng Ge, David Lee Phillips, Jiani Ma*, Yu Fang. J. Phys. Chem. Lett. 2024, DOI: 10.1021/acs.jpclett.4c01875



Basarić 等设计了系列具有空间位阻的醌甲基（Quinone Methide, QM）化合物前体，为两个苯基取代的苯基苯酚衍生物（图 1），其通过溶剂协助光脱水反应生成相应的 QM。取代基的位阻效应阻碍了亲核试剂对 QM 亚甲基位点的进攻，使其在亲核加成反应中具有更长的寿命和更高的选择性，从而在生物体内 DNA 烷基化的应用中表现出巨大潜力。研究表明，系列具有空间位阻的羟基联苯衍生物光致生成的 QMs 对人类癌细胞表现出抗增殖活性。在该项工作中，选取对位和间位羟基联苯衍生物作为空间位阻 QM 前体，并选取了相应的甲氧基化合物作为参照化合物（不发生光脱水反应生成 QM），利用超快光谱学和理论计算研究了它们在水溶液中的反应机理。

实验数据辅以理论计算研究，模拟了反应路径并提供了反应活性位点的分析（图 2）。间位苯基苯酚衍生物 1 和 2 首先发生酚 O–H 的 ESPT 至溶剂水分子中形成酚氧负离子，其随后发生苄基 C–O 键异裂脱去 OH 生成 QM（图 3）。而对位苯基苯酚衍生物 3 则首先发生水协助 ESPT 至苄基醇后脱水形成苄基阳离子中间体，其酚 O–H 进一步脱质子生成终产物 QM（图 4）。

这些结果将有助于化学家进一步了解光化学中的元效应和 ESPT，并帮助合成化学家设计出具有非凡反应活性的 QM 前体，扩大 QM 在生物和医疗系统中的应用。

第一作者：陕西师范大学博士研究生郭燕
通讯作者：陕西师范大学马佳妮教授
文章链接：https://pubs.acs.org/doi/10.1021/acs.jpclett.4c01875

Basarić et al. designed a series of phenylphenol derivatives substituted with the sterically congested adamantyl moiety or two phenyl groups as QM precursors, which undergo solvent-assisted photodehydration reactions to produce their corresponding QMs. The bulkiness of the substituents sterically hindered the attack of nucleophiles to the methylene position of the QMs, making them longer-lived and more selective in reactions with nucleophiles, which renders such QMs potentially useful for applications in biological systems for the alkylation of DNA. A series of sterically congested QMs exhibit photoinduced antiproliferative activity against some human cancer cell lines. To elucidate the structure-reactivity relationship and details of mechanisms of the photogeneration of sterically congested QMs, we chose phenylphenols derivatives 1-3 as

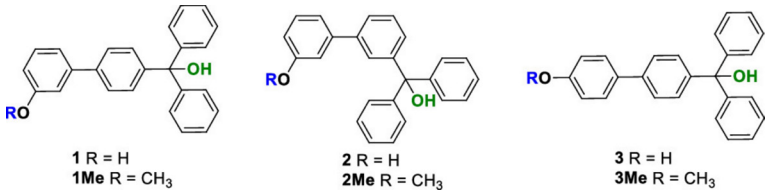


图 1. 空间位阻的 QM 前体 1–3 及参照化合物 1Me–3Me 的化学结构

Figure 1. Investigated Sterically Congested QM Precursors 1-3 and Their Corresponding Methyl Ethers 1Me-3Me Which Cannot Produce QMs.

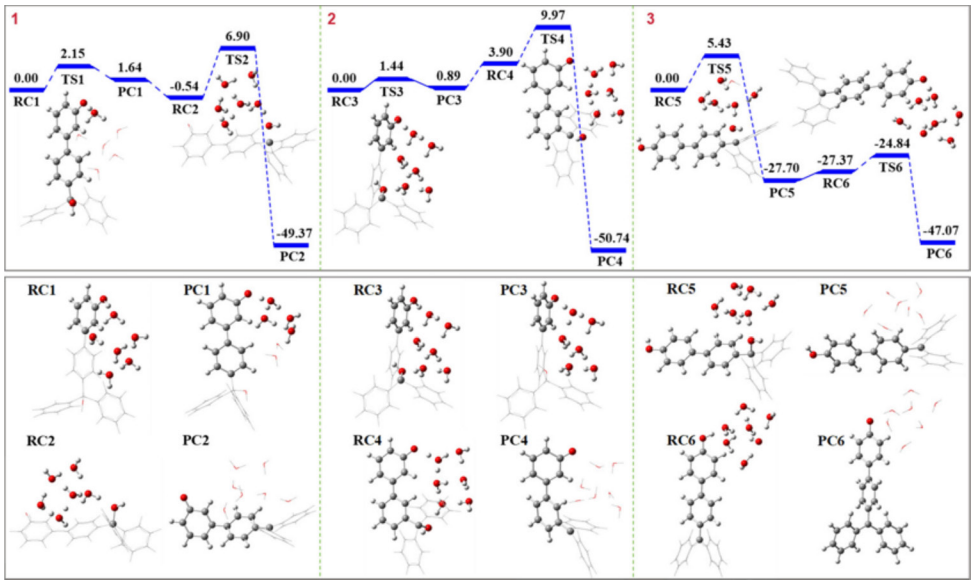


图 2. 采用 TD–B3LYP(D3BJ)/6–311G**/SMD(H_2O) 模拟的苯基苯酚衍生物 1–3 的势能曲线图（能量单位为 kcal mol^{-1}）

Figure 2. PES profiles of phenylphenol derivatives 1-3 with six H2O, mapped employing (TD) B3LYP(D3BJ)/6-311G**/SMD (H_2O) calculations (the energy unit is kcal mol^{-1}).

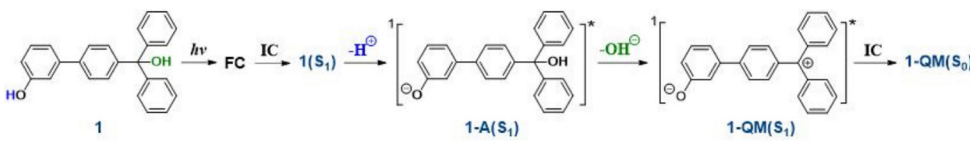


图 3. 间位苯基苯酚衍生物 1 在 $CH_3CN–H_2O$ 中的光致生成 QM 反应机理

Figure 3. Proposed Photoinduced QM Generation Mechanism of 1 in CH_3CN-H_2O

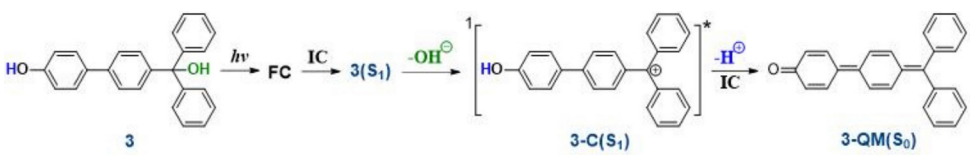


图 4. 对位苯基苯酚衍生物 3 在乙腈 – 水溶液中光致生成 QM 反应机理

Figure 4. Proposed Photoinduced QM Mechanism for Generation of 3 in CH_3CN-H_2O.

QM precursors and investigated their photodehydration processes in aqueous solutions using ultrafast spectroscopy and theoretical computations.

We found that meta-derivatives 1 and 2 undergo water-mediated excited-state proton transfer (ESPT) from the phenol OH, followed by the expulsion of the OH− to form QMs. By comparison, para-derivative 3 proceeds via water-mediated ESPT from H2O to benzyl alcohol coupled with dehydration as the first step, delivering a cation intermediate, which further deprotonates to yield QM.

