陕西师范大学
SHAANXI NORMAL UNIVERSITY

化学化工学院
School of Chemistry & Chemical Engineering

2025年5月
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简报
Newsletter

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

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Liu Taihong and students attend Second National Conference on Nonlinear Optical Technology and Applications

2025 年 5 月 9 至 11 日，第二届全国非线性光学技术及应用学术会议在山东济南召开，新概念传感器与分子材料研究院刘太宏副教授及 4 名研究生参会。

刘太宏副教授作了题为“多偶极双光子荧光探针创制及应用探索”的邀请报告，硕士研究生刘新奥作了题为“方酸菁衍生物的制备与双光子吸收”的口头报告，同时硕士研究生周星彤和陈怡嘉做了墙报展示。

本次会议由中国感光学会非线性光功能材料与器件技术专业委员会主办，旨在打造非线性光学领域的高水平学术平台，推动非线性光学材料、器件及技术高质量发展，助力提升中国在该领域的国际竞争力。

From May 9th to 11th, 2025, Assoc. Prof. Liu Taihong and four master’s students from the Institute of New Concept Sensors and Molecular Materials attended the Second National Conference on Nonlinear Optical Technology and Applications held in Jinan, Shandong Province.

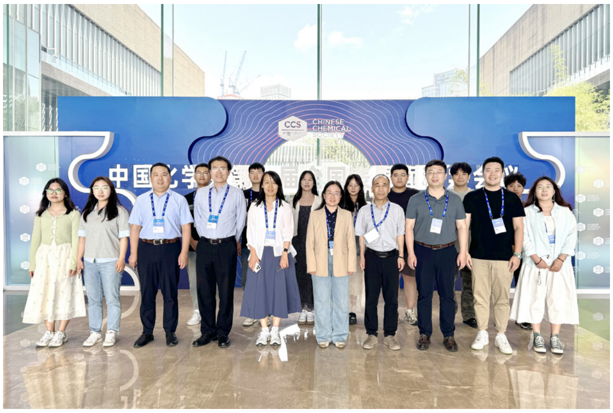
Liu Taihong gave an invited report titled “Creation and Application Exploration of Multidipole Two-Photon Fluorescent Probes”, and master’s student Liu Xin’ao presented an oral report titled “Preparation of Derivatives of Foxylic Acid and Two-Photon Absorption”. Meanwhile, master’s students Zhou Xingtong and Chen Yijia made poster presentations.

Hosted by the Nonlinear Optical Functional Materials and Devices Technology Professional Committee of the Chinese Society for Imaging Science and Technology, this conference aims to build a high-level academic platform in the field of nonlinear optics, promote the high-quality development of nonlinear optical materials, devices and technologies, and help enhance China’s international competitiveness in this field.

研究院师生参加中国化学会第一届全国表界面科学会议

INCSMM teachers and students attend CCS First National Conference on Surface and Interface Science

2025 年 5 月 9 至 12 日，中国化学会第一届全国表界面科学会议在成都召开，新概念传感器与分子材料研究院丁立平教授、刘静教授、刘凯强教授、边红涛教授、彭浩南教授、刘忠山副研究员、薄鑫副研究员和多名学生参会。



丁立平教授、刘静教授、边红涛教授和刘忠山副研究员分别作了题为“界面限域荧光纳米膜创制及其高性能传感应用研究”“分子组装策略调控铂 (II) 配合物的发光行为研究”“水系电解液氢键网络演化动力学的超快红外光谱”和“多级孔表界面的分离与传感”的邀请报告。刘凯强教授主持了“液基材料图案化及器件应用”分会场报告。翟宾宾、闫珍、陈永同学作了墙报展示。

本次会议由中国化学会物理化学学科委员会主办、北京大学纳米器件物理与化学教育部重点实验室承办，旨在

展示我国表界面相关领域的最新研究进展，推动学科发展，涉及作为传感、催化、超导和芯片等国家重大战略需求共性科学基础的物质、能源和信息等基础学科。

From May 9th to 12th, 2025, teachers and students from the Institute of New Concept Sensors and Molecular Materials, including Prof. Ding Liping, Prof. Liu Jing, Prof. Liu Kaiqiang, Prof. Bian Hongtao, Prof. Peng Haonan, A/Prof. Liu Zhongshan, and A/Prof. Bo Xin attended the First National Conference on Surface and Interface Science of the Chinese Chemical Society held in Chengdu.

Ding Liping, Liu Jing, Bian Hongtao and Liu Zhongshan respectively gave invited reports titled “Construction of Interface-Limited Fluorescent Nanofilms and Studites on Their High-Performance Sensing Applications”, “Regulation of the Switchable Luminescence of Platinum(II) Complexes by Controlling the Assembly Process”, “Hydrogen Bonding Evolution Dynamics of Water-Based Electrolytes Investigated by Ultrafast Dynamics” and “Modulating Surface and Interface of Hierarchical Pores for Separation and Sensing”. Liu Kaiqiang presided over the sub-forum on “Patterning of Liquid-based Materials and Device Applications”. Students Zhai Binbin, Yan Zhen and Chen Yong presented their wall posters.

This conference is hosted by the Physical Chemistry Discipline Committee of the Chinese Chemical Society and organized by the Key Laboratory of Nanodevice Physics and Chemistry of the Ministry of Education at Peking University. It aims to showcase the latest research progress in the field of surface and interface in China, promote the development of the discipline, and cover basic disciplines such as materials, energy and information, which serve as the common scientific basis for major national strategic demands such as sensing, catalysis, superconductivity and chips.

刘太宏、乔敏获 2025 年度陕西省科技计划项目资助

Liu Taihong and Qiao Min funded by 2025 Shaanxi Science and Technology Program

近日，陕西省科技厅公布了 2025 年度陕西省科技计划项目资助情况，新概念传感器与分子材料研究院两位教师获得资助。

刘太宏副教授获批省杰出青年科学基金项目（项目名称：激发态动力学行为调控和荧光传感应用，资助金额：50 万元），乔敏博士获批陕西省自然科学基础研究青年项目（项目名称：丰富孔隙高效担载荧光染料纳米膜的可控制备和传感性能研究，资助金额：5 万元）。

Recently, the Science and Technology Department of Shaanxi Province announced the funding of the 2025 Shaanxi Provincial Science and Technology Program projects, and the projects of two faculty members of the Institute of New Concept Sensors and Molecular Materials were awarded funding.

Assoc. Prof. Liu Taihong was approved for the Provincial Outstanding Youth Science Fund Project (Project Title: Regulation of excited state dynamics behavior and fluorescence sensing application, Funding Amount: CNY 500,000 yuan), and Dr. Qiao Min was approved for the Shaanxi Provincial Natural Science Basic Research Youth Project (Project Title: Research on the controllable preparation and sensing performance of nanomembranes of highly efficient stretcher-loaded fluorescent dyes with rich pore space, Funding Amount: CNY 50,000 yuan).

房喻院士获聘超快光科学与技术全国重点实验室第一届学术委员会委员

Fang Yu appointed member of First Academic Committee of National Key Laboratory of Ultrafast Optical Science and Technology

2025 年 5 月 21 日，房喻院士出席在西安召开的超快光科学与技术全国重点实验室第一届学术委员会第一次会议，并获聘学术委员会委员。

实验室主任付玉喜研究员为学术委员会委员颁发了聘书，并作工作报告介绍了实验室基本情况和工作进展。学术委员会主任刘文清院士，副主任顾敏院士、李应红院士、赵卫研究员，委员姜会林院士、王立军院士、洪明辉院士等出席会议。

学术委员会对实验室取得的建设成绩给予肯定，希望实验室力争建设成为超快光科学与技术领域国际一流的学术高地和人才高地。

On May 21, 2025, Prof. Fang Yu attended the first meeting of the First Academic Committee of the National Key Laboratory of Ultrafast Optical Science and Technology in Xi'an and was appointed as a member of the committee.

Prof. Fu Yuxi, director of the laboratory, presented the appointment certificates to the committee members and made a working report to introduce the basic situation and work progress of the laboratory. Academician Liu Wenqing, director of the Academic Committee, Academician Gu Min, Academician Li Yinghong and Researcher Zhao Wei, vice directors, and Academician Jiang Huilin, Academician Wang Lijun and Academician Hong Minghui and other members and officials attended the meeting.

The Academic Committee recognized the construction achievements of the laboratory and hoped that it would strive to become an international first-class academic and talent highland in the field of ultrafast optical science and technology.

边红涛教授参加基于可调谐红外激光的能源化学研究大型实验装置用户会议

Bian Hongtao participates in User Meeting of Large-scale Experimental Device for Tunable Infrared Laser-based Energy Chemistry Research

2025 年 5 月 21 至 22 日，新概念传感器与分子材料研究院边红涛教授参加了在合肥举行的基于可调谐红外激光的能源化学研究大型实验装置用户会议，并作了题为“受限环境中氢键网络的超快振动动力学”的邀请报告。

合肥红外自由电子激光装置是厦门大学、中国科学技术大学、复旦大学、中国科学院大连化学物理研究所联合承建的国家重大科研仪器设备研制专项。该大型装置包含一套可调谐红外自由电子激光光源、一条光束传输线和五条能源化学研究实验线站，是我国首台覆盖中、远红外波段的自由电子激光用户装置，也是国际上首台面向能源化学研究的红外自由电子激光装置。

本次会议主席为厦门大学孙世刚院士，会议旨在探讨如何充分利用合肥红外自由电子激光装置开展高水平研究工作，推动设施和用户共同发展。

On May 21 and 22, 2025, Prof. Bian Hongtao of the Institute of New Concept Sensors and Molecular Materials participated in the User Meeting of the Large-scale Experimental Device for Tunable Infrared Laser-based Energy Chemistry Research in Hefei and presented an invited report titled "Ultrafast Vibrational Dynamics of Hydrogen-Bonded Networks in Confined Environments".

Hefei Infrared Free Electron Laser Device is a special project for the development of national major scientific research instruments and equipment jointly undertaken by Xiamen University, University of Science and Technology of China, Fudan University and Dalian Institute of Chemical Physics, Chinese Academy of Sciences. This large-scale device contains a set of tunable infrared free-electron laser light source, a beam transmission line and five experimental line stations for energy chemistry research, which is the first free-electron laser user device covering the mid- and far-infrared wavelengths in China, and also the first infrared free-electron laser device for energy chemistry research in the world.

This meeting, chaired by Academician Sun Shigang of Xiamen University, aims to discuss how to make full use of the Hefei Infrared Free-Electron Laser Device to carry out high-level research and promote the joint development of the facility and its users.

房喻院士出席第七届智能传感器产业发展大会

Fang Yu attends 7th Intelligent Sensor Industry Development Conference

2025年5月23日，房喻院士应邀出席在安徽省蚌埠市举行的第七届智能传感器产业发展大会开幕式。

大会由安徽省科学技术厅（安徽省人工智能产业推进组办公室）、中国兵器工业集团有限公司民品产业部、蚌埠市人民政府主办。

开幕式上，发布了《2025年中国MEMS产业发展与十大高质量传感器园区报告》、长三角MEMS与传感器新技术新产品，进行了精密微纳制造技术全国重点实验室长三角（蚌埠）产教融合协同中心、安徽省汽车行业协会汽车智能传感专业技术委员会、长三角脑机接口产业联盟揭牌，及为5位智能传感器产业高层次人才颁发了安家补贴。

On May 23, 2025, Prof. Fang Yu was invited to attend the opening ceremony of the 7th Intelligent Sensor Industry Development Conference held in Bengbu, Anhui Province.

The conference is organized by the Science and Technology Department of Anhui Province (Office of the Artificial Intelligence Industry Promotion of Anhui Province), the Civilian Products Industry Department of China North Industries Corporation, and the People’s Government of Bengbu City.

At the opening ceremony, the “2025 Report on China MEMS Industry Development and Top Ten High-Quality Sensor Park”, the Yangtze River Delta MEMS and Sensor new technology and new products were released, the National Key Laboratory of Precision Micro-Nano Manufacting Technology Yangtze River Delta (Bengbu) Industry-Teaching Integration Synergistic Center, the Automotive Intelligent Sensing Professional Technical Committee of the Automobile Industry Association of Anhui Province, the Yangtze River Delta Brain-Computer Interface Industry Alliance were unveiled, and five high-level professionals in the intelligent sensor industry were issued settling-in subsidies.

房喻院士、丁立平教授参加“阿秒看清微观世界”活动

Fang Yu and Ding Liping participate in “Seeing the Microscopic World in Attosecond” event

2025年5月25日，重大科技基础设施与西安产业发展协同对接系列活动——“阿秒看清微观世界”活动在西安市临潼区长安先导国际创新人才交流中心举办，新概念传感器与分子材料研究院房喻院士和丁立平教授应邀参加活动。

中国科学院西安光学精密机械研究所副所长付玉喜介绍了阿秒设施建设进展情况及应用前景。房喻院士在院士交流环节活动作交流发言，丁立平教授作为合作单位代表发言。

陕西省委常委、西安市委书记方红卫出席活动并讲话。中国工程院院士陈志南、先进阿秒激光设施大科学装置首席科学家赵卫，陕西省政府副秘书长、先进技术成果西安转化中心主任冯梓剑等领导及科研院所、高校、行业协会、重点企业代表等参加了活动。

On May 25th, 2025, Prof. Fang Yu and Prof. Ding Liping from the Institute of New Concept Sensors and Molecular Materials participated in the event “Seeing the Microscopic World in Attosecond”, one of a series of collaborative docking activities between major scientific and technological infrastructures and industrial development of Xi’an city, held at Chang’an Pilot International Innovation and Talent Exchange Center in Lintong District, Xi’an, China.

Fu Yuxi, deputy director of Xi’an Institute of Optics and Precision Mechanics, Chinese Academy of Sciences, introduced the progress of the construction of the attosecond facility and its application prospects. Prof. Fang Yu spoke at the Academician Dialog Session, and Prof. Ding Liping spoke as a representative of the cooperative unit.

Fang Hongwei, member of the Standing Committee of Shaanxi Provincial Committee and Secretary of Xi’an Municipal Party Committee, attended the event and delivered a speech. Chen Zhinan, academician of the Chinese Academy of Engineering, Zhao Wei, chief scientist of the Advanced Attosecond Laser Facility Large Scientific Device, Feng Zijian, deputy secretary-general of the Shaanxi Provincial Government and director of the Xi’an Transformation Center for Advanced Technology Achievements, and other officals and representatives of research institutes, universities, industry associations, enterprises attended the event.

