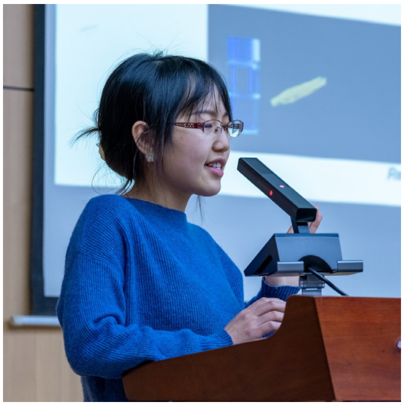
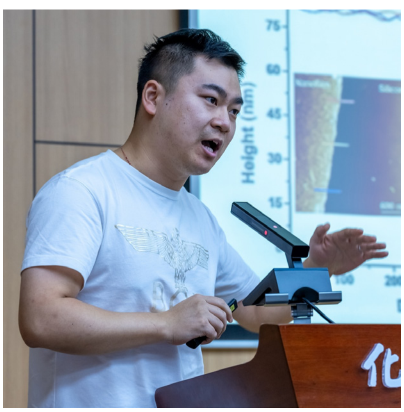
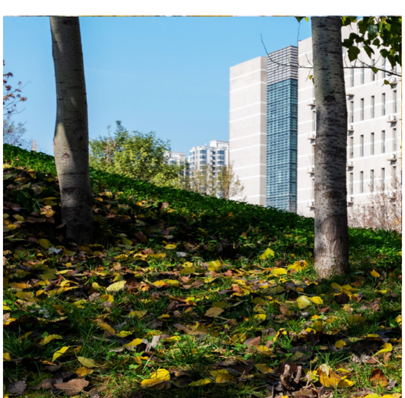
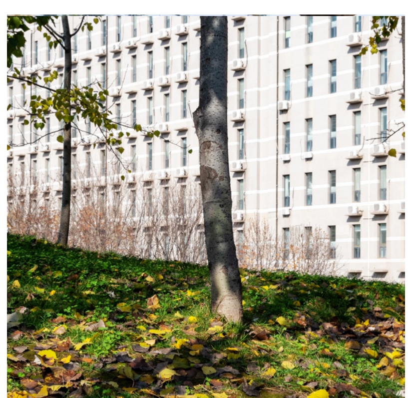
新概念传感器和分子材料研究院简报

Newsletter of Institute of New Concept Sensors and Molecular Materials

11 / 2022






2022 年度 IUPAC 化学领域十大新兴技术正式发布 薄膜荧光传感器位列第四

Film-based fluorescence sensors rank fourth in officially released 2022 IUPAC Top 10 Emerging Technologies in Chemistry

2022 年 11 月 28 日，在主题为“开放·信任·合作”的第四届世界科技与发展论坛闭幕式上，IUPAC 执委会委员、中国化学会副理事长帅志刚正式发布了“2022 年度 IUPAC 化学领域十大新兴技术”，房喻院士团队领衔的“薄膜荧光传感器”位列第四项。

帅志刚副理事长讲到，我们很高兴的看到不断有中国化学家领衔的研究纳入其中，比如今年阎锡蕴院士团队领衔的“纳米酶”、房喻院士团队领衔的“薄膜荧光传感器”、李灿院士团队领衔的“液态太阳燃料”、彭慧胜教授团队领衔的“纤维电池”和“织物显示器”，希望能引起更加广泛的来自中国科技界的关注、支持和参与。

IUPAC 主席 Javier García-Martínez 教授在视频致辞中指出，通过化学领域十大新兴技术的发布，我们希望展示不同的化学技术对于改善人类福祉、促进工业发展、应对气候变化、保障人民健康的重要意义，以及通过化学科学与技术应对全球挑战的重要性。

自 2019 年起，以成立 100 周年为契机，IUPAC 联合包括中国化学会在内的来自世界各个国家和地区的化学学术组织，共同发起“年度化学领域十大新兴技术”这一全球性活动，希望能在全世界范围内遴选出化学及交叉

十一月大事记 Events in November, 2022

领域中从新兴的科学发现到已经被充满冒险精神的初创企业和大胆的工业所采用的具有巨大潜力的创新技术，以此来改变当前的全球化学与工业界格局，推动实现联合国可持续发展目标。

On November 28, 2022, at the closing ceremony of the 4th World Science and Technology Development Forum themed “Openness, Trust and Cooperation”, Shuai Zhigang, member of IUPAC Executive Committee and vice president of the Chinese Chemical Society, officially released the “2022 IUPAC Top Ten Emerging Technologies in Chemistry”, and the Film-based Fluorescence Sensors pioneered by Prof. Fang Yu’s group ranked fourth.