Such results would help chemists understand more about the meta effects in photochemistry and about ESPT and would help synthetic chemists design sterically congested QM precursors with extraordinary reactivities and expand applications of QMs in biological and medical systems.

First Author: Guo Yan, doctoral candidate, Shaanxi Normal University
Correspondence Author: Prof. Ma Jiani, Shaanxi Normal University
Full Text Link: https://pubs.acs.org/doi/10.1021/acs.jpclett.4c01875

ACS SENSORS

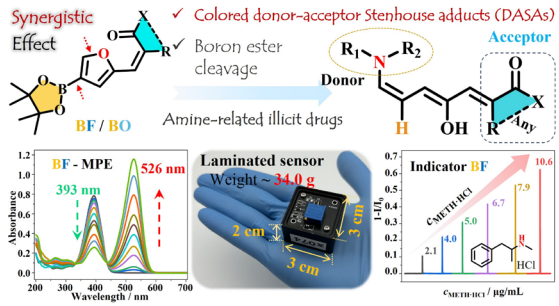
pubs.acs.org/acssensors Article

Integrated Sensing Platform Validated for the Efficient and On-Site Screening of Amine-Containing Illicit Drugs

Jiashuang Yao,§ Chun Yang,§ Ruijuan Wen, Taihong Liu,* Liping Ding,* Zhen Yao, and Yu Fang

高效原位筛查含胺类新精神活性物质的集成式传感平台

Jiashuang Yao#, Chun Yang#, Ruijuan Wen, Taihong Liu*, Liping Ding*, Zhen Yao, Yu Fang. ACS Sens. 2024, DOI: 10.1021/acssensors.4c00787



制毒、贩毒和吸毒等涉毒问题严重危害社会安定、公共安全和公共卫生，引起了社会各界日益广泛关注。建立灵敏、快速并可靠的检测方法，研制能够实施移动检测、快速筛查的技术和装备，对毒品案件侦查和打击毒品犯罪具有非常重要的现实意义。目前世界范围内能够用于隐藏毒品检测的主要技术手段为化学显色、胶体金法、气－质联用（GC/MS）、离子迁移谱（IMS）、表面增强拉曼（SERS）以及专业嗅毒犬等。各种技术手段各有优缺点，与其他方法相比，光谱技术具有灵敏度高、响应速度快和可采集参数丰富等优点，在传感检测方面显示出了极大的优越性。因此，开发高效、快速、现场检测痕量新精神活性物质的分析策略非常必要。

本工作基于对多种呋喃类指示剂的合成和优化，优选了两种硼酯功能化的呋喃指示剂 BF 和 BO，并对其进行了系统结构和光学性质表征。具有受体单元的指示剂（梅氏酸和 CF3– 异恶唑酮）与作为供体单元的含胺类新精神活性物质反应，分别产生第二代和第三代的斯坦豪斯加合物（DASAs）。具体来说，硼酯呋喃衍生化合物中的呋喃环能够与毒品中的胺基基团发生亲核反应，生成具有特征颜色、三烯基团的线性结构衍生物，溶液颜色由无色或者浅黄色变为红棕色，紫外吸收光谱变化明显。因此，在含胺类新精神活性物质存在时，两种呋喃指示剂 BF 和 BO 均表现出明显的可以用肉眼识别的颜色变化（从浅黄色或无色变为红色）；而后给予实验室研究基础，成功实现了叠层式光学液相传感器制备和原型传感平台搭建，并用于部分含胺类新精神活性物质的检测和筛选。

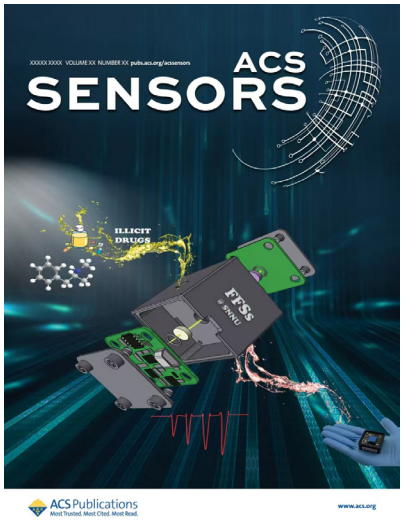
共同第一作者：陕西师范大学硕士研究生姚佳爽、国家毒品实验室陕分中心杨春工程师
通讯作者：陕西师范大学刘太宏副教授、陕西师范大学丁立平教授

全文链接：https://doi.org/10.1021/acssensors.4c00787

Illicit drugs have seriously endangered public health and social safety because of their wide variety, constant structural renewal, vague legal definitions, and rapid adaptation to legal restrictions. Nowadays, a variety of synthetic cannabinoids and new psychoactive substances (NPSs) have drastically appeared on the global market. The World Drug Report 2023 launched by the United Nations Office on Drugs and Crime noted NPSs in the global market increased in 2021 after several years of stabilization and a cumulative number of 1184 substances in 2022. Presently, extensive efforts have been made to efficiently detect illicit drugs. These illicit drugs are detected via popular techniques such as high−performance liquid chromatography, gas chromatography coupled with mass spectrometry (GC−MS), surface−enhanced Raman spectroscopy, fluorescence, and electrochemi−luminescence. However, detection methods for certain aspects of illicit drugs, especially the rapid structural

图 1.（a）叠层式光学传感器硬件结构示意图；（b）叠层式光学传感器实物图；原型传感平台的示意图（c）及真实传感测试图（d）。

Figure 1. Exploded view of the important apparatus (a), small-size and light-weight (b) of the laminated sensor. Schematic representation (c) and picture (d) of the prototype sensing platform.



本研究被选为 ACS Sensors 封面文章。

This study is to be featured on the cover of the journal ACS Sensors.

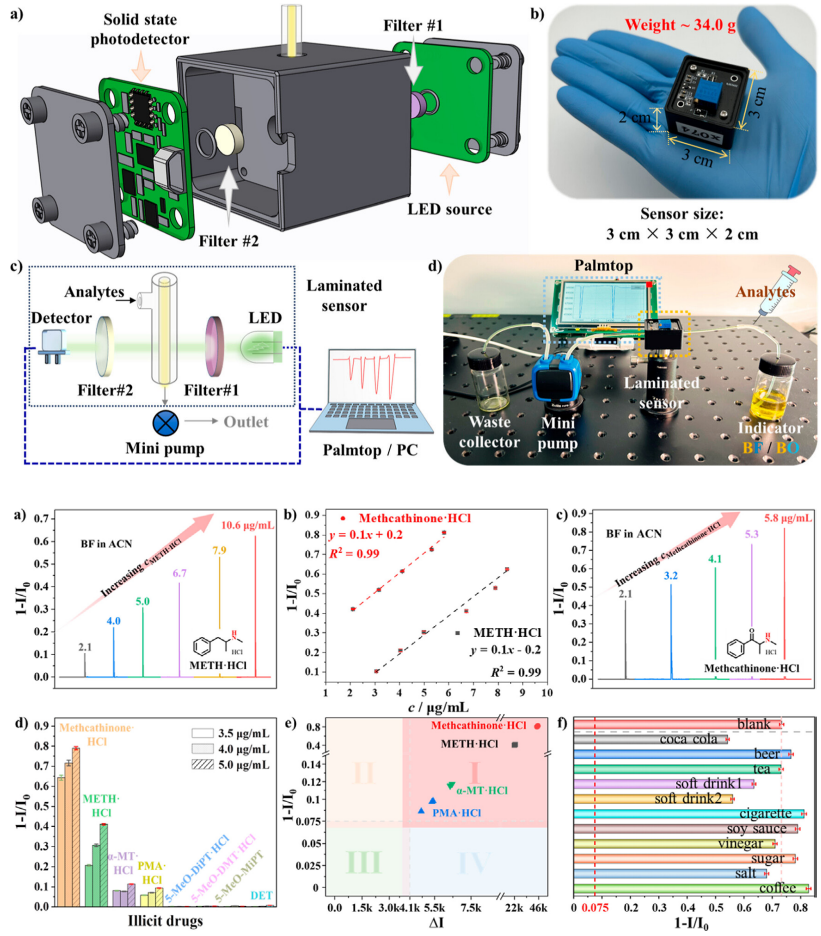


图 2. 基于指示剂 BF 的传感器对不同浓度甲基苯丙胺盐酸盐（a）和甲卡西酮盐酸盐（c）的检测；（b）对不同浓度甲基苯丙胺盐酸盐和甲卡西酮盐酸盐的响应强度图；（d）8 个不同浓度真实样品的传感测试结果；（e）基于综合传感平台的高效筛查新精神活性物质的象限图；(f)常见干扰对综合传感平台检测甲卡西酮盐酸盐(4.0 μg·mL^{-1})的干扰性测试。