房喻院士出席“全国科技工作者日”陕西主场活动

Fang Yu attends “National Science and Technology Workers’ Day” Shaanxi main event

2025 年 5 月 28 日，房喻院士出席在陕西师范大学长安校区举办的 2025 科学家故事舞台剧推广行动展演暨“全国科技工作者日”陕西主场活动。

陕西省委副书记邢善萍、中国科协党组副书记冯身洪出席活动。房喻院士与安芷生院士、邱爱慈院士、彭建兵院士共同为《“陕”耀光芒在陕两院院士风华录（第三辑）》揭幕，并向科技工作者和学生代表赠书。

2025 科学家故事舞台剧推广行动展演剧目《最后一次海试》《永怀之歌》在本次活动中上演。《最后一次海试》取材于首批“全国高校黄大年式教师团队”西北工业大学自主水下航行器团队真实事迹。《永怀之歌》以“两弹一星”功勋奖章获得者郭永怀先生的事迹为内容，弘扬“两弹一星”精神、讴歌家国情怀和奉献精神。

陕西省有关部门负责同志和在陕高校、科研院所、企事业单位科技工作者及部分学生代表约 800 人参加了活动。

On May 28, 2025, Prof. Fang Yu attended the 2025 Scientist Stories Stage Drama Performing Activity and the Shaanxi Main Event of “National Science and Technology Workers’ Day” held at Chang’an Campus of Shaanxi Normal University.

Xing Shanping, deputy secretary of Shaanxi Provincial Party Committee, and Feng Shihong, deputy secretary of the Party Group of China Association for Science and Technology, attended the event.

Academicians Fang Yu, An Zhisheng, Qiu Aici, and Peng Jianbing unveiled the book “Shining Light of Academicians in Shaanxi (Third Series)” and presented the books to representatives of science and technology workers and students.

The two plays “The Last Sea Trial” and “Song of Yonghuai” of the 2025 Scientist Stories Stage Drama Performing Activity were staged in the event. “The Last Sea Trial” is based on the true story of the autonomous underwater vehicle development team of Northwestern Polytechnical University, which is one of the first “National Huang Dainian-style Teacher Teams in Universities”. “Song of Yonghuai” is based on the deeds of Mr. Guo Yonghuai, the recipient of the “Two Bombs and One Star” Medal of Merit, which promotes the spirit of “Two Bombs and One Star” and celebrates patriotism and dedication.

About 800 people attended the event, including officials from relevant departments of Shaanxi Province and scientific and technological workers from universities, research institutes, enterprises and institutions in Shaanxi Province, as well as university students.

博士生谭淑文获国家留学基金委资助赴瑞典隆德大学联合培养

Doctoral Student Tan Shuwen funded by China Scholarship Council for joint program at Lund University

近日，国家留学基金委公布了 2025 年国家建设高水平大学公派研究生项目录取名单，新概念传感器与分子材料研究院博士研究生谭淑文（导师房喻教授，刘小燕副教授）获公派留学奖学金资助，拟赴瑞典隆德大学进行为期一年的联合培养博士学习。

Recently, the China Scholarship Council announced the admission list of 2025 National Postgraduate Study Abroad Program for Construction of High-level Universities, and Tan Shuwen, a doctoral student of the Institute of New Concept Sensors and Molecular Materials (supervised by Prof. Fang Yu and Assoc. Prof. Liu Xiaoyan), has been awarded the scholarship to carry out a year-long joint doctoral program at Lund University, Sweden.

研究院2025届毕业生通过毕业论文答辩

Class 2025 students pass graduation thesis defense

2025年5月29日，新概念传感器和分子材料研究院2025届化学、材料与化工及化学工程与技术三个专业的闫旭东、周建成、张弛、徐晓佳等28名硕士研究生进行了毕业论文答辩。

在同学们的毕业论文陈述之后，由西安交通大学刘峰教授、韦学勇教授、沈少华教授、西北工业大学陈凯杰教授、航天推进技术研究院李万鹏研究员为代表的8位校外专家和12位校内专家组成的答辩委员会的评委专家对同学们进行了提问、评议和点评，并对毕业论文提出了完善修改意见。经讨论，答辩委员会一致认为28位同学研究内容充分，回答问题清楚，逻辑合理，同意通过答辩并建议授予相应的硕士学位。

5月26日、27日和29日，新概念传感器和分子材料研究院2025届化学、化学（师范）、化学（创新实验班）及应用化学等专业的33名本科生分为三组进行了毕业论文答辩。经讨论，答辩委员会一致认为33位本科毕业生同学达到了本科毕业论文相应要求，同意通过答辩。

On May 29, 2025, 28 Class 2025 master’s students, including Yan Xudong, Zhou Jiancheng, Zhang Qi, and Xu Xiaojia, of the Institute of New Concept Sensors and Molecular Materials, who are majoring in Chemistry, Materials and Chemical Engineering and Chemical Engineering and Technology, defended their graduation theses.

After their thesis presentation, eight outside experts, represented by Prof. Liu Feng, Prof. Wei Xueyong and Prof. Shen Shaohua from Xi’an Jiaotong University, Prof. Chen Kaijie from Northwestern Polytechnical University, and Prof. Li Wanpeng from Institute of Aerospace Propulsion Technology, and 12 Shaanxi Normal University experts from the defense committee asked questions, made comments, and gave suggestions for the improvement and modification of the theses. After discussion, the defense committee unanimously agreed that the 28 students had sufficient research

content, clear answers to questions and reasonable logic, and agreed to pass the defense and recommended to award them corresponding master's degrees.

On May 26, 27 and 29, 33 Class 2025 undergraduate students of Chemistry, Chemistry (Teacher Training), Chemistry (Innovative Experimental Class) and Applied Chemistry majors of the Institute of New Concept Sensors and Molecular Materials defended their graduation theses in three groups. After discussion, the defense committee unanimously agreed that the 33 undergraduate students met the corresponding requirements of undergraduate thesis and agreed to pass the defense.

彭浩南教授受邀担任国际期刊 Responsive Materials 青年编委

Peng Haonan appointed young editorial board member of Responsive Materials

近日，新概念传感器与分子材料研究院彭浩南教授受邀担任国际期刊 Responsive Materials 青年编委。

Responsive Materials 是 Wiley 旗下一本聚焦刺激响应功能材料领域的首个跨学科专业英文期刊，涵盖材料在物理、化学、生物、环境等多种刺激下的响应行为与应用研究，致力于推动智能材料与前沿功能系统的基础研究与技术转化。

Recently, Prof. Peng Haonan of the Institute of New Concept Sensors and Molecular Materials was invited to serve as a young editorial board member of the international journal Responsive Materials.

Responsive Materials is Wiley's first interdisciplinary English-language journal focusing on stimulus-responsive functional materials, covering research on the responsive behaviors and applications of materials under physical, chemical, biological, and environmental stimuli, and is dedicated to promoting the basic research and technological transformation of smart materials and cutting-edge functional systems.

Responsive Materials

CERTIFICATE OF APPOINTMENT

To

Haonan Peng

as **Youth Editorial Board Member** for

Responsive Materials from May 2025 to May 2027

Editor-in-Chief:

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Letter

Improved Solvatochromism and Quantum Yields in Acridine through Polarity-Enhanced π-Conjugation

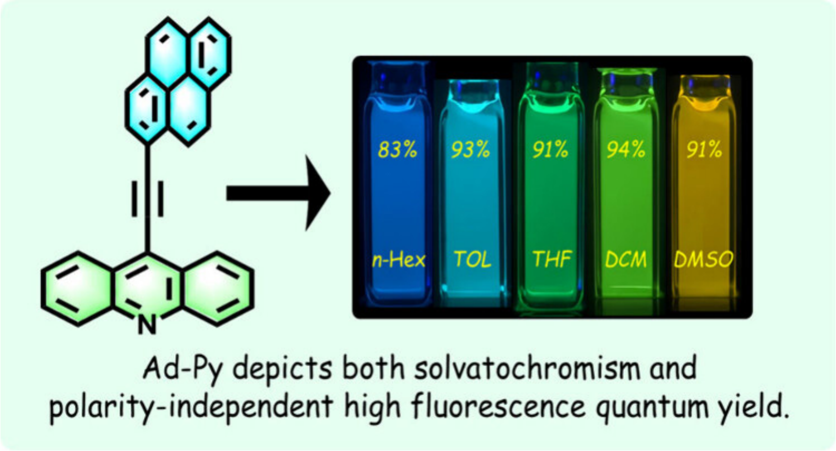
Jiancheng Zhou,[∇] Yan Jiang,[∇] Qingwei Jiang, Simin Lin, Zhouyu Chen, Mengyu Ji, Xinyu Gou, Lingya Peng,* and Yu Fang*

Cite This: *J. Phys. Chem. Lett.* 2025, 16, 4853−4860

Read Online

通过极性增强的 π 共轭体系提升吖啶的溶剂致变色效应与量子产率研究

Jiancheng Zhou, Yan Jiang, Qingwei Jiang, Simin Lin, Zhouyu Chen, Mengyu Ji, Xinyu Gou, Lingya Peng, Yu Fang. J. Phys. Chem. Lett. 2025, 16, 4853-4860. DOI: 10.1021/acs.jpclett.5c00803.



Ad-Py depicts both solvatochromism and polarity-independent high fluorescence quantum yield.

有机荧光染料的探索因其在生物成像、光电器件和传感等领域的广泛应用而受到广泛关注。通过调控其几何结构与电子结构，这些化合物的多样性得到了极大的拓展。其中，溶剂致变色分子作为非侵入性可视化工具具有特别重要的前景，这主要归因于它们对微环境的高度敏感性。典型的溶剂致变色染料包括尼罗红、丙烷荧光素和月桂荧光素，这些染料在高极性环境中表现出显著的荧光颜色变化。然而，此类染料在高极性环境中的应用受到其较低量子产率的显著限制，主要原因在于增强的非辐射跃迁途径被激活，从而导致荧光猝灭。

在本研究中，我们介绍了一种基于吖啶衍生的荧光团 Ad–Py，该化合物在多种溶剂中表现出显著的溶致变色效应以及较高的荧光量子产率。在低极性溶剂中，局部激发态（LE）占主导地位，从而导致较高的荧光量子产率；而在高极性溶剂中，由 π 电子体系扩展所促进的电荷转移态（CT）则在精细调节能隙与发射波长方面发挥了关键作用，使 Ad–Py 对微环境的极性变化具有高度敏感性。通过在这些状态之间实现微妙的平衡，Ad–Py 充分利用了两种电子结构的优势，既增强了辐射跃迁效率，又提升了对环境的敏感性。此外，基于其对极性变化的敏感特性，我们开发了一种用于检测二氧化硫（SO_2）的荧光薄膜传感器，实现了低于 10 ppb 的检测限。这

一策略成功设计出一种新型荧光团，不仅能够展现对极性敏感的发射颜色变化，同时还能保持对极性不敏感的发射强度稳定性。

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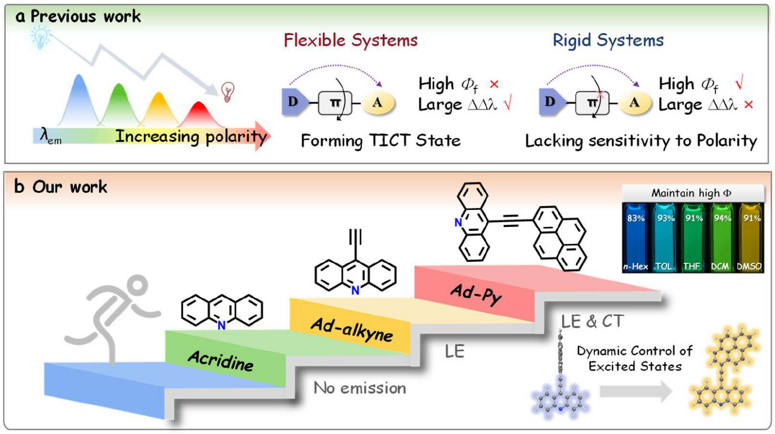

图 1 (a) 已报道的溶剂致变色策略示意图；(b) Ad−Py 分子设计策略的示意图。
Figure 1. (a) Illustrations of the reported strategies for solvatochromism; (b) Schematic representation of the molecular design strategy for Ad-Py.

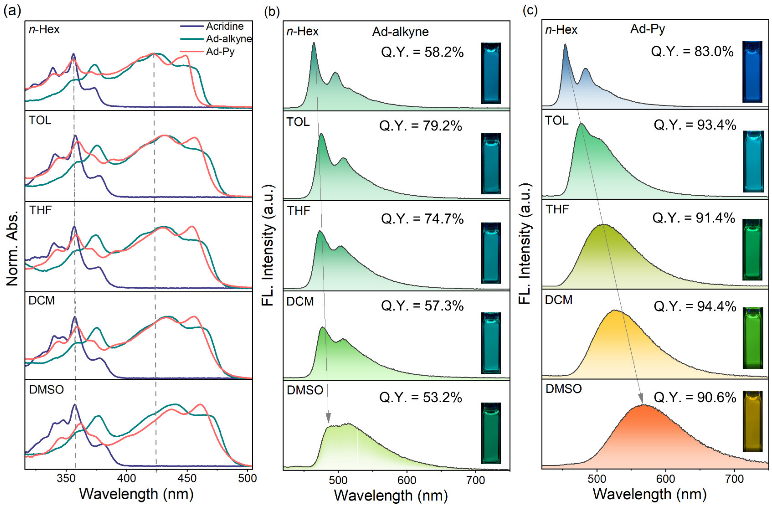

图 2 (a) Acridine, Ad−alkyne, 及 Ad−Py 在不同溶剂中的紫外−可见吸收光谱（浓度为 5 × 10^{-6} M）；(b) Ad−alkyne 在不同溶剂中的荧光光谱(激发波长为 360 nm，浓度为 5 × 10^{-6} M)。插图：在紫外灯照射下(激发波长为 365 nm）拍摄的 Ad−alkyne 在不同溶剂中的照片。(c) Ad−Py 在不同溶剂中的荧光光谱（激发波长为 360 nm，浓度为 5 × 10^{-6} M）。插图：在紫外灯照射下（激发波长为 365 nm）拍摄的 Ad−Py 在不同溶剂中的照片。
Figure 2. (a) UV-vis absorption spectra of Acridine, Ad-alkyne, and Ad-Py in various solvents (c = 5 × 10^{-6} M); (b) Fluorescence spectra of Ad-alkyne (λex = 360 nm) in various solvents (c = 5 × 10^{-6} M). Inset: the photographs of Ad-alkyne in various solvents taken under UV light (λex = 365 nm). (c) Fluorescence spectra of Ad-Py (λex = 360 nm) in various solvents (c = 5 × 10^{-6} M). Inset: the photographs of Ad-Py in various solvents taken under UV light (λex = 365 nm).

The exploration of organic fluorescent dyes has been widely noted due to their extensive applications in bioimaging, optoelectronic devices, and sensing. Significant expansion in the diversity of these compounds has been achieved through modulation of their geometric and electronic structures. Among them, solvatochromic molecules have been recognized as particularly promising non-invasive visualization tools, primarily because of their high sensitivity to microenvironments. Typical solvatochromic dyes, including Nile Red, propanofluorone, and laurofluorone, exhibit notable fluorescence color changes in highly polar environments. However, the application of such dyes in highly polar environments is considerably restricted by their low quantum yields, which are largely attributed to the activation of enhanced non-radiative decay pathways, leading to fluorescence quenching.