Shuai Zhigang said “we are very happy to see that there are more research led by Chinese chemists in the top ten technologies, such as this year’s nanozymes by Prof. Yan Xiyun’s group, film-based fluorescent sensor by Prof. Fang Yu’s group, liquid solar fuels by Prof. Li Can’s group, and fiber batteries and textile displays by Prof. Peng Huisheng’s group”. He hoped that it can attract more attention, support and participation from China’s scientific and technological circles.

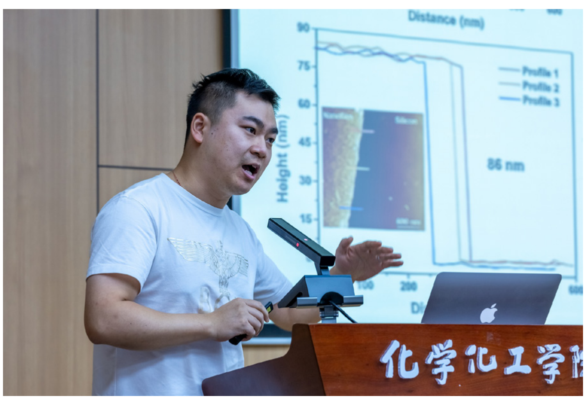
IUPAC President Prof. Javier García-Martínez said in his video speech that “through the release of the top ten emerging technologies in chemistry, we hope to showcase how different chemistry technologies are so vital to improve our well-being, to have a more competitive industry, to fight climate change and emerging illnesses, and even more important to engage in a global conversation about the importance in chemistry in tackling our more present challenges.”

Since 2019, the 100th anniversary of its establishment, IUPAC has collaborated with chemical organizations from various countries and regions around the world, including the Chinese Chemical Society, to jointly launch the global annual activity “Top Ten Emerging Technologies in Chemistry”, in the hope to change the current global chemistry and industry landscape and contribute to the achievement of the United Nations Sustainable Development Goals by selecting from emerging scientific discoveries to innovative technologies with great potential that have been adopted by adventurous start-ups and bold industries around the world.

研究院科研经验与感悟分享会举行

Research experience and reflection sharing session held

2022 年 11 月 14 日下午，新概念传感器与分子材料研究院在致知楼 1668 报告厅举行科研经验与感悟分享会，邀请刘凯强老师，博士生唐嘉琪、乔敏、黄蓉蓉为研究院师生作报告和分享。



分享会由刘静老师主持，院长房喻院士，学院老师和博士、硕士研究生出席。

唐嘉琪同学介绍了自己的科研工作，并分享了在科研中遇到的一些挫折以及自己解决这些问题的经验。

乔敏同学介绍了阴离子判别的交叉反应、荧光传感器的构建等领域内的科学问题，通过变温光谱、扫描电镜等的数据分析和实验验证，提出了解决方案。她还从如何高效阅读文献、合理安排实验、以及撰写论文等方面提出了建议。

黄蓉蓉同学从自己的研究工作出发，介绍了自己的科研工作进展、未来规划，以及在学习和实验过程中遇到的问题，建议低年级同学要多读文献，多与他人交流讨论，同时树立积极向上的心态。

刘凯强老师从研究思路与目标谈起，图文并茂、生动形象地讲述了科研探索、科研之苦、心态调整策略及科研之美。他建议同学们要力争做一个有理想追求的人、潜心做有深度的科研，告诉大家面对科研过程中的挫败与焦虑要如何积极调整心态、如何进行自我反思与鞭策，鼓励同学们要热爱科研、敢于吃苦、学会沟通，勇于挑战自我，在探索中奋进，在思考中成长。

房喻院士分享了自己的教育理念，包括基础教育与高等教育的关系以及博士生毕业后的择业等方面的思考，提出今后要多举办这种分享活动。

最后，刘静老师在总结讲话中感谢了刘凯强老师与三位博士生，希望同学们从他们的经验、感悟和建议中能够有所收获，在今后的科研和生活中成长成才。

On November 14, 2022, the Institute of New Concept Sensors and Molecular Materials held a research experience and reflection sharing meeting in the 1668

lecture hall of Zhizhi Building, inviting Prof. Liu Kaiqiang and doctoral students Tang Jiaqi, Qiao Min and Huang Rongrong to report and share for teachers and students of the institute.