Figure 2. Detection test of the BF-based sensor to the analytes METH•HCl (a) and methcathinone•HCl (c) at different concentrations. (b) Plot of response intensity against the different concentrations of METH•HCl and methcathinone•HCl. (d) Test results of the eight real samples with different concentrations. (e) Efficient screening results based on the integrated sensing platform. (f) Influence of the common interferences to the detection of methcathinone•HCl (4.0 μg•mL-1) using the integrated sensing platform.

modifications of NPSs, are still scarce. In situ and on−site detection evoked challenges for traditional techniques owing to various drawbacks such as time −consuming, slow response, complicated operations, and bulky and sophisticated equipment. Presumptive tests are critical for prompt qualitative identification of a suspected substance in real−life scenarios, enabling immediate action at the scene. Thus, the first step for the rapid screening of suspected substances in field tests involves the use of drug testing kits or portable devices. Therefore, developing efficient, fast, and on−site analytical strategies for detecting trace illicit drugs is highly desirable.

In this study, based on the comprehensive synthetic optimization, two furanic indicators (BF and BO) modified with boron ester groups were synthesized and characterized properly. The indicators with the acceptor units (Meldrum's acid and CF3-isoxazolone) reacted with the amine-containing illicit drug donors, generating the second- and third-generation DASAs, respectively. Both indicators exhibited distinct color changes from light yellow or colorless to red in the presence of amine-containing illicit drugs, which could be identified with the naked eye. A laminated sensor and prototype sensing platform were successfully realized to detect and screen real illicit drug samples.

This study is to be featured on the cover of the journal ACS Sensors.

First Authors: Yao Jiashuang, master's candidate, Shaanxi Normal University; Yang Chun, National Anti-Drug Laboratory Shaanxi Regional Center
Correspondence Authors: Assoc. Prof. Liu Taihong, Prof. Ding Liping, Shaanxi Normal University
Full Text Link: https://doi.org/10.1021/acssensors.4c00787

LANGMUIR

pubs.acs.org/Langmuir Article

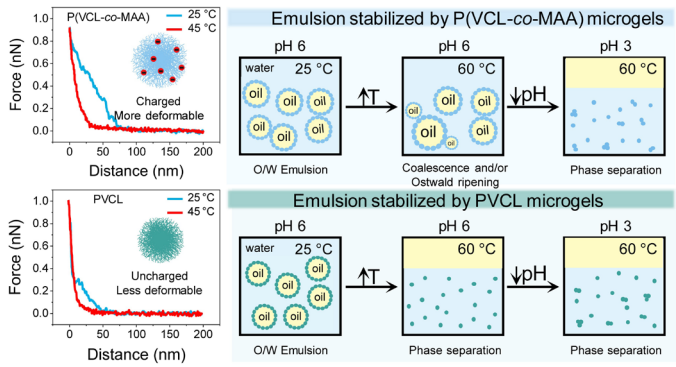
Emulsion Stabilized by Biocompatible and Stimuli-Responsive Poly(*N*-vinylcaprolactam)-Based Microgels: Effects of Electrostatic Repulsion and Deformability on Emulsion Stability

Shuwen Tan, Xiaojia Xu, Ting Zhang, Min Li, Xiaoyan Liu,* Per M. Claesson, and Yu Fang

Cite This: *Langmuir* 2024, 40, 16946−16958 Read Online

聚 (N– 乙烯基己内酰胺) 微凝胶乳液稳定性受静电斥力和微凝胶变形性的影响

Shuwen Tan, Xiaojia Xu, Ting Zhang, Min Li, Xiaoyan Liu*, Per M. Claesson, and Yu Fang. Langmuir 2024, DOI: 10.1021/acs.langmuir.4c01743



微凝胶纳米颗粒具有可变形性和刺激响应性被广泛用于制备乳液。然而，静电相互作用和纳米颗粒的变形性对乳液稳定性的影响仍具有争议需要更深入的研究。

本研究利用电中性的聚 (N– 乙烯基己内酰胺)(PVCL) 和带负电的聚 (N– 乙烯基己内酰胺) 甲基丙烯酸 (P(VCL–co–MAA)) 微凝胶纳米颗粒分别作为稳定剂制备了具有超高稳定性且具有温度和 pH 响应的乳液。DLS 和 AFM 研究表明 P(VCL–co–MAA) 微凝胶在水中的溶胀程度高于 PVCL 微凝胶。并利用原子力显微镜对两种微凝胶颗粒的纳米力学性能进行了系统表征，发现 P(VCL–co–MAA) 微凝胶具有更高的变形能力和粘附力，以及更低的弹性模量。乳液稳定性的研究发现在微凝胶的体积相变温度以下，两种微凝胶制备的乳液都具有很好的稳定性。值得注意的是，所制备的乳液在相变温度以上仍然具有较好的稳定性，这将拓宽温度响应型乳液的应用场景。将温度升高到 60 °C，PVCL 微凝胶乳液会发生相分离，P(VCL–co–MAA) 微凝胶乳液在 pH 低高于 MAA 的 pKa 时保持稳定，表明静电斥力有利于稳定乳液。另外，P(VCL–co–MAA) 微凝胶颗粒较高的变形性也对稳定乳液具有重要的贡献。我们的研究表明微凝胶的静电斥力和较高的变形性对稳定乳液发挥着重要的作用，对软物质纳米颗粒稳定乳液机理的深入理解将为设计和制备具有超高稳定性的乳液提供新思路。

第一作者：陕西师范大学博士研究生谭淑文
通讯作者：陕西师范大学刘小燕副研究员
全文链接：https://doi.org/10.1021/acs.langmuir.4c01743

Microgels have been widely used for stabilizing emulsions due to their softness and stimulus responsiveness. Although ultrastable emulsions have been prepared by microgel nanoparticles, the role of electrostatic interactions on emulsion stability is still a controversial topic and further investigation of the effect of microgel deformability is required.

In the present study, neutral poly(N-vinylcaprolactam) (PVCL) and charged

poly(N-vinylcaprolactam)-co-methacrylic acid (P(VCL-co-MAA)) microgels were synthesized and further used as emulsifiers to stabilizing emulsion. The P(VCL-co-MAA) microgel has a swelling ratio larger than that of the PVCL microgel in water. The nano-mechanical properties of the microgels in water were characterized by atomic force microscopy with using the tip of different radii. The result reveals that the P(VCL-co-MAA) microgel is more deformable than the PVCL counterpart. Stability tests of the emulsions showed that below the volume phase transition temperature (VPTT) of the microgels, both microgel types can stabilize the emulsions under various conditions. Unexpectedly, most of the emulsions still remain stable above the VPTT. Further increasing the temperature to 60 °C, P(VCL-co-MAA) microgel emulsions remained stable at a pH value above the pKa of MAA while the emulsion was unstable below the pKa. However, phase separation occurs in PVCL microgel-stabilized emulsions at 60 °C. These results demonstrate that electrostatic repulsion and deformability of the microgels can enhance the emulsion stability, providing insights into the rational design and preparation of ultrastable Pickering emulsions.