In this study, an acridine-derived fluorophore, Ad-Py, is introduced, demonstrating significant solvatochromic effects and high fluorescence quantum yields across various solvents. In low-polarity solvents, the locally excited state (LE) is observed to dominate, resulting in high fluorescence quantum yields. In contrast, in high-polarity solvents, the charge-transfer state (CT), promoted by the extension of the π-electron system, plays a critical role in fine-tuning the energy gap and emission wavelength, making Ad-Py highly sensitive to changes in environmental polarity. A delicate balance between these states allows both electronic configurations to be effectively utilized, enhancing radiative transition efficiency while improving environmental sensitivity. Additionally, based on its sensitivity to polarity variations, a fluorescent thin-film sensor for the detection of sulfur dioxide (SO_2) has been developed, achieving a detection limit below 10 ppb.

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Precision Molecular Engineering of Compact Near-Infrared Fluorophores

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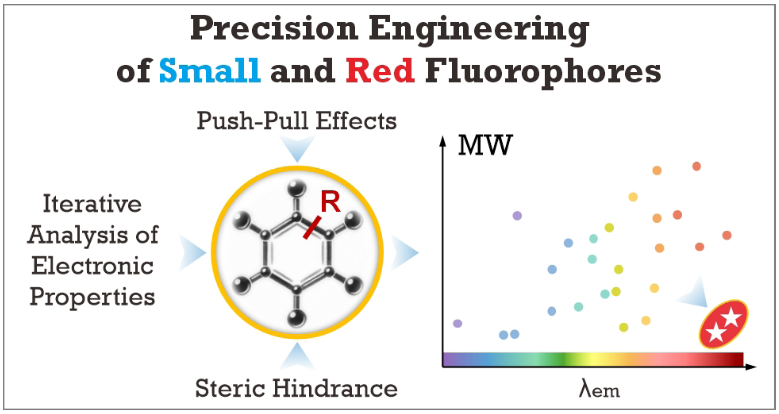
小分子尺寸近红外荧光染料的精准设计

Rongrong Huang,# Qinglong Qiao,# Deborah Seah, Tianruo Shen, Xia Wu, Fabio de Moliner, Chao Wang, Nannan Ding, Weijie Chi, Huaming Sun, Marc Vendrell,* Zhaochao Xu,* Yu Fang,* and Xiaogang Liu*. J. Am. Chem. Soc. 2025, 147, 5258-5268. DOI: 10.1021/jacs.4c16087



有机荧光染料在生命科学和生物医学研究中具有广泛应用，例如疾病诊断、蛋白质定量和细胞动态研究。然而，传统荧光染料通常存在分子尺寸大、发射波长短等问题，限制了其在深层组织成像和高分辨率显微技术中的应用。开发兼具小分子尺寸和近红外发射特性的荧光染料一直是科学界的重大挑战。

本工作通过量化计算和结构－性质关系分析，建立了一种迭代设计方法，实现了对单苯环基近红外荧光染料的精准结构设计。该方法通过逐步引入电子给体（D）和电子受体（A），优化推拉电子效应和空间位阻，从而确定取代基位置、取代基数目和取代基类型，最终设计出分子量极低但发射波长较长的荧光染料。例如，SR-1的分子量仅为192 g/mol，发射波长为724 nm；SR-3的发射波长更是达到759 nm。

这些新型荧光染料展现出独特的环境敏感性: 在水溶液中几乎不发光，而在脂质环境中表现出高荧光强度。这一特性使其能够实现免洗活细胞成像，简化了实验流程并可获得较高信噪比。此外，染料的光稳定性和选择性使其适用于超分辨成像，能够长时间追踪脂滴动态。研究团队进一步将染料与D-丙氨酸结合，开发出荧光非天然氨基酸ASR-5，成功用于细菌细胞壁生物合成的标记。这一成果为细菌研究和抗生素开发提供了新工具。此外，染料的小分子尺寸使其能够穿透分子筛等微小空腔，为材料科学和三维成像提供了新可能。

这项研究突破了荧光染料领域长期存在的“小分子尺寸与长发射波长难以兼容”这一技术瓶颈，通过精准分子工程策略，为高分辨率生物成像技术开辟了创新路径。随着性能优化与应用场景的拓展，此类超紧凑近红

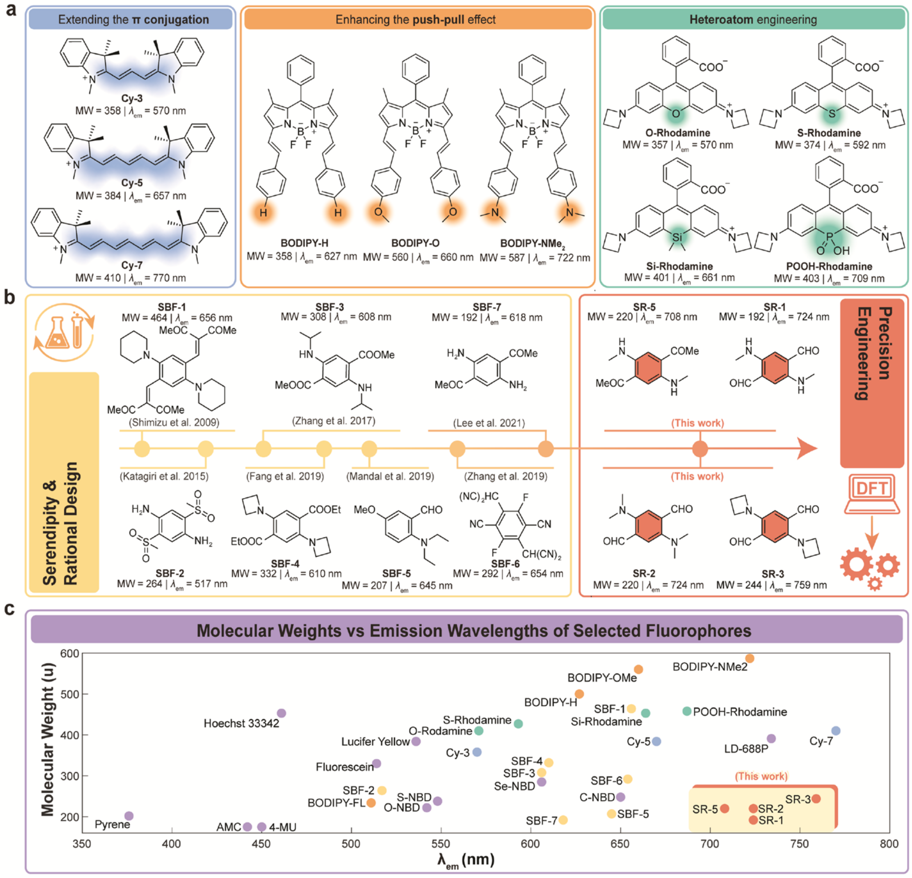


图 1. 用于开发红色 / 近红外荧光染料及单苯环荧光染料的示意图。

Figure 1. Schematic Representation for Developing Red/NIR Fluorophores and Single-Benzene Fluorophores.

外荧光染料有望成为生命科学研究和临床精准诊断的关键工具。尽管在摩尔吸光系数提升与功能化修饰方面仍需突破，但其提出的迭代设计范式展现了强大的普适性——通过量化计算指导的分子精准设计，为功能导向型荧光染料的理性设计提供了全新范式。

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Organic fluorophores are widely used in life sciences and biomedical research, including applications in disease diagnosis, protein quantification, and studies of cellular dynamics. However, traditional fluorophores often suffer from large molecular sizes and short emission wavelengths, limiting their utility in deep-tissue imaging and high-resolution microscopy. Developing fluorophores that combine compact molecular dimensions with near-infrared (NIR) emission has remained a significant scientific challenge.

In this work, we established an iterative design methodology through quantum chemical calculations and structure-property relationship analysis, enabling precise structural engineering of single-benzene-based NIR fluorophores. By systematically introducing electron donors (D) and acceptors (A), optimizing push-pull electronic effects, and managing steric hindrance, we determined optimal substituent positions, quantities, and types. This approach yielded fluorophores with ultra-low molecular weights and extended emission wavelengths. For example, SR-1 exhibits a molecular weight of 192 g/mol and an emission peak at 724 nm, while SR-3 achieves an emission wavelength of 759 nm.

These novel fluorophores demonstrate unique environmental sensitivity: they are nearly non-emissive in aqueous solutions but highly fluorescent in lipid environments. This property enables wash-free live-cell imaging, simplifying experimental workflows while maintaining high signal-to-noise ratios. Their photostability and selectivity further facilitate super-resolution imaging, allowing prolonged tracking of lipid droplet dynamics. By conjugating the fluorophores with D-alanine, the team developed ASR-5, a fluorescent unnatural amino acid that successfully labels bacterial cell wall

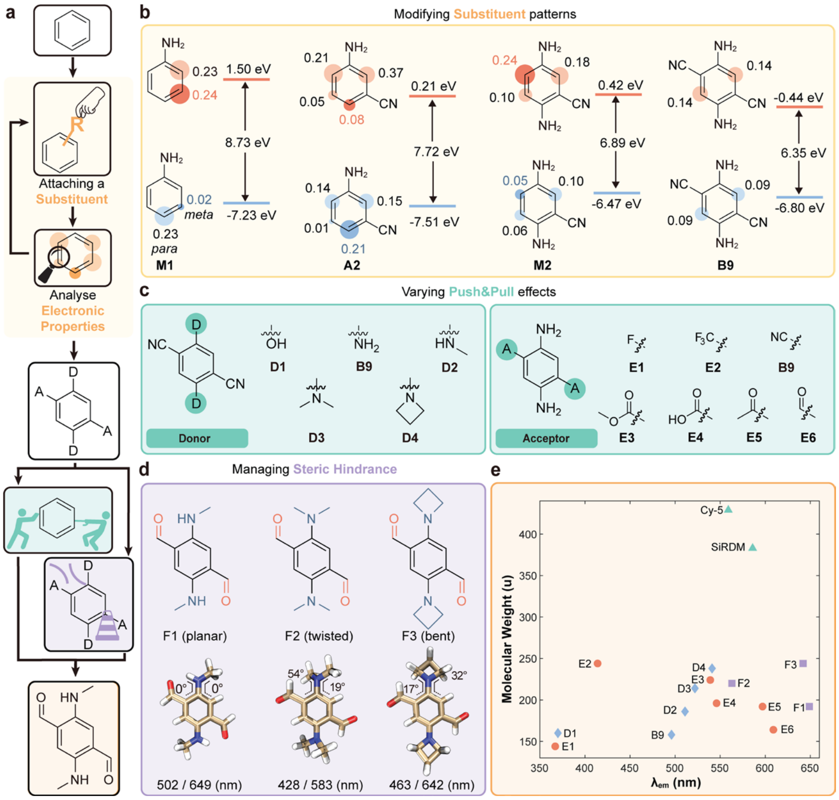

图 2. 小而红荧光染料的迭代精准设计。

Figure 2. Iterative precision molecular engineering of small and red/NIR fluorophores.

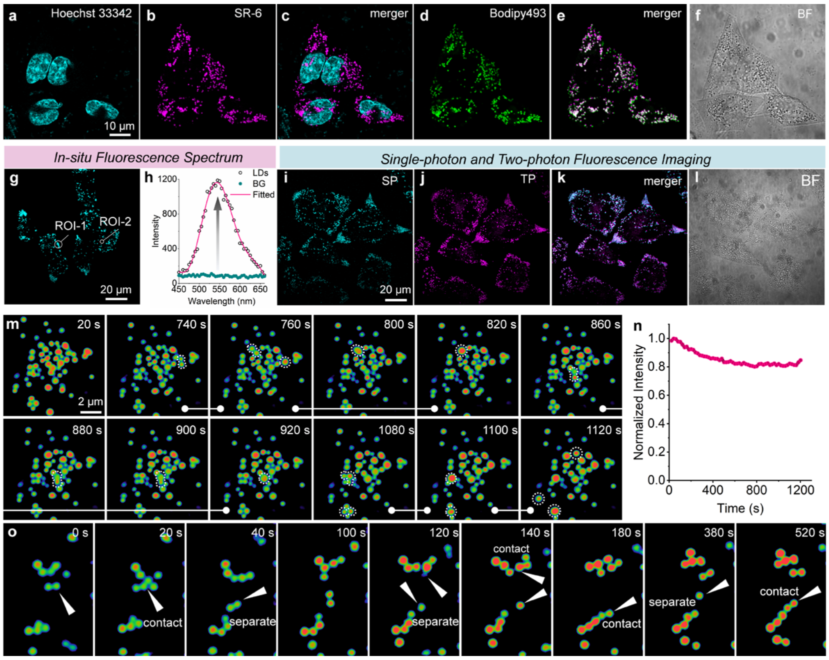

图 3. 本工作中所报道的 SR 荧光分子用于活细胞中脂滴的动态成像。

Figure 3. Wash-free imaging of lipid droplets (LDs) in live cells using SR fluorophores.

biosynthesis. This innovation provides a powerful tool for bacterial research and antibiotic development. Additionally, the compact molecular size of these dyes permits penetration into microcavities (e.g., molecular sieves), opening new possibilities for materials science and 3D imaging.

This study not only resolves the long-standing contradiction between small molecular size and long emission wavelengths in fluorophore design but also expands the frontiers of bioimaging through precision molecular engineering. With further optimization and application exploration, these compact NIR fluorophores hold promise for advancing scientific research and clinical diagnostics. Although improvements in molar absorption coefficients and functionalization are still needed, the universal applicability of this design paradigm establishes a new framework for the rational development of functional fluorescent probes.

By overcoming the technical bottleneck of reconciling compact molecular dimensions with NIR emission, this work pioneers an innovative pathway for high-resolution bioimaging. As performance enhancements and application scenarios evolve, these ultra-compact NIR fluorophores are poised to become pivotal tools in life science research and precision clinical diagnostics. While challenges in boosting molar absorptivity and functional modifications persist, the proposed iterative design strategy—guided by quantum chemical calculations—offers a transformative paradigm for the rational design of function-oriented fluorescent dyes.