Prof. Fang Yu joined the teachers, doctoral and master students of the institute at the session, which was hosted by Prof. Liu Jing.

Tang Jiaqi presented his research work, and shared his story of suffering setbacks in research and solving these problems.

Qiao Min introduced the scientific problems in the fields of cross-reactivity of anion discrimination and the construction of fluorescence sensors, and proposed solutions through data analysis and experimental verification of variable temperature spectroscopy and scanning electron microscopy. She also gave suggestions on efficient literature reading, reasonable experiment arrangement, and paper writing.

Starting from her own research work, Huang Rongrong introduced the progress of her research work, future planning, and problems encountered in the process of learning and experimentation, and suggested that junior students should read more literature, communicate and discuss with others, and establish a positive attitude.

Prof. Liu Kaiqiang, starting from research ideas and goals, vividly described the research exploration, the pain of research, the strategy of mentality adjustment and the beauty of scientific research. He suggested that students should strive to be a person with ideals and pursuits, concentrate on in-depth scientific research, telling them how to actively adjust their mentality, how to carry out self-reflection and encouragement in the face of frustration and anxiety in the process of research, and encouraged students to love research, get ready to endure hardships, learn to communicate, dare to challenge themselves, forge ahead in exploration, and grow in thinking.

Fang Yu shared his educational philosophy, including the relationship between basic education and higher education, and the career choice of doctoral students after graduation, and proposed to hold more such sharing activities in the future.

In the end, Liu Jing thanked Prof. Liu Kaiqiang and the three doctoral students, hoping that the students could learn something from their experiences, reflections and suggestions, and grow into talents in future research and life.

博士研究生唐嘉琪、黄蓉蓉通过毕业论文答辩

Doctoral students Tang Jiaqi and Huang Rongrong pass graduation dissertation defense

2022年11月29日下午，新概念传感器与分子材料研究院在致知楼1568教室进行了博士研究生毕业论文答辩会，唐嘉琪和黄蓉蓉通过了答辩。

博士毕业生唐嘉琪进行了题为“动态酰腙键基新型软物质材料的制备及其应用探索”的答辩报告，博士毕业生黄蓉蓉进行了题为“具有分子内电荷转移特性的邻碳硼烷衍生物设计合成、发光性质调控及应用”的答辩报告。

答辩委员会由华东理工大学田禾院士担任主席，英国利物浦大学肖建良教授、新加坡科技设计大学刘晓刚教授、西安交通大学何刚教授、西北大学李剑利教授、陕西师范大学薛东教授和曹睿教授担任委员，陕西师范大学刘忠山老师担任答辩秘书。

答辩委员会由华东理工大学田禾院士担任主席，英国利物浦大学肖建良教授、新加坡科技设计大学刘晓刚教授、西安交通大学何刚教授、西北大学李剑利教授、陕西师范大学薛东教授和曹睿教授担任委员，陕西师范大学刘忠山老师担任答辩秘书。

On November 29, 2022, the Institute of New Concept Sensors and Molecular Materials held a doctoral dissertation defense session in Room 1568 of Zhizhi Building, and doctoral students Tang Jiaqi and Huang Rongrong passed the defense.

Tang Jiaqi’s report is titled Dynamic Acylhydrazone-based Soft Materials: Preparation and Application Exploration, and Huang Rongrong’ report is titled Design, Synthesis, Luminescence Property Regulation and Application of Oo-cCarborane Derivatives with

Intramolecular Charge Transfer Characteristics.