First Author: Tan Shuwen, Doctoral candidate, Shaanxi Normal University
Correspondence Author: Assoc. Prof. Liu Xiaoyan, Shaanxi Normal University
Full Text Link: https://doi.org/10.1021/acs.langmuir.4c01743

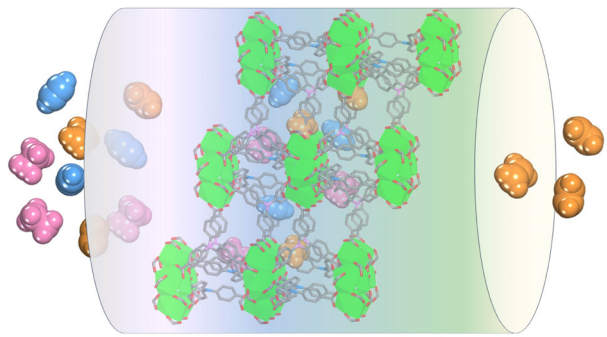
Inorganic Chemistry
pubs.acs.org/IC Article

A Propeller-Like Ligand-Directed Construction of a Tetranuclear Cerium-Organic Framework for Single-Step Ethylene Purification from Ternary C_2 Mixtures

Ning Yang,[▽] Hong-Xin Li,[▽] Logan Ritter, Guo-Tong Du, Xin-Ai Guo, Brian Space, and Dong-Xu Xue*

螺旋桨型配体诱导构筑的四核铈基有机骨架材料及其从三组分 C_2 气体中一步纯化乙烷性能

Ning Yang#, Hong-Xin Li#, Logan Ritter, Guo-Tong Du, Xin-Ai Guo, Brian Space, Dong-Xu Xue*. Inorg. Chem. 2024, DOI: 10.1021/acs.inorgchem.4c02473



乙烯（C_2H_4），作为石化产品的基石，在高价值有机化学品的合成中起到重要作用。乙烯产品中含有的乙烷和乙炔杂质使其纯度达不到工业使用要求，传统的获取高纯度乙烯的方法能耗高、成本大，阻碍了其实际应用。因此，寻找低成本高效率的乙烯分离技术具有重要意义。

金属有机骨架（MOF）作为一类新兴晶态多孔材料，由于其孔径可调控、功能基团丰富和结构多样化等特征而被人们广泛关注。基于 MOF 材料的吸附分离技术，具有提高能源效率和降低操作成本的潜力，是一种非常有前景的气体分离技术。尽管 MOF 材料已被用于二元混合物的分离研究，如 C_2H_2/C_2H_4 或 C_2H_6/C_2H_4 的分离，但是从三元混合物中同时除去 C_2H_2 和

C_2H_6 的分离仍是一项更加复杂和具有挑战性的任务。这主要是由于 C_2H_4 的四极矩和极化率均介于 C_2H_2 和 C_2H_6 之间，从而导致 C_2H_2 和 C_2H_6 很难一步同时脱除。虽然已有一些关于 MOF 材料从三组分气体中一步纯化乙烯的文献被相继报道，但是这类材料的设计合成仍然是一项紧迫而艰巨的挑战。

在本课题组近期工作中，聚焦利用配体构象异构体策略构筑新颖 MOF 材料，例如，通过在三羧酸配体中引入酰胺或者亚胺键，分别获得了三维朝向的链基和多级孔锆基 MOF 材料。铈是一种无毒、经济且含量丰富的稀土金属，与其他稀土金属相比，其在新型 MOF 构筑方面却研究较少。已报道的铈基 MOF 结构主要以无机链构筑单元形式存在，而基于铈簇的材料则报道较少。这为扩大铈基 MOFs 的范围及其应用研究提供了机会。

基于以上考虑，我们引入螺旋桨型三酸配体（H_3NTB）作为有机连接体，用铈作为金属源，成功构筑一例新型铈基 MOF 材料，即 Ce–NTB–rtk。在该结构中，原位生成一种从未报道过的四核铈簇 [$Ce_4F_2(O_2C–)_{12}$]，其与 NTB 配体的连接模式为 μ5–η2:η1:η1:η2:η1。拓扑分析表明该结构是一种新的 3,3,12–c 的网络。结构中存在两种晶体学独立的 NTB，因此可将其拆分为一个二维 3,6–c 的 kgd 网络和一个三维 3,6–c 的 rtl 网络，最终结构是 3,3,12–c 的 rtk 网络。低压气体吸附等温线、IAST 选择性和吸附焓数据结果均表明 Ce–NTB–rtk 具有从三组分 C_2 气体中一步纯化乙烯的潜力，进一步通过穿透测试及 GCMC 理论计算得以验证。Ce–NTB–rtk 良好的分离效果主要归因于该材料微孔孔径和非极性的孔环境。该项研究工作进一步说明了配体构象异构体策略在新金属簇和多孔材料构筑方面的作用，为基于该类 MOF 材料的前沿应用打下基础。

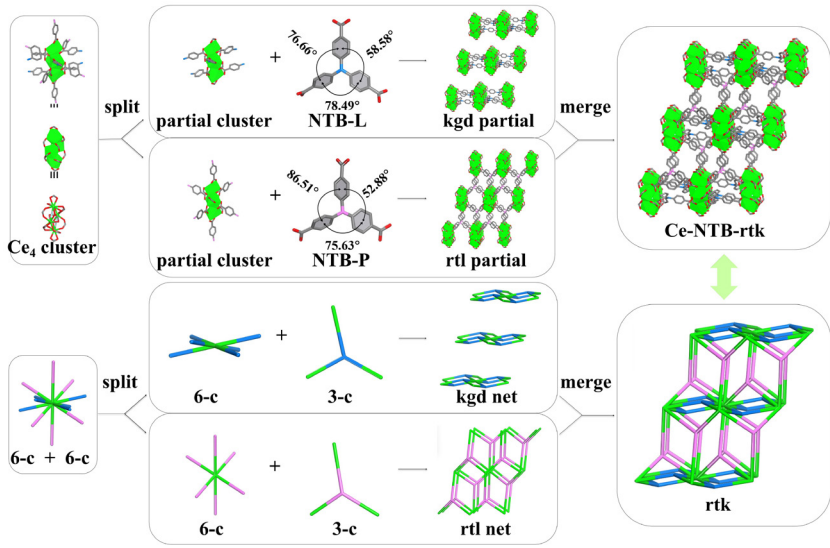


图 1. Ce–NTB–rtk 的组装示意图。顶部：kgd 和 rtl 框架被拆分出来并组合形成 Ce–NTB–rtk；底部：kgd 和 rtl 网络合并形成 rtk 网络。Ce = 绿色，C = 灰色，N = 蓝色 / 粉色，O = 红色，F = 蓝绿色。为了清晰，氢原子和末端配位的甲醇分子被删除。

Figure 1. Schematic representation showing the assembly of Ce-NTB-rtk. Top: the frameworks of kgd and rtl are split and then merged to form Ce-NTB-rtk; bottom: kgd and rtl nets are merged to form rtk network. Ce = green, C = gray, N = blue/pink, O = red and F = cyan. Hydrogen atoms and the terminally coordinated methanol molecules are omitted for clarity.