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Generation, Capture, Storage, and Release of Singlet Oxygen from a Perylene Diimide-Based Metallacage for Oxygen Sensing

Dr. Yali Hou, Yingjie Li, Dengke Han, Dr. Zeyuan Zhang, Dr. Jinping Zhang, Shijin Jian, Zixuan Li, Prof. Dr. Xianglong Duan, Prof. Dr. Haonan Peng, Prof. Dr. Yu Fang, Prof. Dr. Mingming Zhang

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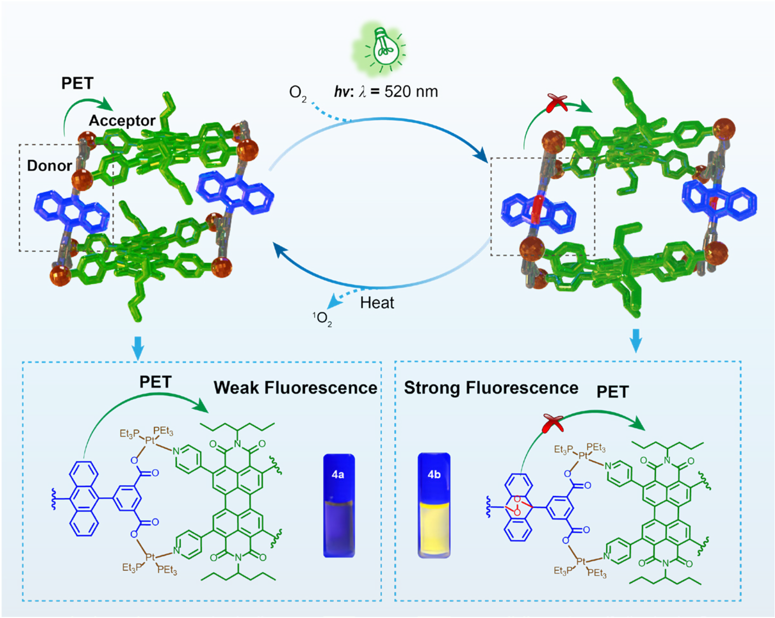
基于苝二酰亚胺金属笼在氧传感中实现单线态氧的生成、捕获、存储与释放

Yali Hou+, Yingjie Li+, Dengke Han+, Zeyuan Zhang, Jinping Zhang, Shijin Jian, Zixuan Li, Xianglong Duan*, Haonan Peng*, Yu Fang, and Mingming Zhang*. Angew. Chem. Int. Ed. 2025, e202507112. DOI: 10.1002/anie.202507112.



单线态氧 ($^1O_2$) 作为分子氧的激发态，凭借其强氧化性和高反应活性，在光动力疗法(通过选择性破坏癌细胞)、工业废水处理(降解有机污染物)及光催化氧化合成等领域展现出重要价值。然而，$^1O_2$ 的极短寿命(微秒级)和高扩散性使其难以直接捕获和存储，限制了其可控利用。传统内过氧化物 (EPOs) 虽可存储 $^1O_2$，但稳定性差且需额外光敏剂生成 $^1O_2$。金属有机框架 (MOFs) 已实现 $^1O_2$ 的可控释放，但分子级金属笼体系尚未突破。相比之下，金属笼 (metallacages) 作为分子级超分子容器，兼具结构精确性和动态响应性，有望通过模块化设计将光敏、捕获、存储与释放功能集成于单一体系，为 $^1O_2$ 的精准操控及多功能应用提供全新平台。

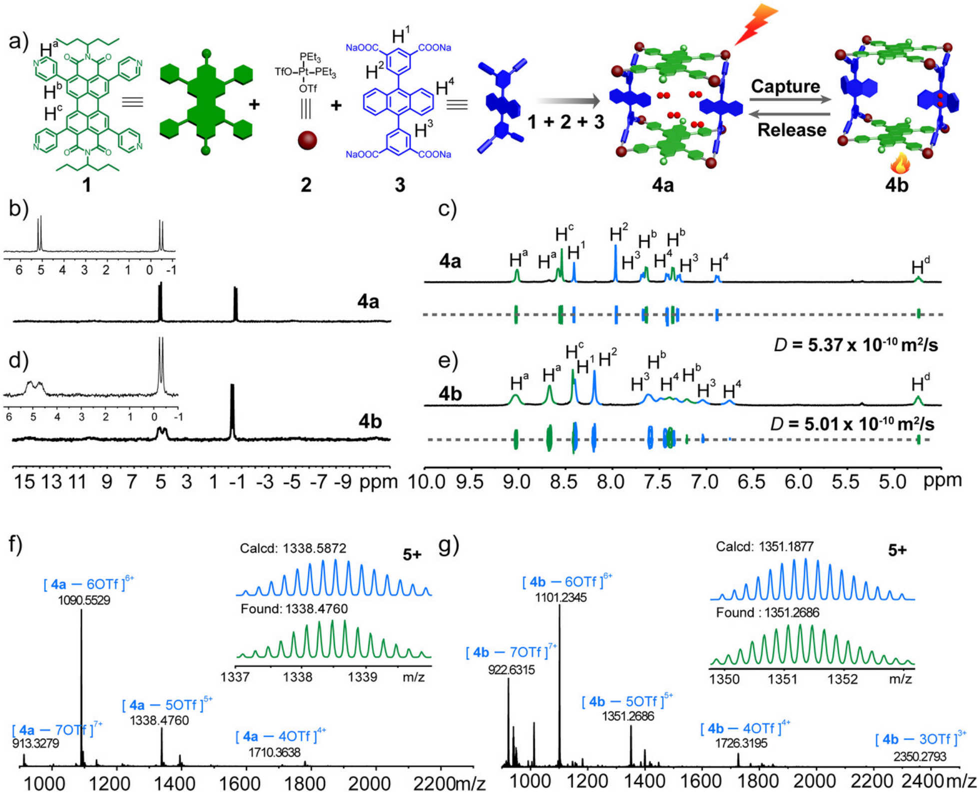


图 1. PDI 基金属笼 4a 的自组装及其过氧化生成金属笼 4b 的过程。

Figure 1. Self-assembly of PDI-based metallacage 4a and its peroxidation to metallacage 4b.

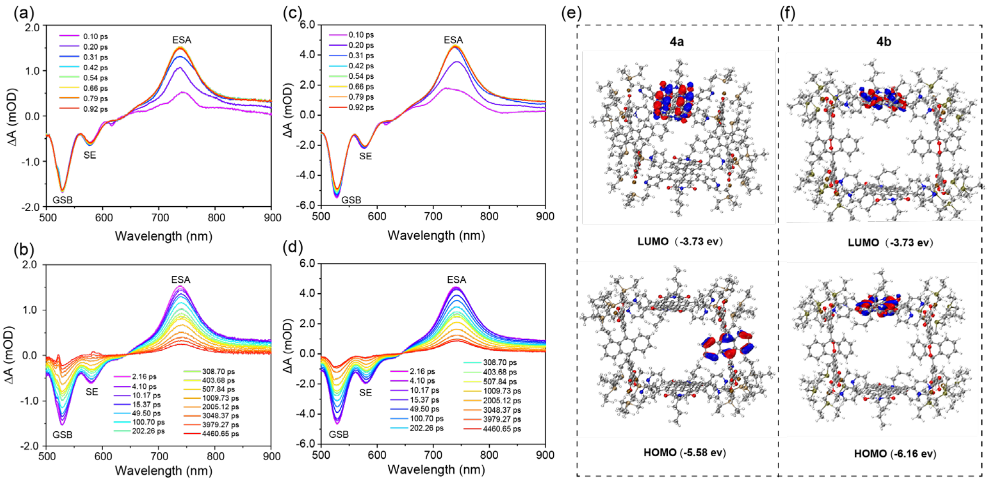


图 2. PDI 基金属笼 4a 和 4b 的 fs–TA 光谱及 HOMO–LUMO 计算能级分布图。

Figure 2. fs-TA spectra and diagram of the HOMO–LUMO calculated energy profiles of 4a and 4b.

本研究采用四吡啶花二酰亚胺 (PDI) 和四羧酸蒽分子作为功能基元，通过多组分配位组装构建了高对称性桶状金属笼 4a。其中，PDI 平面作为高效光敏剂，在光照下通过系间窜越激活氧气生成 $^1O_2$；同时，蒽基羧酸柱作为 $^1O_2$ 捕获位点，与其反应生成稳定的内过氧化物金属笼 4b。X 射线单晶衍射证实，两种金属笼在室温下均保持高度稳定的刚性结构，且在加热时 $^1O_2$ 可定量释放并恢复 4a 原始结构，实现动态循环。通过飞秒瞬态吸收 (fs–TA) 和密度泛函理论 (DFT) 分析，揭示了蒽羧酸柱到 PDI 的光致电子转移 (PET) 路径，证明 4a 中电子转移导致 PDI 荧光淬灭，而 4b 因内过氧化物阻断 PET 过程，恢复强荧光特性。

金属笼的荧光特性与 $^1O_2$ 状态紧密关联：4a 因 PET 作用仅显示微弱发射，而 4b 因 PET 抑制呈现明亮荧光。这种可逆的荧光“开关”行为使 4a 能够作为灵敏的溶解氧探针，其检测限达 1.1×10^{-3} mg/L，并可通过荧光强度实时监测氧浓度变化。此外，金属笼的循环性能与结构稳定性保障了其在重复光照–加热过程中的功能一致性，并首次在分子笼体系中实现了 $^1O_2$ 生

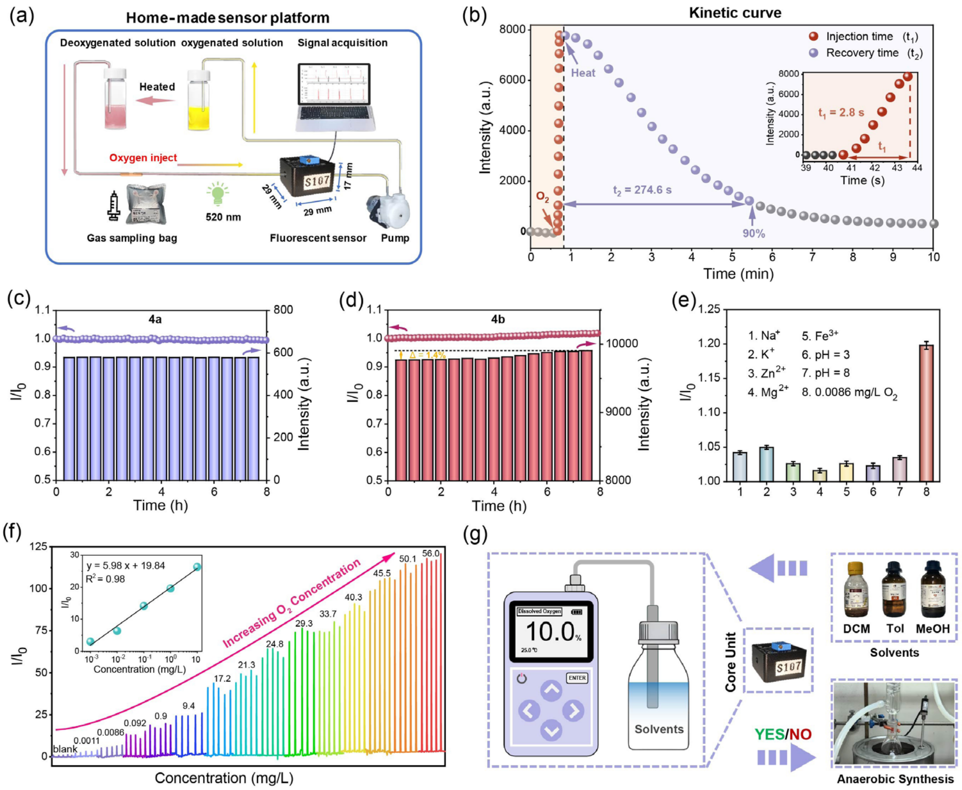


图 3. 荧光传感器的超低溶解氧检测性能。

Figure 3. Sensing performance of the PDI-based sensor for trace dissolved oxygen detection.

成、捕获、存储与释放的全过程集成。该设计不仅为精准调控 $^1O_2$ 动力学提供了模型体系，还通过整合光敏、储能与荧光响应的多功能特性，推动了动态智能材料在环境传感与生物医学等领域的应用创新。

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Singlet oxygen ($^1O_2$), an excited state of molecular oxygen, is widely used in photodynamic therapy, wastewater treatment, and photocatalytic oxidation due to its oxidative properties. However, its short lifetime and challenges in controlled storage/release limit practical applications. Aromatic compounds like anthracene derivatives react with $^1O_2$ to form endoperoxides (EPOs) for reversible storage, but their instability and poor solubility hinder optimization. Additionally, external photosensitizers are often required to generate $^1O_2$. Integrating $^1O_2$ generation, capture, storage, and release into a single system remains critical for advancing applications.

Coordination-driven self-assembly allows precise construction of supramolecular architectures, such as metal-organic frameworks (MOFs), which enable controlled $^1O_2$ release. However, molecular metallacages have not yet achieved this functionality. Metallacages could combine $^1O_2$ dynamics with optical properties for real-time monitoring, but integrating photosensitizers and EPO precursors into a single cage requires precise ligand design.

Here, we design a box-shaped metallacage (4a) via self-assembly of tetrapyridyl perylene diimide (PDI) and tetracarboxylate anthracene. Upon irradiation, PDI generates $^1O_2$, which reacts with anthracene pillars to form peroxidized metallacage 4b, storing $^1O_2$. Heating releases $^1O_2$ and regenerates 4a, confirmed by X-ray diffraction. Photoinduced electron transfer (PET) from anthracene to PDI in 4a quenches fluorescence, while peroxidation in 4b inhibits PET, restoring emission.

This reversible emission change enables the metallacage to function as a “turn-on” fluorescence sensor for dissolved oxygen, with a detection limit of 1.1×10^{-3} mg/L. This study demonstrates a metallacage that can generate, capture, store, and release $^1O_2$ for oxygen sensing, offering insights for designing stimuli-responsive smart materials.