Chaired by CAS academician Prof. Tian He of East China University of Science and Technology, the defense committee is comprised of Prof. Xiao Jianliang of the University of Liverpool, Prof. Liu Xiaogang of Singapore University of Technology and Design, Prof. He Gang of Xi'an Jiaotong University, Prof. Li Jianli of Northwest University, and Prof. Xue Dong and Prof. Cao Rui of Shaanxi Normal University, and Dr. Liu Zhongshan of Shaanxi Normal University acted as the secretary.

After their presentations, the two doctoral students answered the questions raised by the defense committee, discussed relevant issues and further research and work prospects with the committee members. The defense committee unanimously agreed that the research done by the students was solid, the answers to the questions were clear and logical, and agreed to accept their defenses and award them doctoral degree.

简讯动态 News in Brief

房喻院士应邀赴西北大学作报告

Fang Yu speaks on Film-based Fluorescence Sensors at Northwest University

2022 年 11 月 16 日下午，房喻院士应邀做客西北大学，在“杨钟健学术讲座”第 205 讲上作了题为《薄膜荧光传感器－从基础研究到产业应用》的报告。

On the afternoon of November 16, 2022, Prof. Fang Yu was invited to be a guest speaker at Northwest University in Xi'an and gave a report titled “Film-based Fluorescence Sensors - From Basic Research to Industrial Application” at the 205th session of NWU's Yang Zhongjian Lectures.

房喻院士受邀担任上海交通大学教育学院顾问委员会主任

Fang Yu to serve as Advisory Committee director of SJTU's School of Education

2022 年 11 月 24 日，房喻院士应邀在线参加上海交通大学教育学院召开的 “2022 年学科专业建设咨询会”和“聚焦高质量・教育向未来——上海交通大学教育学院 2022 年顾问委员战略咨询会”，并受邀担任上海交通大学教育学院顾问委员会主任。

On November 24, 2022, Prof. Fang Yu was invited to participate in the “2022 Consultation Meeting for Discipline and Major Construction” and “Focus on High-quality Education for the Future - 2022 Strategic Consultation Meeting of Advisory Committee Members of the School of Education of Shanghai Jiaotong University” via online conference, and was invited to serve as the director of the Advisory Committee of SJTU's School of Education.

简讯动态 News in Brief

研究院副院长和办公室主任获任命

Vice dean and administrative office director appointed

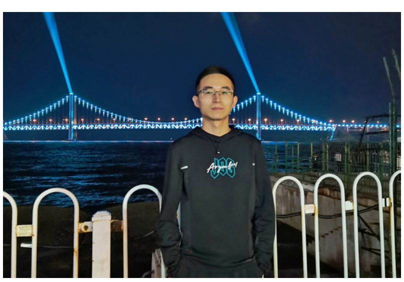
2022 年 11 月 10 日，新概念传感器与分子材料研究院召开会议，宣布陕西师范大学人事任命，由丁立平任研究院副院长，杨小刚任研究院办公室主任。

On November 10, 2022, at a meeting held by the Institute of New Concept Sensors and Molecular Materials, the appointment of Shaanxi Normal University that Ding Liping as the vice president and Yang Xiaogang as the director of the administrative office was announced.

院友动态 Alumni News

博士毕业生王朝龙获中科院大连化物所两项资助

Wang Zhaolong funded by CAS Dalian Institute of Chemical Physics



2022 年 11 月 28 日，中国科学院大连化学物理研究所发布 2022 年第二批优秀博士后支持计划和特别研究助理资助项目资助人选名单，研究院毕业生王朝龙博士入选上述两个项目，获得相应的经费资助用于科研及访问交流等支出。

王朝龙，2022 届博士毕业生，师从房喻院士，于 2022 年 6 月从陕西师范大学毕业，获理学博士学位。同年 8 月加入中科院大连化物所分子反应动力学国家重点实验室吴凯丰教授课题组从事博士后研究，目前主要研究方向为胶体量子点 – 有机分子界面电荷 / 能量转移动力学。他以第一作者身份在 Angew. Chem. Int. Ed.、Adv. Funct. Mater. 等专业期刊发表论文 5 篇，获得陕西省普通高等学校优秀毕业生荣誉称号。

On November 28, 2022, the Dalian Institute of Chemical Physics, Chinese Academy of Sciences released the list of candidates for its 2022 second outstanding postdoctoral support program and special research assistant funding project, and Dr. Wang Zhaolong, a graduate of the Institute of New Concept Sensors and Molecular Materials, was selected for the above two projects and will receive financial support for scientific research, visits and exchanges.