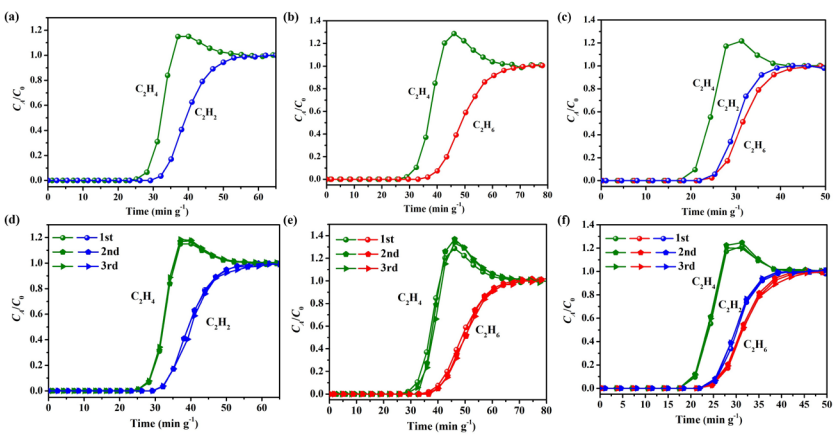


图 2. 在 298 K 和 1.0 bar 条件下，(a) 流速 2 mL min^{-1} 下的 C_2H_2/C_2H_4/He (25/25/50) 穿透实验曲线，(b) 流速 2 mL min^{-1} 下的 C_2H_6/C_2H_4/He (25/25/50) 穿透实验曲线，(c) 流速 2 mL min^{-1} 下的 $C_2H_2/C_2H_4/C_2H_6$/He (16.5/16.5/16.5/50) 穿透实验曲线，(d), (e) 和 (f) 分别表示上述三种穿透曲线的重复实验。

Figure 2. Experimental column breakthrough curves for (a) C_2H_2/C_2H_4/He (25/25/50) mixture under a flow of 2 mL min^{-1}, (b) C_2H_6/C_2H_4/He (25/25/50) mixtures under a flow of 2 mL min^{-1} and (c) $C_2H_2/C_2H_4/C_2H_6$/He (16.5/16.5/16.5/50) mixture under a flow of 1.2 mL min^{-1} in an absorber bed packed with Ce-NTB-rtk at 298 K and 1.0 bar. (d), (e) and (f) are their regenerative tests, respectively.

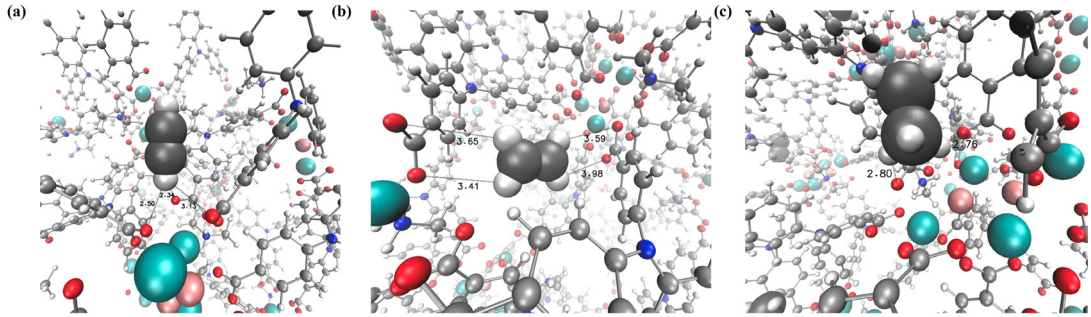


图 3. 基于 GCMC 理论计算模拟获得的 (a) C2H2，(b) C2H4，和 (c) C2H6 分子在 Ce−NTB−rtk 中的优先结合位点。
Figure 3. Preferential (a) C2H2, (b) C2H4, and (c) C2H6 molecule binding sites within Ce-NTB-rtk simulated with GCMC.

第一作者：陕西师范大学硕士研究生杨宁、博士研究生李洪昕
通讯作者：陕西师范大学薛东旭教授
全文链接：https://pubs.acs.org/doi/10.1021/acs.inorgchem.4c02473

Ethylene (C_2H_4), a cornerstone in the pantheon of petrochemical products, is instrumental in the synthesis of a plethora of valuable organic compounds and polymers. The impurities of ethane and acetylene in ethylene products can´t meet the requirements of industrial use. The traditional method of obtaining high purity ethylene has high energy consumption and high cost, which hinders its practical application. Therefore, it is of great significance to find a low cost and high efficiency ethylene separation technology.

Metal-organic frameworks (MOFs), a new class of crystalline porous materials renowned for their tunable pore sizes, diverse chemical functionalities, and high surface areas. Adsorptive purification technology based MOFs, with its potential for energy efficiency and operational cost reduction, has been hailed as a promising avenue for the future of gas separation. While MOFs have been explored for the separation of binary mixtures such as C_2H_2/C_2H_4 or C_2H_6/C_2H_4, respectively, the simultaneous removal of C_2H_2 and C_2H_6 from a ternary mixture is a more complex and challenging task. This is largely due to the intermediate quadrupole moment and polarizability of C_2H_4, which fall between those of C_2H_2 and C_2H_6, making it difficult to simultaneously remove C_2H_2 and C_2H_6 in a single step. Although a few MOF materials have been reported to enable single-step purification of ethylene from a ternary C_2 mixture, the design and synthesis of such materials remains a pressing need and a formidable challenge.

In our recent work, we have focused on the development of innovative MOFs through a ligand-conformer strategy. By utilizing amide or imine inserted tritopic carboxylate ligands, novel three-way rod and multi-cage zirconium-based MOFs have been successfully constructed. Additionally, cerium, a non-toxic, cost-effective, and abundant metal element, has been less explored in the construction of new MOFs compared to other rare-earth metals. Most cerium-based MOFs reported in the literature are structured from rod inorganic building units, while cluster-based cerium MOFs are relatively scarce. This presents an opportunity to expand the scope of cerium-based materials and to investigate their potential in various applications.

Building on above considerations, we have introduced a propeller-like ligand as the connecting node and utilized cerium as the metal source to construct a new cerium-based MOF material, i.e., Ce-NTB-rtk. In this structure, in situ generate a rare tetranuclear cerium cluster of $[Ce_4F_2(O_2C\text{-})_{12}]$, such cluster is observed for cerium ion for the first time, which is further connected via NTB linkers in a mode of μ5-η2:η1:η1:η2:η1. Topological analysis reveal that it is a new (3,3,12)-c net. Considering the occurrence of two crystallographically independent NTB linkers (i.e., ligand conformer) within Ce-NTB-rtk, such (3,3,12)-c framework can be split into a 2D (3,6)-c kgd net and a 3D (3,6)-c rtl one, consequently resulting in a merged (3,3,12)-c rtk network. The results of low-pressure gas adsorption isotherms, IAST selectivity and adsorption enthalpy data indicate that Ce-NTB-rtk has the potential to purify ethylene from ternary C_2 gas in one step, which is further verified by breakthrough test and GCMC theoretical calculation. The good separation performance of Ce-NTB-rtk is mainly due to its suitable microporous cavity and nonpolar microenvironment. This discovery further illuminates the efficacy of the ligand-conformer approach in the synthesis of novel metal clusters and the subsequent creation of porous frameworks, paving the way for their application in cutting-edge technologies.