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Functional Thin Films: From Interfacial Preparation to Applications

Yan Luo, Xiaoyan Liu,* and Yu Fang*

功能薄膜：从界面制备到应用

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界面聚合法（IP）制备的功能薄膜因其独特的结构特点和巨大的应用潜力而备受关注。这些薄膜通常在气－液、液－液界面上制备，界面的限域效应创造了有利于聚合和薄膜形成的独特环境。在气－液界面聚合（ALIP）过程中，反应单体在缩聚之前在界面自组装，允许材料的受限生长。通过合理的选择构筑单元、调节单体浓度和反应时间，可以制备出大面积、自支撑、无缺陷、厚度和孔隙率可调的几十到几百纳米厚度的薄膜。这些薄膜具有很强的粘附性、优异的机械稳定性，在分离技术、光学、催化和环境保护方面的发挥着重要的作用。液－液界面聚合（LLIP）进一步扩大了可用于薄膜制备的构筑单元的可选择性。两种互不相溶的液体之间的界面为处于两相的反应分子提供了一个理想的反应平台，促进了具有丰富孔隙率的，大面积、均匀、自支撑薄膜的生长。薄膜的物理化学性质可以通过对构筑单元分子结构的理性设计、调控单体浓度和反应时间来实现调控，这将推动功能薄膜的制备和应用。

本综述介绍了我们课题组通过 ALIP 和 LLIP 方法在功能薄膜制备和应用方面取得的最新研究进展。首先讨论了通过希夫碱和 Katritzky 反应制备多种具有特定性能的薄膜。此外，介绍了薄膜在荧光和比色传感、吸附、分离、催化、软致动器、柔性表面增强拉曼散射（SERS）衬底和非线性光学（NLO）等方面的应用。最后，针对目前高性能薄膜制备和应用所面临的挑战，对界面限域方法制备薄膜的未来研究方向进行了展望，旨在推动具有独特物理化学性质的薄膜的创新。

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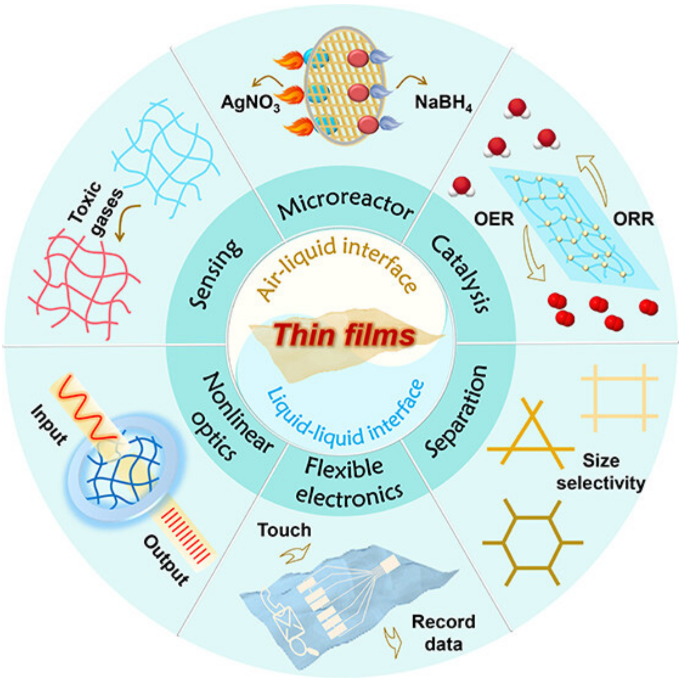

图 1. 功能性纳米膜的制备及其应用
Figure 1. Preparation and application of functional thin films

Functional thin films prepared through interfacial polymerization (IP) have garnered significant attention due to their unique structural characteristics and wide-ranging application potential. These films are typically fabricated at air–liquid or liquid–liquid interfaces, which create distinctive environments conducive to polymerization and thin film formation. In the air-liquid interfacial polymerization (ALIP) process, reactive monomers self-assemble at the interface prior to polycondensation, allowing for the confined growth of two-dimensional materials. By carefully adjusting the monomer concentration, building block structure, and reaction time, it is possible to produce large-area, freestanding, defect-free thin films with a tunable thickness and porosity.

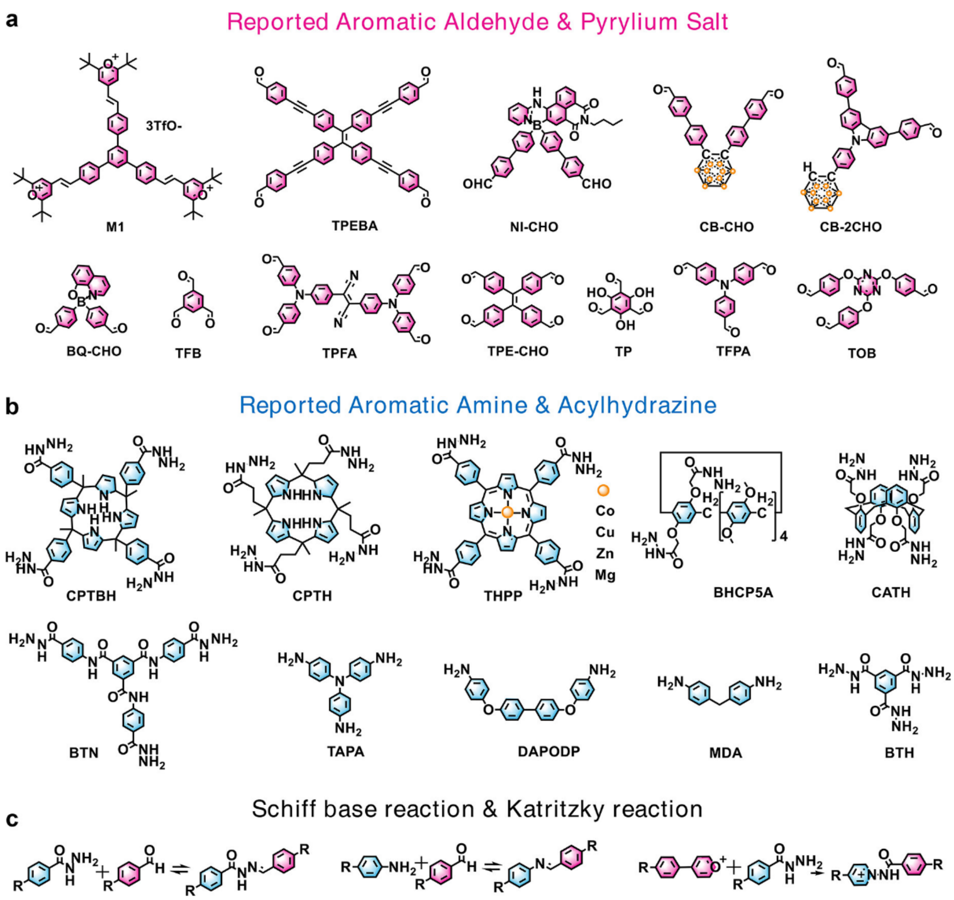

图 2. 制备薄膜的典型分子单元：(a) 醛和吡啶盐单体，(b) 氨基和肼单体，(c) 通过希夫碱和 Katritzky 反应制备薄膜的典型反应

Figure 2. Typical molecular building blocks in the fabrication of thin films: (a) Aldehyde and pyrylium salt monomers, (b) amino and hydrazide monomers, and (c) typical linkage bonds of the thin films prepared through Schiff base and Katritzky reactions.

These thin films exhibit strong adhesion, flexibility, and geometric continuity, making them particularly suitable for advanced applications in separation technologies, soft optics, catalysis, and environmental protection. Liquid–liquid interfacial polymerization (LLIP) further expands the range of building blocks available for thin film preparation. The interface between two immiscible liquids provides an ideal platform for reactive molecules residing in different phases to interact, facilitating the growth of large-area, uniform, free-standing films with extensive porosity. The properties can be finely controlled by varying the building block structure, monomer concentration, and reaction time, highlighting their potential for scalable production of functional thin films. The IP method effectively addresses challenges in thin film production such as substrate effects and mass transfer limitations, thereby enhancing the sensitivity and reliability of high-performance films. These advantages underscore the pivotal role of IP in the development of multifunctional thin films, offering distinct benefits over conventional top-down or bottom-up synthesis methods.

This Account presents recent research advancements achieved by our group in developing functional thin films via ALIP and LLIP. We first explore the preparation of various thin films with specific properties through Schiff base and Katritzky reactions. We then discuss their applications in fluorescence and colorimetric sensing, adsorption, separation, catalysis, soft actuators, flexible surface-enhanced Raman scattering (SERS) substrates, and nonlinear optics (NLO). Finally, we address the current challenges in developing interfacially confined films and propose future research directions aimed at advancing the innovation of thin films with unique physicochemical properties.

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Separate Control Model for Tailoring Ultralong Organic Room-Temperature Phosphorescence with Highly Efficient Energy Transfer to Rhodamine B

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基于分离调控模型定制超长有机室温磷光材料以及与罗丹明 B 的高效能量转移研究

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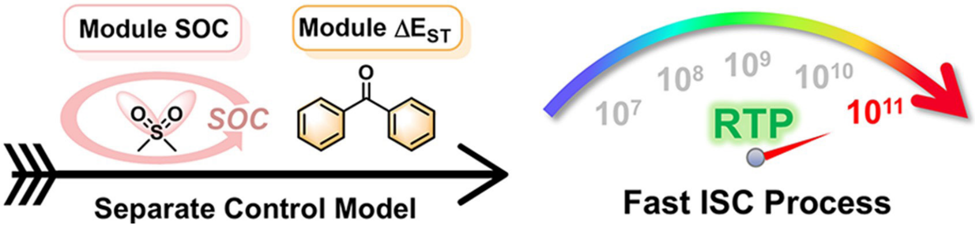

有机室温磷光（RTP）材料在光电显示、生物成像和防伪加密等领域展现出重要的应用价值，然而获得高效 RTP 分子仍然具有很大的挑战性。较大的旋轨耦合常数和较小的能差可以促进系间窜跃（ISC）过程的发生，但是同时实现比较困难。本研究提出“分离调控模型”，通过独立优化 SOC 和 ΔEST，实现对两个关键参数的精准调控。为了获得高效的 RTP 分子，通过将不同的给体与受体进行组合，构成了 D-A 分子数据集，并结合密度泛函理论（DFT）与高精度多参考态微扰理论进行高通量筛选，确定出磷光候选分子 PPTZO-CO。

本研究也系统考察了前驱体 PPTZ-CO 的光物理性质，并与 PPTZO-CO 进行对比分析。PPTZO-CO 表现出 RTP 特性，而 PPTZ-CO 仅为常规的荧光分子。通过飞秒瞬态吸收光谱（fs-TAS）对两种化合物薄膜的激发态动力学进行分析，PPTZO-CO 薄膜在 ps 尺度范围内即可观测到明显的 ISC 过程；对于 PPTZ-CO 薄膜，仅观察到单重激发态（S1）的吸收（550 nm）与辐射衰减过程，未检测到三重态相关信号，与荧光分子特性一致。

为了更深入地了解两种化合物激发态的弛豫路径，我们选取相同的活化空间 CASPT2//CASSCF（8e/7o）进行理论计算，揭示了 PPTZ-CO 和 PPTZO-CO 的光物理性质和 ISC 速率。PPTZO-CO 的 SOC 比 PPTZ-CO 高 6 倍，同时 kISC 从 1.4 × 108 s–1 增加到 5.6 × 1011 s–1。而且，通过测定 PPTZ-CO 和 PPTZO-CO 的 2- 甲基四氢呋喃溶液在 77 K 时的稳态光谱和延迟光谱，准确测定了 S1 及 T1 能级。PPTZ-CO 和 PPTZO-CO 的 ΔEST 分别为 0.38 eV 和 0.55 eV。尽管 ΔEST 增加，但 SOC 值没有显著降低。这一实验结果验证了我们提出的分离调控模型策略，证实了该模型能够突破传统设计限制，成功实现 RTP 性能的精准调控。

而且，当将磷光单元 PPTZO-CO 掺杂在聚甲基丙烯酸甲酯（PMMA）时，表现出光激活室温磷光的性质，其磷光寿命可达 700 毫秒。由于 PPTZO-CO@PMMA 的磷光光谱与 RB 的吸收光谱存在很大程度的重叠，可以作为

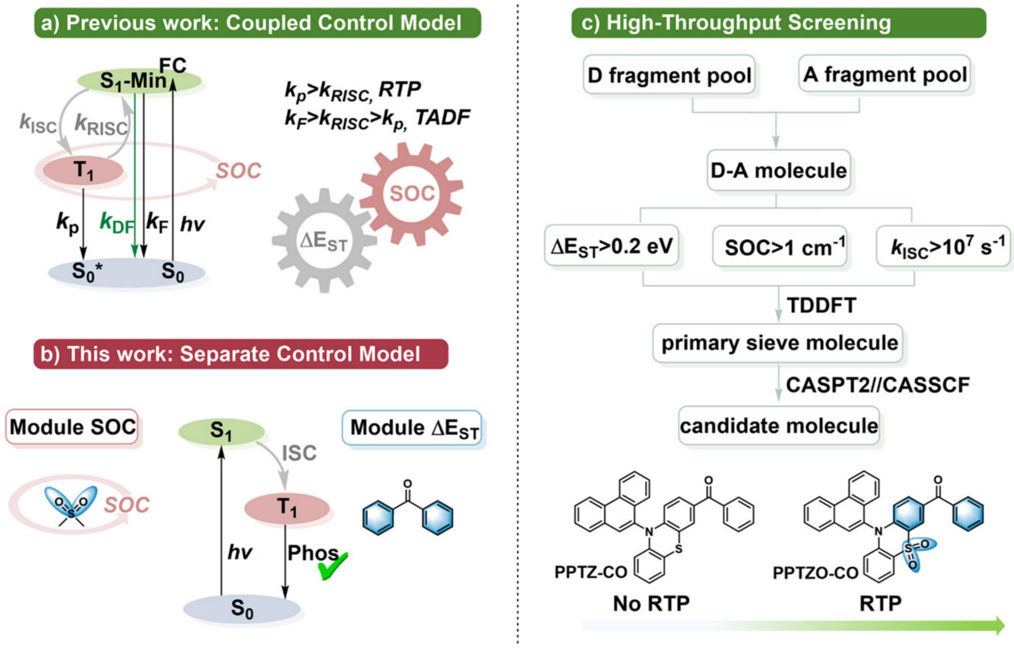

图 1. a) 传统的耦合调控模型（之前的工作）：同时调控 SOC 和 ΔEST，导致这两个参数相互影响。b) 提出的分离调控模型策略（本研究）：图示展示了本研究采用的新策略，其中 SOC 和 ΔEST 通过分离调控模型进行独立优化，从而能够更精确地调控这两个参数以实现 RTP。c) 高通量筛选过程及结果：流程图展示了根据 D–A 分子的 SOC、ΔEST 及 kISC 的高通量筛选过程，从而确定出潜在的 RTP 候选分子，包括 PPTZO–CO 单元。

Figure 1. a) Typical coupled control model (previous work): Illustration of the conventional approach where the SOC and ΔEST are controlled simultaneously, leading to interdependent modulation of both parameters. b) Proposed separate control model strategy (this work): Diagram depicting the novel strategy employed in this study, where SOC and ΔEST are independently optimized through separate control model, allowing for more precise tuning of both parameters to achieve RTP. c) High-throughput screening process and results: Flowchart illustrating the process of high-throughput screening used to evaluate the SOC and ΔEST of various D-A molecules, leading to the identification of promising RTP candidates, including the PPTZO-CO unit. Results of the screening process are also summarized, showcasing the efficiency of the proposed strategy.