First Authors: Ying Ning, master's candidate, Li Hongxin, doctoral candidate, Shaanxi Normal University
Correspondence Author: Prof. Xue Dongxu, Shaanxi Normal University
Full Text Link: https://pubs.acs.org/doi/10.1021/acs.inorgchem.4c02473

The Journal of Organic Chemistry > Vol 89/Issue 16 > Article

Subscribed

Cite Share Jump to

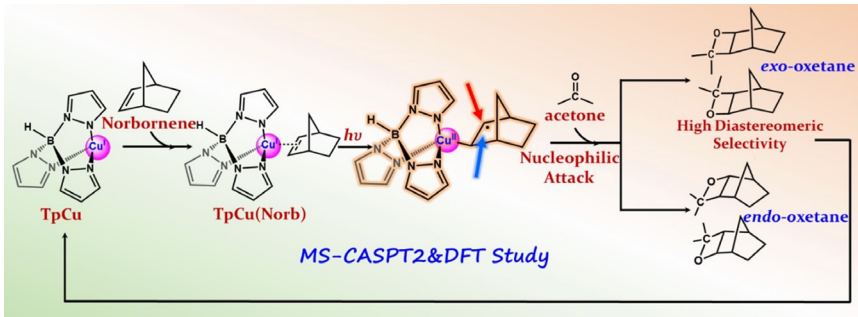
ARTICLE | August 2, 2024

Roles of Nonadiabatic Processes, Reaction Mechanism, and Selectivity in Cu-Catalyzed [2 + 2] Photocycloaddition of Norbornene and Acetone to Oxetane

Ling-Ya Peng, Rui Jin, Shi-Ru Zhang, Xiang-Yang Liu*, Wei-Hai Fang, and Ganglong Cui*

铜配合物光催化 [2+2] 环加成反应的非绝热过程、反应机理和选择性研究

Ling-Ya Peng#, Rui Jin#, Shi-Rui Zhang, Xiang-Yang Liu*, Wei-Hai Fang, Ganglong Cui*. J. Org. Chem. 2024, 89, 11334-11346. DOI: 10.1021/acs.joc.4c00990



氧杂环丁烷因其在药物化学中的重要应用而受到广泛研究。近期，实验课题组报道了一篇 Cu 催化的 [2+2] 光环加成反应生成氧杂环丁烷的工作，并且实验上推测其机理与传统的 Patern ò –B ü chi 反应机理不同。然而，其在原子水平上的机制尚不清楚。

为深入理解产物选择性来源，我们采用多态完全活性空间二阶微扰理论（MS–CASPT2）和密度泛函理论（DFT）相结合的方法，系统地研究了反应机理，阐明了影响非对映异构选择性的因素。反应初期，三（吡唑基）硼酸铜（TpCu）和降冰片烯在基态下发生强相互作用，生成 TpCu(Norb) 配合物。在光激发下，TpCu(Norb) 最终布居到 T_1 态，随后 TpCu(Norb) 进攻丙酮引发后续反应，生成最终的 exo– 或 endo– 氧杂环丁烷产物。

计算发现，反应初期在 T_1 态发生 C–C 成键，生成开环中间体。随后经过无辐射跃迁回到 S_0 态，生成五元环中间体，并在基态发生进一步的 C–O 成键，最终生成 exo– 产物。相反，endo– 氧杂环丁烷由于空间位阻较大，在 C–C 键生成后需要发生重排反应。因此，生成 exo– 产物和 endo– 产物的反应路径在自由能势垒上表现出很大的差异，从而导致了实验观察到的非对映异构选择性。此外，我们发现无辐射跃迁在反应路径中起着至关重要的作用。我们的计算研究为 Cu 催化的光环加成反应的理解提供了有价值的理论洞察。

第一作者：陕西师范大学彭灵雅博士，北京师范大学硕士毕业生金蕊

通讯作者：北京师范大学崔刚龙教授，四川师范大学刘向洋副教授

全文链接：https://pubs.acs.org/doi/10.1021/acs.joc.4c00990

Oxetane has been extensively studied for its applications in medicinal chemistry and as a reactive intermediate in synthesis. Experiments report a Cu-catalyzed [2+2] photocycloaddition of acetone and norbornene to oxetane, which is proposed to deviate from the conventional Paternò-Büchi reaction. However, its mechanism at the atomic level is not clear.

In this study, we used a combination of multi-state complete active space second-order perturbation theory (MS-CASPT2) and density functional theory (DFT) to systematically investigate the reaction mechanism and elucidate the factors contributing to the diastereomeric selectivity. Initially, the formation of the TpCu(Norb) complex is achieved by strong interaction between tris(pyrazolyl) borate Cu(I) (TpCu) and norbornene in the ground state (S_0). Upon photoexcitation, TpCu(Norb) eventually decays to the T_1 state, in which TpCu(Norb) attacks acetone to initiate subsequent reactions and produces final endo- or exo-oxetane products.

All these reactions initially involve the C-C bond formation in the T_1 state thereto leading to a ring-opening intermediate. This intermediate then undergoes a nonradiative transition to the S_0 state, producing a five-membered ring intermediate, from which the C-O bond is formed, leading to the experimentally dominant exo-product. In contrast, the endo-oxetane formation requires a rearrangement process after the C-C bond is formed because of the large steric effects. As a consequence, the different reaction pathways generating exo- and endo-products exhibit large differences in the free-energy barriers, which results in a diastereomeric selectivity observed experimentally. Additionally, the nonradiative transition is found to play an important role in facilitating these reaction steps. The present computational study provides valuable mechanistic insights into Cu-catalyzed photocycloaddition reactions.

First Authors: Dr. Peng Lingya, Shaanxi Normal University; Jin Rui, master's graduate, Beijing Normal University
Correspondence Authors: Prof. Cui Ganglong, Beijing Normal University; Assoc. Prof. Liu Xiangyang, Shaanxi Normal University
Full Text Link: https://pubs.acs.org/doi/10.1021/acs.joc.4c0990

ELSEVIER
Available online at www.sciencedirect.com
ScienceDirect
Current Opinion in Colloid & Interface Science

Advances of surfactant aggregates in constructing cross-reactive fluorescent sensors and arrays for discriminative application

Zhen Yan, Min Qiao, Liping Ding and Yu Fang

表面活性剂聚集体在构建交互响应性荧光传感器和阵列以及区分识别应用中的进展

Zhen Yan, Min Qiao, Liping Ding* and Yu Fang. Curr. Opin. Colloid Interface Sci. 2024, 73:101831

表面活性剂是一类两亲性分子化合物，其分子结构包含亲水头基和疏水尾链（图 1a）。这使得表面活性剂分子在水溶液中具有独特的组装行为，可自组装形成各种聚集体，如胶束、囊泡、脂质体等。这些聚集体具有疏水内核和与亲水外表面，且处于动态组装平衡，易受离子强度、pH 值、化学物质等外界刺激的影响。表面活性剂聚集体的异质微结构使其能够在水溶液中增溶有机染料，在构建荧光化学 / 生物传感器得到广泛应用。荧光传感器可分为选择性和交互响应式（图 1b）。前者通常含有特异性受体结构，可在多种检测样本中选择性结合并识别目标分析物。后者则通常是由一些非特异性传感单元的组合，传感单元对所有分析物的响应程度不同而具有交互响应性。所有传感器单元输出信号的组合可产生针对特定分析物的特定识别指纹图谱，通过主成分分析、线性判别分析等多变量数据分析方法可实现对多种分析物的区分识别。因此，交互响应荧光传感器不仅可以鉴别相似分析物，而且可以分析生物流体或混合物等复杂样品，这使其在实际应用中更具吸引力。

表面活性剂聚集体已被广泛应用于构建荧光传感器，它们可以提供疏水核心来封装荧光团或与荧光团共组装，使用表面活性剂聚集体具有多种优势（图 1c），例如增加有机荧光团的水溶性，增强被包封荧光团的荧光稳定性和量子产率等。此外，将两亲性表面活性剂聚集体与荧光团结合，不仅可以保持荧光性质，而且由于其动态组装特性，可以提供对外界刺激的敏感性。可灵活选择和组装不同的表面活性剂聚集体和荧光团，使集成传感器系统表现出不同的结构 / 光物理性能，具有多重相互作用、聚集行为可变、组装条件温和多刺激响应性等优点。