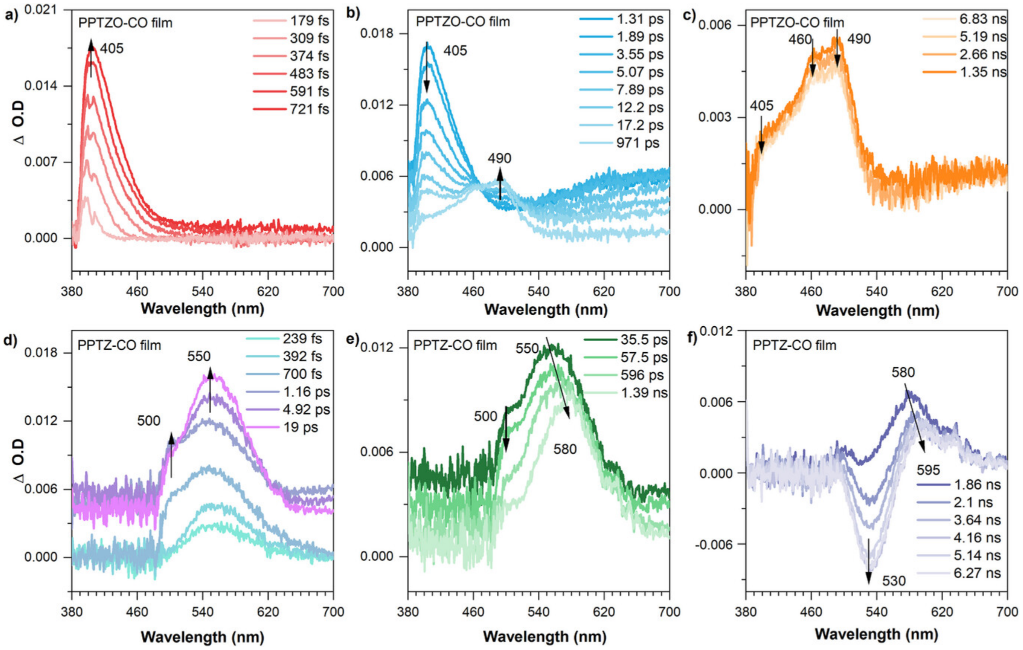

图 2. a–c) PPTZO–CO 薄膜和 d–f) PPTZ–CO 薄膜的瞬态吸收（λ ex=330 nm）。

Figure 2. fs-TA spectra for thin film of a-c) PPTZO-CO and d-f) PPTZ-CO under the excitation of 330 nm at room temperature.

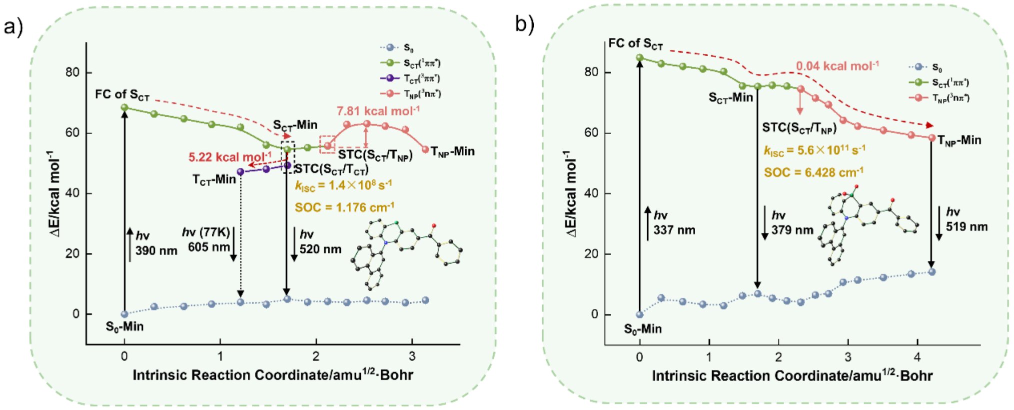

图 3.（a）PPTZ–CO 和（b）PPTZO–CO 的最低能量势能面。计算结果基于 CASPT2//IRC/CASSCF(8e/7o) 理论水平获得。
Figure 3. Minimum-energy profiles for the a) PPTZ-CO and b) PPTZO-CO. These computational results were obtained at the CASPT2//IRC/CASSCF (8e/7o) level of theory.

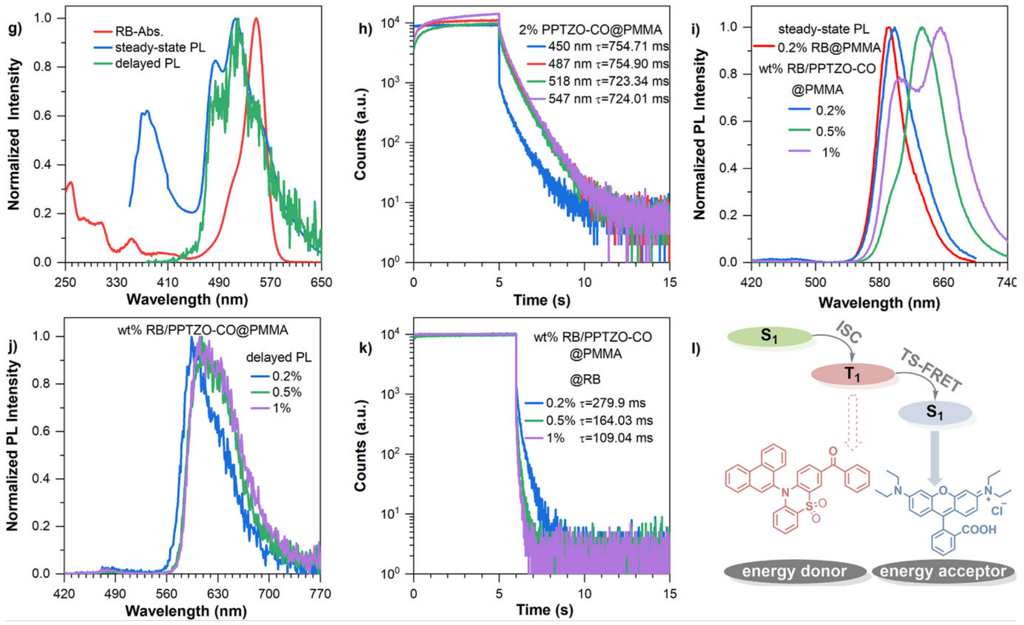

图 4. g) 2% PPTZO–CO@PMMA 薄膜的稳态光谱（λ ex = 330 nm）与延迟光谱（λ ex = 365 nm），罗丹明 B（RB）在乙醇溶液中的紫外 – 可见吸收光谱。h) 2% PPTZO–CO@PMMA 薄膜的磷光寿命。i) 0.2% RB@PMMA 的稳态光谱（λ ex = 520 nm）与不同含量 RB/PPTZO–CO@PMMA 的稳态光谱（λ ex = 365 nm）。j) RB/PPTZO–CO@PMMA 掺杂薄膜的延迟光谱（λ ex = 365 nm）。k) RB/PPTZO–CO@PMMA 薄膜的时间分辨光谱曲线。l) 基于共振能量转移机制的罗丹明 B 持久发光示意图。
Figure 4. g) Steady-state (λex = 330 nm) and delayed PL (λex = 365 nm) spectra of 2% PPTZO-CO@PMMA, UV-vis spectrum of RB in CH3CH2OH. h) Time-resolved delayed PL decay spectra of 2% PPTZO-CO@PMMA film. i) Steady-state PL spectra of 0.2% RB@PMMA (λex = 520 nm) and wt% RB/PPTZO-CO@PMMA (λex = 365 nm). j) Delayed PL spectra of wt% RB/PPTZO-CO@PMMA (λex = 365 nm). k) Time-resolved delayed PL decay spectra of wt% RB/PPTZO-CO@PMMA film; l) Schematic diagram of RB persistent luminescence through phosphorescence resonance energy transfer. All measurements were conducted at room temperature.

一种潜在的能量给体。当在 PPTZO–CO@PMMA 中掺杂罗丹明（RB）时，PPTZO–CO@PMMA 的磷光峰几乎消失，观察到的是红色余晖，其能量转移效率接近 100%。而且，PPTZO–CO@PMMA 薄膜在动态防伪领域表现出很大的应用潜力，其对温度比较敏感，加热至 120℃时磷光淬灭，冷却后恢复肉眼可见的绿色余晖；薄膜在水相环境中发光仍然保持稳定，适用于多重加密防伪。

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Organic room-temperature phosphorescence (RTP) materials demonstrate significant application

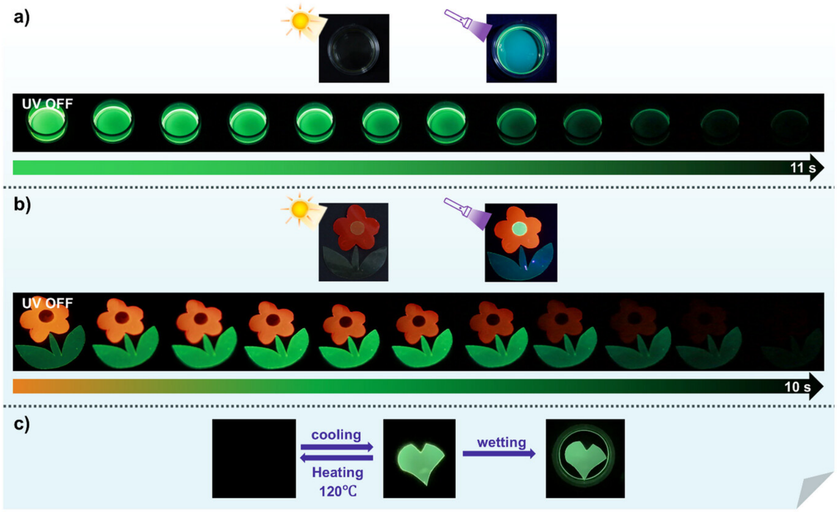

图 5. 掺杂 PMMA 防伪体系的潜在应用。a) PPTZO−CO@PMMA 在玻璃培养皿中于日光下、紫外灯开启和紫外灯关闭状态下的照片；b) 由 PPTZ−CO@PMMA（花蕊）、0.2% RB@PPTZO−CO@PMMA（花瓣）和 2% PPTZO−CO@PMMA（托叶）组成的花卉在日光下、紫外灯开启和紫外灯关闭状态下的照片；c) 紫外灯关闭状态下 PPTZO−CO@PMMA 的温度和水相相应 RTP。当加热到 120 ° C 时，余辉完全消失。
Figure 5. Potential applications of doping PMMA systems for anti-counterfeiting. a) Photographs of PPTZO-CO@PMMA in a glass petri dish at room temperature under daylight, UV on and UV-OFF state; b) Photographs of pattern of the flower, which is composed of PPTZ-CO@PMMA (stamens), 0.2% RB@PPTZO-CO@PMMA (petals), and 2% PPTZO-CO@PMMA (stipules) at room temperature under daylight, UV on and UV-OFF state, respectively; c) Reversible temperature and wetting-responsive RTP of PPTZO-CO@PMMA under UV-OFF state. The afterglow completely disappears when heated to 120 °C.

potential in optoelectronic displays, bioimaging, and anti-counterfeiting encryption. However, achieving high-performance RTP molecules remains challenging. Larger spin-orbit coupling (SOC) values and smaller ΔEST are more prone to ISC processes, but it is difficult to achieve both simultaneously. This study proposed a “separate control model” strategy that independently optimizes SOC and ΔEST to achieve precise control over these two critical parameters. To develop efficient RTP molecules, a comprehensive dataset of donor-acceptor (D-A) structured molecules is developed using D and A fragment pools. Promising phosphorescent candidates PPTZO-CO can be efficiently identified through high-throughput screening that combines density functional theory (DFT) with high-precision multireference perturbation theory calculations.

This study systematically investigated the photophysical properties of the precursor PPTZ-CO in comparison with PPTZO-CO. While PPTZO-CO exhibits RTP characteristics, PPTZ-CO demonstrates only conventional fluorescence behavior. The excitation-state dynamics of the two compounds were analyzed by femtosecond transient absorption spectroscopy (fs-TAS). Obvious intersystem crossing (ISC) processes could be observed in the PPTZO-CO film within the ps scale range. For the PPTZ-CO film, only the absorption (550 nm) and stimulated emission signal of the single excited state (S1) were observed, and no triplet state-related signals were detected, which were consistent with the characteristics of fluorescent molecules.

To gain deeper insight into the photophysical properties of PPTZ-CO and PPTZO-CO, theoretical calculations were performed using the CASPT2//CASSCF (8e,7o) method. These theoretical investigations into PPTZ-CO and PPTZO-CO reveal their distinct photophysical properties and the efficiency of their ISC processes, which are characterized by significant SOC values and rapid transition rates. The SOC of PPTZO-CO is 6 times higher than that of PPTZ-CO, accompanied by a dramatic increase in kISC from 1.4×108 s-1 to 5.6×1011 s-1, consistent with the ISC process of 6.7 ps in TAS. The steady-state and delayed spectra of PPTZ-CO and PPTZO-CO in 2-methyltetrahydrofuran solution at 77 K were measured to accurately determine the S1 and T1 energy levels. The ΔEST of PPTZ-CO and PPTZO-CO were found to be 0.38 and 0.55 eV, respectively. These findings highlight a crucial observation: despite the increase in ΔEST, there was no significant reduction in the SOC value. This observation represents the first detailed experimental confirmation of our proposed strategy, demonstrating the successful utilization of the separate control model to effectively achieve RTP.

When PPTZO-CO was doped into polymethyl methacrylate (PMMA), the doped systems exhibit photoactivated RTP property with long lifetime up to 700 ms. In the case of PPTZO-CO@PMMA, its phosphorescence spectrum shows a substantial overlap with the absorption spectrum of rhodamine B (RB), suggesting the potential for effective energy transfer. When 0.2% RB was incorporated into the PPTZO-CO@PMMA film, the emission exhibited only a red afterglow with energy transfer efficiency approaching 100%. Moreover, PPTZO-CO@PMMA film shows practical application potential in the field of dynamic anti-counterfeiting. It is sensitive to temperature. When heated to 120℃ , it undergoes phosphorescent quenching and regains a visible green afterglow to the naked eye upon cooling. The film remains stable in luminescence in an aqueous environment and is suitable for multiple encryption anti-counterfeiting.