文中系统介绍了表面活性剂聚集体在构建交互响应性荧光传感器和阵列方面的研究进展，重点介绍了基于非荧光表面活性剂聚集体和类表面活性剂荧光两亲体的不同构建策略（图

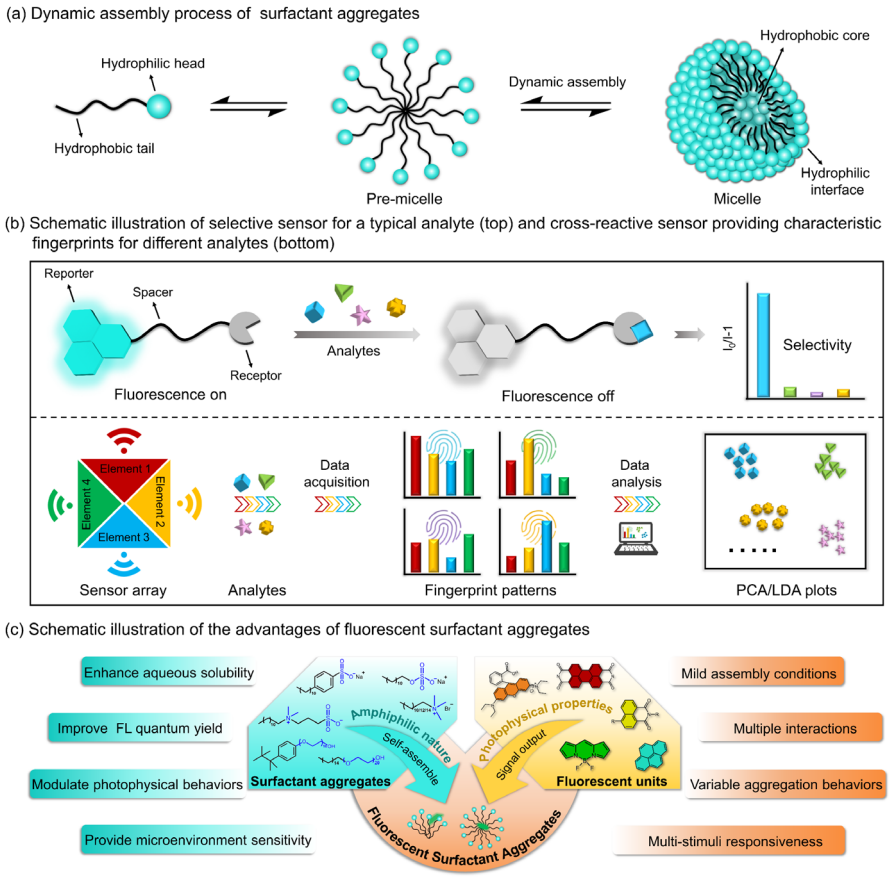


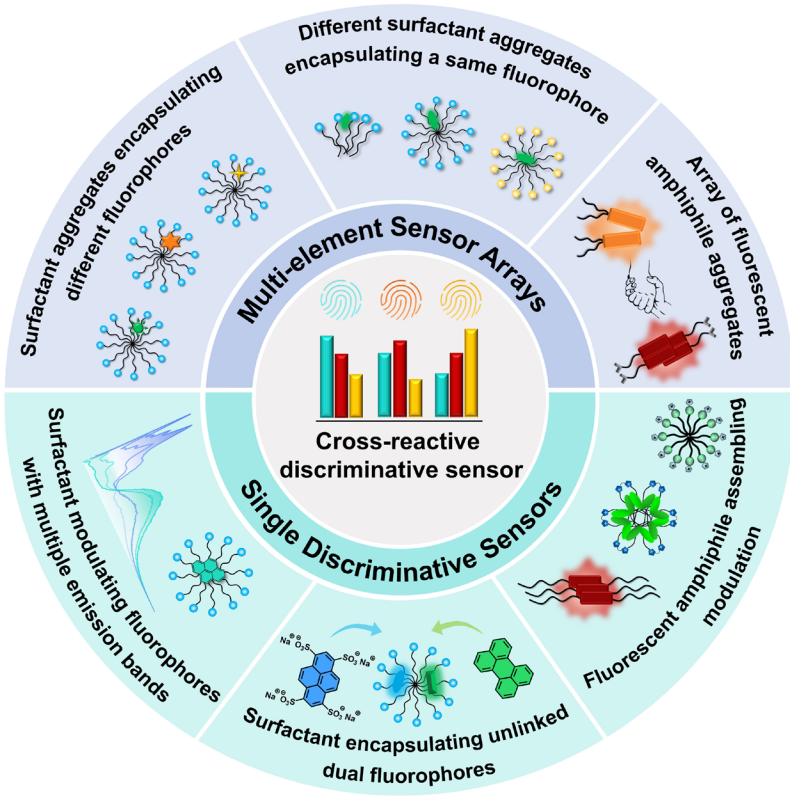
图 1（a）表面活性剂聚集体在水溶液中的动态组装过程的示意图。（b）选择性传感器（荧光团 – 连接臂 – 受体传感器）和传感器阵列（由一组传感器元件组成）示意图。（c）表面活性剂聚集体在构建荧光传感器方面的优点。

Figure 1 (a) A simple diagram depicting the dynamic assembly process of surfactant aggregates in aqueous solution. (b) Schematic illustration of selective sensor (fluorophore-spacer-receptor sensor) and sensor array (composed of a set of sensor elements). (c) Schematic illustration of the advantages of surfactant aggregates in generating fluorescent sensors.

2）。采用了三种方法来改变基于表面活性剂聚集体的传感单元构建传感器阵列：1）使用特定的表面活性剂聚集体来封装不同的荧光团以产生多个传感单元；2）使用不同类型的表面活性剂聚集体来封装一个特定的探针以提供不同的传感单元；3）使用不同的荧光两亲性聚集体提供多个传感单元。建立基于单一体系的交互响应性传感器的方法有 :1）具有多发射带的荧光团的组合；2）封装两个光物理性质相关但未连接的荧光团（FRET 对，D–A 对等）；3）采用具有多个发射带的荧光两亲性聚集体。虽然表面活性剂组件在构建交互响应性荧光传感器和阵列方面显示出了各种优势，但这种方法以及表面活性剂在交互响应性传感中的作用仍需要更多的探索。

第一作者：陕西师范大学博士研究生闫珍
通讯作者：陕西师范大学丁立平教授
全文链接：https://doi.org/10.1016/j.cocis.2024.101831

Surfactant is characterized with amphiphilic molecular structure, containing a hydrophilic head group and a hydrophobic tail (Figure 1a). This endows surfactant molecules' unique assembling behaviors in aqueous solution, where they can self-assemble into various colloidal aggregates, such as micelles, vesicles, and liposomes, etc. These colloidal aggregates are heterogeneous as having a hydrophobic core and a hydrophilic outer interface with water. Moreover, they are in dynamic assembling balance and are easy to be influenced by external stimuli like ionic strength, pH, and chemicals, etc. The heterogeneous microstructure of surfactant aggregates enables them to solubilize organic dyes in aqueous solutions and have been widely applied



图图 2 得益于表面活性剂的微观非均相结构和动态组装特性，表面活性剂聚集体通过不同的策略被广泛应用于构建交互响应性传感器和阵列

Figure 2 Due to the heterogeneous microstructure and dynamic assembling nature, surfactant aggregates have been widely applied in constructing cross-reactive sensors and arrays through different strategies.

in fabrication of fluorescent chemo/biosensors Fluorescent sensors can be either selective or cross-reactive (Figure 1b). For the former kind, it usually contains a specific receptor structure for selectively binding and recognizing the target analyte among a variety of detecting samples. For the latter type, it is generally an array of a number of nonspecific sensor elements, where each sensor element responds to all the analytes with different extent of responses. The combination of output signals from all the sensor elements generates a specific recognition pattern to a particular analyte. Such fluorescent sensor arrays are known as “optical nose” or “optical tongue”, and can identify and differentiate multiple analytes through multivariate data analysis methods such as principal component analysis and linear discriminant analysis. Thus, cross-reactive fluorescent sensors can not only discriminate similar analytes but also analyze complex samples such as in biofluids or mixtures, which makes them more attractive in practical applications.