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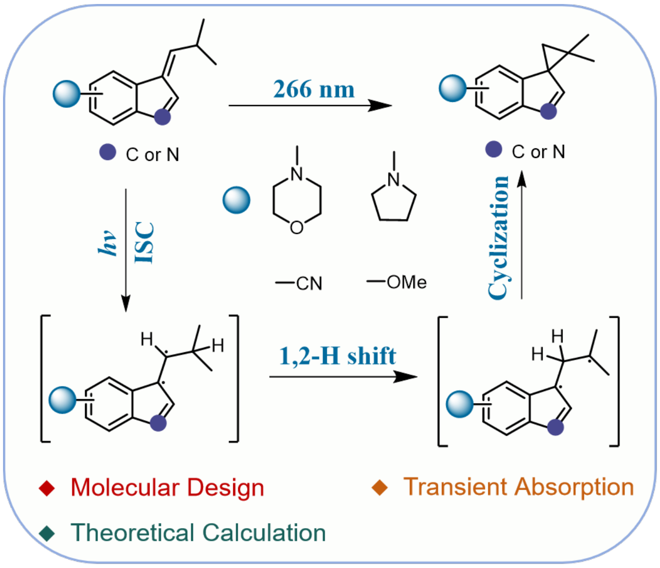
Rational Design and Reaction Mechanism Study of the Photochemical Rearrangement of Fulvene Derivatives

Shuang Xu, Tianhe Yang, Shu-Lin Zhang, Yifan Su, Yang Cheng, David Lee Phillips, Le Yu*, Jiani Ma*, and Yu Fang

富烯衍生物光化学重排的合理设计与反应机理研究

Shuang Xu, Tianhe Yang, Shu-Lin Zhang, Yifan Su, Yang Cheng, David Lee Phillips, Le Yu*, Jiani Ma*, and Yu Fang. J. Phys. Chem. Lett. 2025 DOI: https://doi.org/10.1021/acs.jpclett.5c00720



光化学是有机合成中最高效、可重复的技术之一。近期，List 及合作者报道了一种由不同取代基的富烯光化学合成螺[2,4]庚二烯的方法（Angew. Chem. Int. Ed. 2023, 62, e202303119）（图 1B）。为了促进这一新型光化学反应的应用，我们从理论上设计了系列具有不同母体分子骨架的富烯衍生物分析其取代效应，并合成了其中两种具有代表性的富烯分子，利用时间分辨瞬态吸收光谱和激发态理论计算研究反应机理。研究发现，要对所研究的富烯进行可靠的理论表征，必须使用二阶 n 电子价态扰动理论来代替密度泛函理论。光反应产物分析表明，我们设计的富烯会发生光重排环丙烷化反应。利用瞬态吸收光谱分析了参与光重排反应中分子内氢原子转移和环化过程的中间产物，并提出了完整的反应途径。我们的工作不仅揭示了该光重排反应的详细机理，还证明了适当的理论方法对于合理分子设计的重要意义。

本研究利用理论计算对 34 个候选分子进行合理设计和筛选后（图 2），成功合成了两个新的富烯分子 1 和 31。理论分析表明，对于带有 –MOP 和 –THP 取代基的衍生物 DFT/TDDFT 筛选并不准确，证实了在合理设计其他具有类似分子骨架的光化学反应时使用 NEVPT2/CASSCF 计算的必要性。

借助超快光谱技术和高水平的 ab initio 计算，确定了这两种分子的详细光重排机理。实验检测到了底物的三重态和参与分子内 HAT 过程的双自由基中间体。计算结果表明，当分子被激发到单线激发态后，在三线态发生 HAT 的能垒过高，因此在 ISC 点附近发生 HAT 过程，之后环化生成产物。不同的是，31 的 HAT 过程能垒比 1 高 13.7 kcal mol^{-1}，1 与 31 的反应速率常数比为 $k_1/k_{31}=74.4$。其次，31（$3.03 \times 10^5\ s^{-1}$）的 ISC 反应速率常数小于 1（$1.73 \times 10^8\ s^{-1}$），这些结果表明 31 的反应速率较慢。

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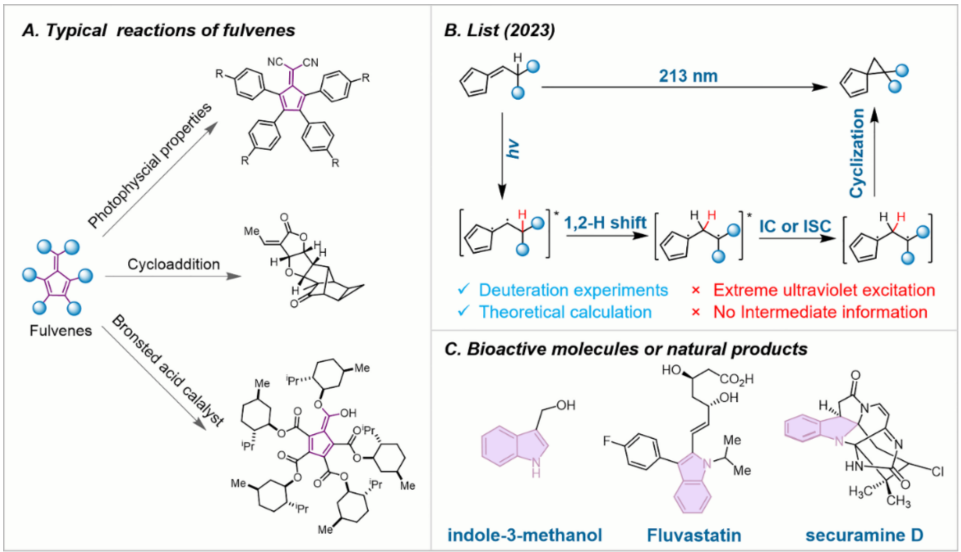

图 1.（A）富烯类化合物的典型反应实例，（B）List 提出的富烯的光重排机理；（C）含杂环的药物和天然产物分子。

Figure 1. (A) Examples of typical reactions of fulvenes, (B) proposed photo-rearrangement mechanism for the fulvenes by List, (C) heterocyclic-containing drug and natural product molecules.

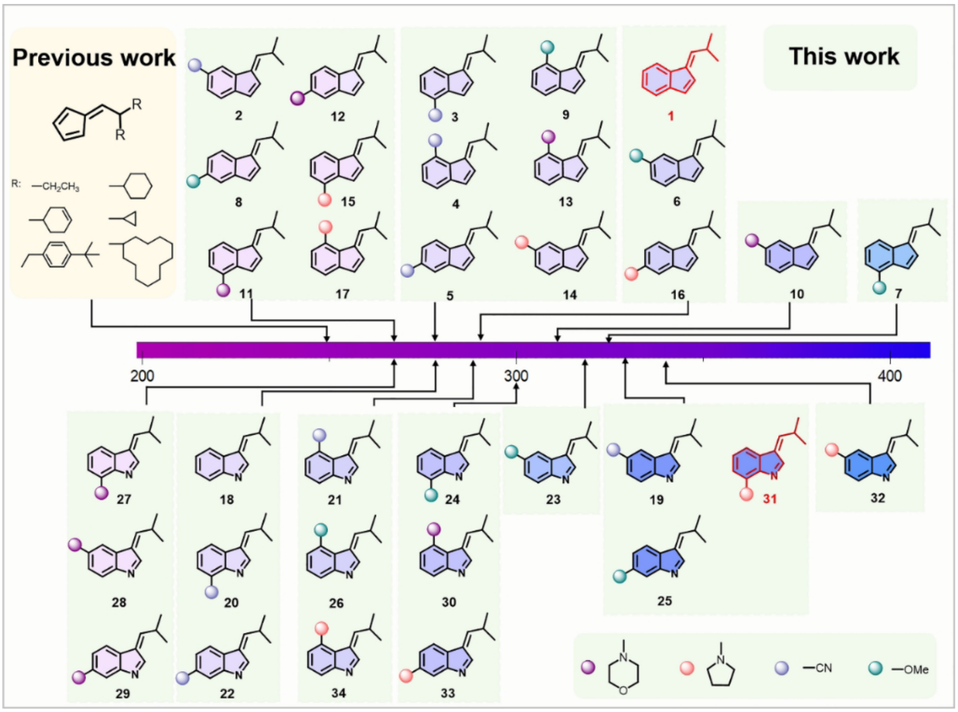

图 2. 由 NEVPT2(8,8)/def2−TZVP//CASSCF(6,6)/6−31G(d) 计算的 34 种富烯分子的吸收光谱。

Figure 2. The structures of the screened fulvene molecules with electronic absorbance simulated by NEVPT2(8,8)/def2-TZVP//CASSCF(6,6)/6-31G(d).

Photochemistry is considered one of the most efficient and reproducible techniques in organic synthesis. Recently, List and co-workers reported an efficient UV light triggered photochemical synthesis of spiro[2,4]heptadiene from fulvenes with different substituents (*Angew. Chem. Int. Ed.* 2023, 62, e202303119); however, the mechanistic details remain unclear, and the intermediates have not been characterized. To facilitate the applications of this novel photochemical reaction, we theoretically designed a series of fulvene derivatives with different parent molecular skeletons for analyzing the substitution effects, and two of the representative fulvenes were synthesized for investigating the reaction

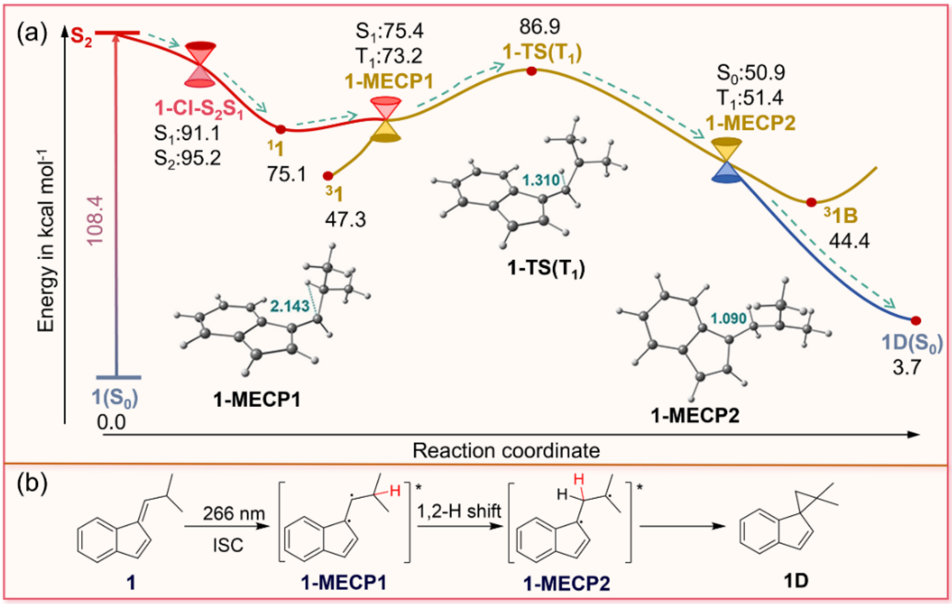

图 3. （a）在 NEVPT2(8,8)/def2−TZVP//CASSCF(6,6)/6−31G(d) 理论水平上计算的 1 的势能曲线（能量为 kcal mol−1，1(S0) 的基态能量作为估算相对能量的零能量，过渡态 1−TS(T1) 的几何形状通过 TDDFT 优化），1−MECP1 为 ISC 通道，（b）1 的光化学反应机理。

Figure 3. (a) Potential energy profile of 1 computed at NEVPT2(8,8)/def2-TZVP//CASSCF(6,6)/6-31G(d) level of theory (the energy is kcal mol-1 and ground state energy of 1(S0) was used as zero energy for estimating relative energies, the geometry of the transition state 1-TS(T1) was optimized by TDDFT) and ISC channels at 1-MECP1, (b) the proposed photochemical reaction mechanism of 1.

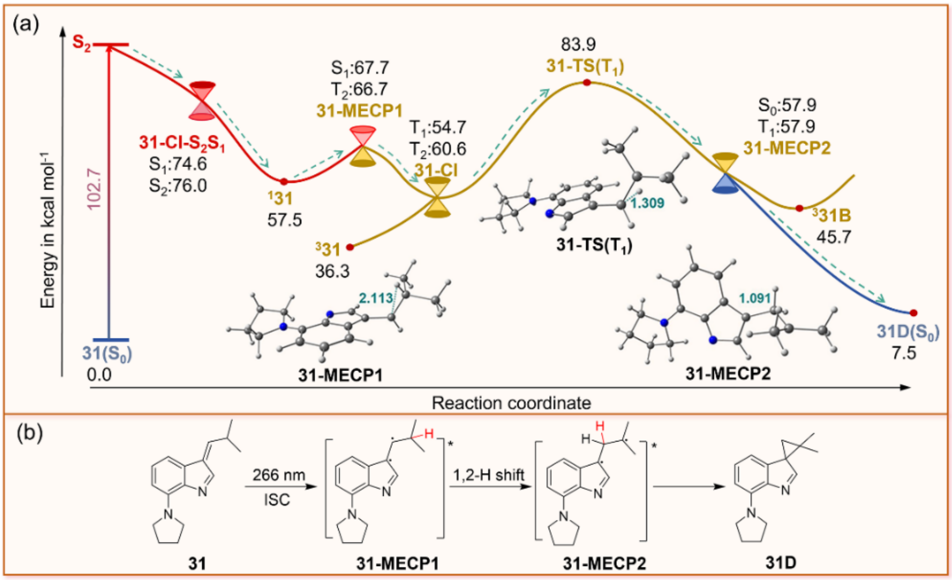

图 4. （a）在 NEVPT2(8,8)/def2−TZVP//CASSCF(6,6)/6−31G(d) 理论水平上计算的 31 的势能曲线（能量为 kcal mol−1，31(S0) 的基态能量作为估算相对能量的零能量，过渡态 31−TS(T1) 的几何形状通过 TDDFT 优化），31−MECP1 为 ISC 通道，（b）31 的光化学反应机理。

Figure 4. (a) Potential energy profile of 31 computed at NEVPT2(8,8)/def2-TZVP//CASSCF(6,6)/6-31G(d) level of theory (the energy is kcal mol-1 and ground state energy of 31(S0) was used as zero energy for estimating relative energies, the geometry of the transition state 31-TS(T1) was optimized by TDDFT) and ISC channels at 31-MECP1, (b) the proposed photochemical reaction mechanism of 31.

mechanisms by employing time-resolved transient absorption spectroscopy (TA) experiments. It has been found that instead of density functional theory, the second-order n-electron valence state perturbation theory is necessary to acquire reliable theoretical characterization of the fulvenes examined. Our designed fulvenes were found to undergo the photorearrangement cyclopropanation reaction on the basis of photoproduct analysis. The intermediate species involved in the intramolecular hydrogen atom transfer and cyclization processes within the photorearrangement reaction were characterized by TA spectroscopy, and the full reaction pathways were proposed. Our work not only reveals the detailed mechanism of this photorearrangement reaction but also demonstrates the significance of appropriate theoretical methods for rational molecular design.

After rational design and screening of 34 candidates using theoretical computations, two new fulvene molecules were successfully synthesized. The molecular design increases greatly, expanding the scope of spiro[2,4] heptadiene synthesis upon irradiation of ~300 nm. Moreover, the theoretical analysis reveals that for derivatives with −MOP and −THP substituents, the inaccuracy of the DFT/TDDFT screening for fulvenes with −MOP and −THP substitutions confirmed the necessity of utilizing NEVPT2/CASSCF computations in the rational design of other photochemical reactions with similar molecule backbones.

With the help of state-of-the-art ultrafast spectroscopies and high-level ab initio computations, the detailed photorearrangement mechanism was determined for both molecules. 1 and 31 follow a similar reaction mechanism to generate the photorearrangement product. The triplet state of the substrate and the diradical species involved in the intramolecular HAT process were directly detected experimentally. The calculation results show that after the molecule is excited to the singlet excited state, a HAT process occurs around the ISC point, followed by a cyclization to generate the product. On the other hand, it was found that the reaction rate of 31 was much slower, compared to that of 1. First, the energy barrier of the HAT process for 31 is 13.7 kcal mol^{-1} higher than that for 1, and the reaction rate constant ratio of 1 to 31 is calculated to be $k_1/k_{31} = 74.4$ using the Arrhenius formula. Second, the ISC rate constant for 31 (3.03×10^5 s^{-1}) is smaller than that for 1 (1.73×10^8 s^{-1}), further demonstrating the slower reaction rate of 31.

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Issue 10, 2025

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From the journal:
Analyst

Recent advances in active chromophores for detecting gamma-hydroxybutyric acid (GHB)-related illicit drugs

Check for updates

Chun Yang,[a] Hongxian Yang,[b] Zhen Yao*[a] and Taihong Liu *[c]

γ– 羟基丁酸毒品检测中光学活性物质的研究进展

Chun Yang, Hongxian Yang, Zhen Yao,* and Taihong Liu*. Analyst, 2025, 150, 1972-1985. DOI: 10.1039/D5AN00167F

涉毒问题对社会安定、公共安全和公共卫生造成的危害具有系统性和持续性，引起了社会各界日益广泛关注。随着近年来新型毒品犯罪手段不断迭代，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

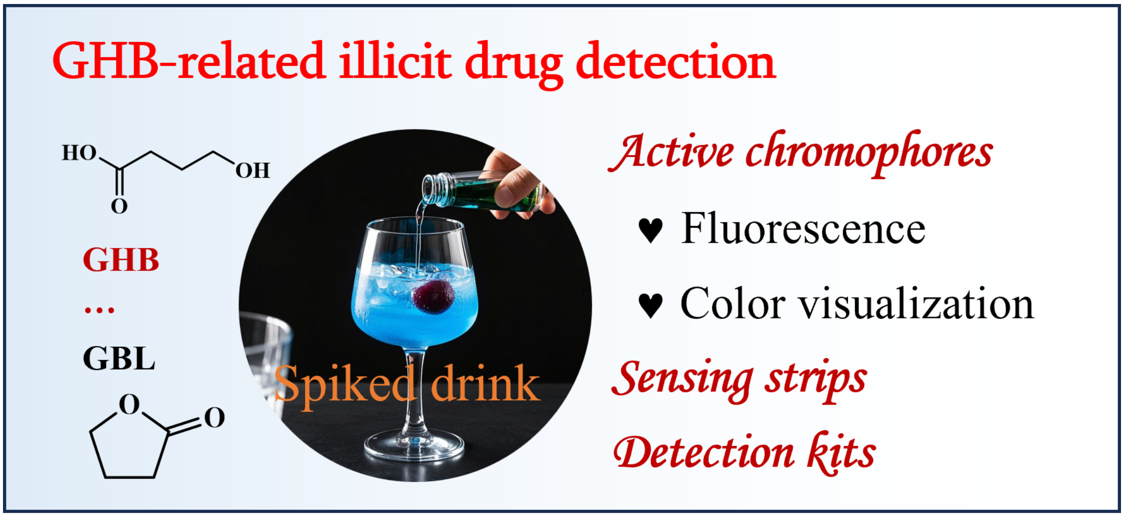

图 1. 本工作概述了 γ– 羟基丁酸（GHB）在人体内的内源性背景水平和可能的生物代谢途径，并总结了适用于 GHB 的光学活性检测物质的最新进展。

Figure 1. This minireview outlines the possible metabolism pathways of GHB in body and summarizes the recent advances of active chromophores.

速筛查的技术和装备，不仅是完善法医物证鉴定体系的关键环节，更是提升毒品犯罪打击效能的核心支撑。γ–羟基丁酸（GHB）及其衍生物作为典型的第三代合成毒品，具有强烈的中枢神经系统抑制作用，被我国列入《麻醉药品及精神药品品种目录》第一类精神药品严格管控。这类毒品在体内呈现代谢速度快、代谢产物多样性高以及有效检验窗口期短等特点，导致执法过程中样本采集、保存及检测面临严峻挑战。因此，开发适用于 γ–羟基丁酸及其衍生物的实时现场检测技术，已成为破解此类犯罪侦查取证难题的关键突破口。

基于荧光和比色原理的光学检测技术，凭借高灵敏度、高特异性、易于操作以及累积信号效应等多种技术优势，在新型毒品现场检测领域展现出独特应用价值。本文系统梳理了 γ–羟基丁酸在人体内的内源性背景水平和可能的生物代谢途径，总结了光学活性检测物质的最新进展，阐释了相应的传感特性，并举例说明了目前常见的光学传感试纸和检测试剂盒。此外，该工作还详细讨论了相关研究前景，以期为我国公安禁毒部门构建现代化毒品检测技术体系提供理论依据与实践参考。

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Gamma-hydroxybutyric acid (GHB) and its related illicit drugs are of particular forensic interest owing to their abuse as recreational drugs and implications in drug-facilitated sexual assault. The rapid and complete metabolism of GHB in the body results in a short evidence collection window for forensic experts, and challenges exist in simultaneously differentiating between exogenous addition in spiked drinking and low endogenous levels of GHB. Consequently, the development of real-time and on-site detection strategies for GHB plays vital roles in tackling drug-facilitated crimes. Recently, fluorescent and colorimetric strategies have emerged as promising approaches in this field, offering multiple merits of high sensitivity and specificity, ease of handling, and cumulative signaling effects. This minireview outlines the endogenous levels of GHB in the body and possible metabolism pathways, summarizes the recent advances in active chromophores, elucidates the corresponding sensing characteristics, and then exemplifies the developed sensing strips and detection kits based on the optimized chromophores mostly in the past five years. Additionally, the perspectives of the relevant studies are discussed in detail.

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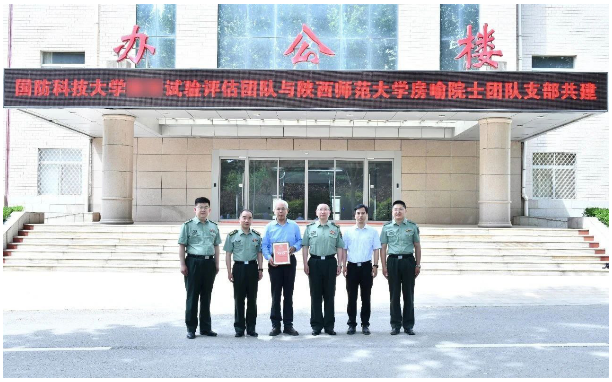
研究院赴国防科技大学试验训练基地开展支部共建活动

INCSMM carries out Party branch co-construction with NUDT Experimental Training Base



2025 年 5 月 7 日，新概念传感器与分子材料研究院房喻院士团队赴国防科技大学试验训练基地与某试验评估团队开展支部共建活动，以学术研讨形式促进双方交流合作。

首先，全体人员来到试训馆，实地观摩某试验场、训练场条件建设情况，听取了基地在新质战斗力建设中取得的进展、突破、创新等方面介绍，双方就技术、装备等进行了讨论交流。

在随后的座谈会上，房喻院士作了题为《传感器驱动的分子材料创新》的专题报告，介绍了团队的最新研究成果及未来发展方向。基地某试验评估团队作了专题汇报，重点阐述了团队在科研攻关方面取得的技术进展与合作前景。

交流环节，双方围绕“某技术如何赋能提升新质战斗力”展开探讨，并就未来联合攻关、人才培养等合作方向初步达成共识。双方表示，将以此次合作为契机，进一步深化交流，共同推动军地融合创新发展。

基地主任侯中喜、政委董远中，陕西师范大学党委常委、副校长陈新兵，西安交通大学刘峰教授、何刚教授，研究院副院长丁立平教授、副院长杨小刚、刘凯强教授、彭浩南教授、刘太宏副教授、刘小燕副教授、薄鑫副教授、赵智豪博士，研发工程师王佩、何怡楠、罗艳彦、马剑飞和行政秘书左振男参加了活动。

On May 7, 2025, the team led by Prof. Fang Yu from the Institute of New Concept Sensors and Molecular Materials visited the Experimental Training Base of National University of Defense Technology to carry out a joint Party branch co-construction activity with a certain experimental evaluation team, promoting exchanges and cooperation between the two sides in the form of academic discussions.

First, the participants went to the trial and training hall to observe the conditions of a certain test field and training ground on the spot, and listened to the introduction of the progress, breakthroughs and innovations made by the base in the construction of new combat effectiveness. Both sides discussed and exchanged views on technology, equipment and other aspects.

At the subsequent symposium, Fang Yu gave a report titled “Innovations in Sensor-driven Molecular Materials”, introducing the latest research achievements and future development direction of the team. A certain experimental evaluation team from the base presented a report, highlighting the technological progress and cooperation prospects achieved by the team in scientific research breakthroughs.

During the exchange session, both sides discussed how a certain technology can empower and enhance new combat effectiveness, and reached a preliminary consensus on future cooperation directions such as joint research and development and talent cultivation. Both sides expressed that they would take this cooperation as an opportunity to further deepen exchanges and jointly promote the innovative development of military-civilian integration.

The base director Hou Zhongxi and political commissar Dong Yuanzhong, Chen Xinbing, a member of the Standing Committee of the Party Committee and vice president of Shaanxi Normal University, Prof. Liu Feng and Prof. He Gang from Xi’an Jiaotong University, INCSMM vice dean Prof. Ding Liping, vice dean Mr. Yang Xiaogang, Prof. Liu Kaiqiang, Prof. Peng Haonan, A/Prof. Liu Taihong, A/Prof. Liu Xiaoyan, A/Prof. Bo Xin, Dr. Zhao Zhihao, and R&D engineers Wang Pei, He Yinan, Luo Yanyan, Ma Jianfei and administrative secretary Zuo Zhennan attended the event.

中国科学院物理所曹则贤研究员应邀作报告

Researcher Cao Zexian of CAS Institute of Physics invited to give a report

2025 年 5 月 15 日，应新概念传感器与分子材料研究院房喻院士邀请，中国科学院物理所曹则贤研究员做客陕西师范大学高端学术论坛，作了题为“量子力学是怎么创立的？”的专题科普报告。

曹则贤研究员从物理学家沃尔夫冈·泡利的学习历程讲起，和同学们探讨大学学什么，未来作为教师怎么教，进而引出量子力学的创立，循着量子力学发展的历史脉络，用关键的人物、物理事件与数学思想构筑量子力学的知识体系，从普朗克的能量量子化假设，到爱因斯坦的光子理论，再到德布罗意的物质波概念，以及薛定谔方程和海森堡矩阵力学的诞生等，将量子力学建立过程中的关键节点一一呈现。

在互动环节，同学们就对量子力学的一些困惑、概念理解以及与其他学科交叉应用等问题与曹则贤研究员展开交流。曹则贤研究员鼓励学生们保持对科学的好奇心和探索精神，勇于挑战传统思维，为未来的科研之路奠定坚实基础。

房喻院士高度评价曹则贤研究员的精彩报告，他强调量子力学不仅是科学，更是重要的一门学科，如何将科学知识与教学实践相结合是学校未来发展的重要探索之路，他鼓励科研人员与广大师生们要积极奋进，共同推进学校的良性发展。

报告由学校科学技术处、校科协、物理学与信息技术学院、化学化工学院和材料科学与工程学院联合主办，500 余名师生参加。房喻院士出席报告会并作点评。报告会由校党委常委、物理学与信息技术学院院长李贵安主持。

On May 15, 2025, at the invitation of Prof. Fang Yu of the Institute of New Concept Sensors and Molecular Materials, Researcher Cao Zexian of the Institute of Physics of the Chinese Academy of Sciences was invited to give a special science popularization report titled “How was Quantum Mechanics Founded?” at the High-end Academic Forum of Shaanxi Normal University.

In the report, Cao Zexian, staring from the learning history of Physicist Wolfgang Pauli, discussed with students what to study in the university, how to teach as a teacher in the future, and then introduced the creation of quantum mechanics, following the historical vein of quantum mechanics development, with key figures, physical events and mathematical ideas to construct the knowledge system of quantum mechanics, from Planck’s quantization of energy assumptions, to the theory of photon of Albert Einstein, and then to the concept of matter waves of De Broglie, and the birth of Schrödinger equation and Heisenberg matrix mechanics, presenting the key points in the process of establishing quantum mechanics.

During the interactive session, students exchanged views with Cao Zexian on some confusions in quantum mechanics, conceptual understanding, and cross-applications with other disciplines. Cao encouraged the students to maintain their curiosity and spirit of exploration in science, and to challenge the traditional thinking, so as to lay a solid foundation for their future scientific research.

Fang Yu highly praised Cao Zexian’s report, and emphasized that quantum mechanics is not only science, but also an important discipline, saying how to combine scientific knowledge with teaching practice is an important exploration path for the future development of the school, and encouraged the researchers, students and faculty members work hard in order to promote the benign development of the university together.

The report was co-sponsored by the Science and Technology Department, the School of Physics and Information Technology, the School of Chemistry and Chemical Engineering and the School of Materials Science and Engineering of the university, and was attended by more than 500 teachers and students. Prof. Fang Yu attended the presentation and made comments. The presentation was hosted by Li Guian, member of the Standing Committee of the Party Committee of the university and dean of the School of Physics and Information Technology.

西安市人才工作局、西安人才集团来访

Xi’an Talent Work Bureau and Xi'an Talent Group guests received

2025年5月27日，西安市委组织部副部长、市人才工作局局长张凯，西安城市发展集团董事长、西安人才集团董事长焦振华一行到访新概念传感器与分子材料研究院，了解了研究院概况和理念，参观了研究院展厅，并与房喻院士进行了会谈交流。

西安人才集团人力资本部部长朱碧颖、长安先导产业创新中心科技金融中心主任王瑾、物质科学中心主任王强，西安远诺技术转移中心总经理王海栋；新概念传感器与分子材料研究院丁立平副院长、杨小刚副院长和彭军霞教授参加了会谈交流。

On May 27, 2025, Zhang Kai, vice director of Organization Department of Xi’an Municipal Party Committee and director of Talent Work Bureau of Xi’an Municipal Government, Jiao Zhenhua, chairman of Xi’an Urban Development Group and chairman of Xi’an Talent Group, visited the Institute of New Concept Sensors and Molecular Materials, and Prof. Fang Yu introduced the overview and concept of the Institute, showed them the exhibition room, and had a talk with them.

Zhu Biying, director of Human Capital Department of Xi’an Talent Group; Wang Jin, director of Science and Technology Finance Center, Wang Qiang, director of Center for Material Science of Chang’an Pilot Industry Innovation Center; Wang Haidong, general manager of Xi’an Yuannuo Technology Transfer Center; and INCSMM vice dean Prof. Ding Liping, vice dean Mr. Yang Xiaogang, and Prof. Peng Junxia participated in the meeting.

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