Surfactant aggregates have been widely applied in constructing fluorescent sensors as they can provide hydrophobic core to encapsulate fluorophores or co-assemble with fluorophores. Variety of advantages were accompanied with using surfactant aggregates (Figure 1c), e.g., increasing aqueous solubility of organic fluorophores, enhancing fluorescence stability and quantum yield of the encapsulated fluorophores, etc. Moreover, combining amphiphilic surfactant aggregates with fluorophores can not only retain the fluorescence properties, but also provide external stimuli sensitivity due to the dynamic assembling characteristics. Different surfactant aggregates and fluorophores can be flexibly selected and assembled to make the ensemble sensor system exhibit different structural/photophysical properties, which have the merits of multiple interactions, variable aggregation behaviors, mild assembly conditions and multi-stimuli responsiveness.

In this short review, we intent to systematically introduce the advances of surfactant aggregates in constructing cross-reactive fluorescent sensors and arrays, specially focusing on introducing different construction strategies based on using non-fluorescent surfactant aggregates and surfactant-like fluorescent amphiphiles (Figure 2). To generate sensor arrays, three ways were employed to vary the surfactant aggregate-based sensor elements: 1) use one particular surfactant aggregate to encapsulate different fluorophores to generate multiple sensor ensembles; 2) use different types of surfactant aggregates to encapsulate one particular probe to provide different sensor ensembles; 3) use different fluorescent amphiphile aggregates to offer multiple sensor elements. To build cross-reactive single-system-based sensors, there are also three ways that were attempted using surfactant aggregates: 1) ensembles with fluorophores exhibiting multiple emission bands; 2) encapsulation of two photophysical-related but unlinked fluorophores (FRET pair, D-A pair, etc.); 3) employing fluorescent amphiphile assemblies with multiple emission bands. Although surfactant assemblies have shown a variety of advantages in constructing cross-reactive fluorescent sensors and arrays, this methodology is still less developed and the roles of surfactant assemblies in the cross-reactive sensing is still less explored.

First Author: Yan Zhen, doctoral candidate, Shaanxi Normal University
Corresponding Author: Prof. Ding Liping, Shaanxi Normal University
Full Text Link: https://doi.org/10.1016/j.cocis.2024.101831

中电科 39 所研发中心曹燕华一行来访

CETC No. 39 Institute visitors received

2024 年 8 月 19 日下午，中国电子科技集团有限公司第 39 研究所研发中心副主任曹燕华一行 4 人到访新概念传感器与分子材料研究院，与房喻院士团队进行了座谈交流，随后参观了综合展厅。

曹燕华副主任介绍了中心的基本情况和需求，双方进行了交流讨论。

研究院对外联络与行政办公室主任杨小刚，专职科研人员何怡楠和秘书左振男参加了座谈交流。

On August 19, 2024, four visitors from the 39th Research Institute of China Electronics Technology Group Co., Ltd., headed by its R&D Center deputy director Cao Yanhua, visited the Institute of New Concept Sensors and Molecular Materials, and had a discussion and exchange with Prof. Fang Yu, before visiting the comprehensive exhibition room.

The two sides exchanged ideas after Cao Yanhua introduced the basic information and needs of the center.

INCSMM Outreach and Administrative Office director Yang Xiaogang, full-time research assistant He Yinan, and secretary Zuo Zhennan, participated in the meeting.

汉威科技集团首席专家张小水一行来访

Hanwei Technology Group chief expert Zhang Xiaoshui received

2024 年 8 月 27 日上午，汉威科技集团首席专家张小水先生一行到访新概念传感器与分子材料研究院，参观了综合展厅，并与房喻院士进行了座谈交流。

汉威集团炜盛研究院化学传感器研发总监刘红霞从发展历程、荣誉资质、应用领域、企业核心能力四个方面介绍了汉威集团情况。

汉威研究院平台技术部研发总监郭远龙介绍了公司基本情况、产品与方案、应用与案例和企业愿景。

随后双方进行了座谈交流。张小水先生希望双方今后能加强联系，相互交流，在不同的应用领域达成一些合作。最后房喻院士总结讲话。

汉威集团炜盛研究院周建奎经理、郑岩岩经理和刘萍项目经理陪同来访。新概念传感器与分子材料研究院彭军霞教授、彭浩南教授、对外联络与行政办公室主任杨小刚、专职科研人员王佩、罗艳彦和秘书左振男参加座谈。

On August 27, 2024, Mr. Zhang Xiaoshui, chief expert of Hanwei Technology Group, and his delegation visited the Institute of New Concept Sensors and Molecular Materials, and had a discussion meeting with Prof. Fang Yu, after touring the INCSMM comprehensive exhibition room.

Liu Hongxia, R&D director of chemical sensor of Hanwei Group Weisheng Research Institute, briefed about Hanwei Group from four aspects: development history, honors and qualifications, application fields and core capabilities.

Guo Yuanlong, R&D director of Platform Technology Department of Hanwei Research Institute, briefed about

the company, its products and solutions, applications and cases, and corporate vision.

In the following discussion session, Zhang Xiaoshui hoped that the two sides could strengthen contacts and exchange in the future, and reach some cooperation in different application fields. Finally, Prof. Fang Yu summed up the meeting.

Weisheng Research Institute manager Zhou Jiankui, manager Zheng Yanyan and project manager Liu Ping accompanied Zhang Xiaoshui during the visit. INCSMM Prof. Peng Junxia, Prof. Peng Haonan, Office of Liaison and Administration director Yang Xiaogang, researcher assistants Wang Pei and Luo Yanyan, and secretary Zuo Zhennan attended the meeting.

上海众合创投聂新勇董事长一行来访

Shanghai Unity Asset Management chairman Nie Xinyong received

2024 年 8 月 30 日上午，陕西师范大学杰出校友、上海众合创业投资管理有限公司董事长聂新勇先生一行在校党委副书记卢胜利的陪同下到访新概念传感器与分子材料研究院，并与房喻院士进行了座谈交流。

陕西风润智能制造研究院有限公司总经理李博陪同来访。校友工作办公室主任刘洪超、研究院对外联络与行政办公室主任杨小刚参加会谈。

On August 30, 2024, Mr. Nie Xinyong, distinguished alumnus of Shaanxi Normal University and chairman of Shanghai Unity Asset Management Co., Ltd., accompanied by Lu Shengli, deputy secretary of SNNU Party Committee, visited the Institute of New Concept Sensors and Molecular Materials, and had a meeting with Prof. Fang Yu.

Shaanxi Fengrun Intelligent Research Institute Co., Ltd. general manager Li Bo accompanied Nie during the visit. SNNU Alumni Work Office director Liu Hongchao, and INCSMM Liaison and Administration Office director Yang Xiaogang attended the meeting.

总策划：房喻教授
Producer & Editor-in-Chief: Prof. Fang Yu
责任编辑：刘小燕 冯伟
Executive Editors: Liu Xiaoyan, 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