Wang Zhaolong, a 2022 doctoral graduate of Prof. Fang Yu, graduated from Shaanxi Normal University in June 2022 with a doctorate degree in science. In August, he joined the research group of Prof. Wu Kaifeng, of the State Key Laboratory of Molecular Reaction Kinetics at CAS Dalian Institute of Chemical Physics to engage in postdoctoral research, and his current research direction is interfacial charge/energy transfer dynamics of colloidal quantum dots-organic molecule systems. He published five papers as the first author in professional journals such as Angew. Chem. Int. Ed. and Adv. Funct. Mater., and won the honorary title of outstanding graduate of Shaanxi Province colleges and universities.

Angewandte Chemie International Edition
GDCh A Journal of the German Chemical Society

Communication

Large-area Free-standing Metalloporphyrin-based Covalent Organic Framework Films by Liquid-air Interfacial Polymerization for Oxygen Electrocatalysis

Jiaqi Tang, Dr. Zuozhong Liang, Haonan Qin, Xiangquan Liu, Binbin Zhai, Zhen Su, Qianqian Liu, Dr. Haitao Lei, Prof. Dr. Kaiqiang Liu, Prof. Dr. Chuan Zhao, Prof. Dr. Rui Cao, Prof. Dr. Yu Fang

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大面积、自支撑金属卟啉 COF 薄膜的气液界面聚合及高效氧电催化

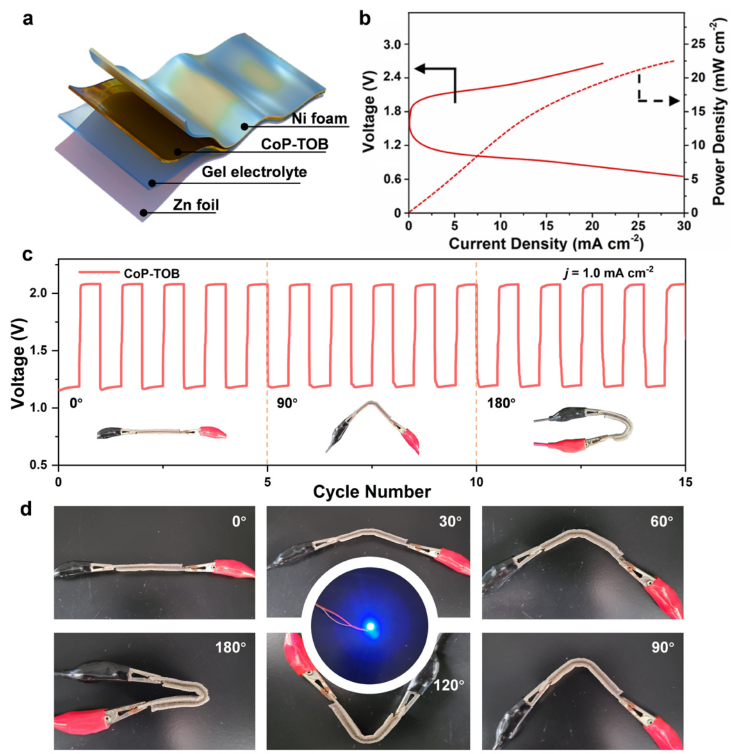
作为结构明确、孔径可调的一类新兴多孔材料，COF 膜具有巨大的应用潜力，然而柔性自支撑大面积 COF 膜的缺失严重制约着 COF 材料在催化、气体分离和传感等方面的应用。因此，发展大面积 COF 膜的制备技术具有重要的实践意义。

金属空气电池、燃料电池和水裂解技术能否走向产业应用在很大程度上取决于 ORR 和 OER 效率，而 ORR 和 OER 过程的发生离不开催化剂的使用。已有研究表明，金属卟啉是一类高效双功能催化剂，但金属卟啉的存在形式极大的影响着催化作用的发生。不难想象，将金属卟啉的高效催化作用与 COF 膜的高通透性结合，无疑可以提高离子传输速率，增加催化作用位点与底物作用几率，大幅度提高催化作用效率。大面积钴卟啉 COF 膜的高效电催化性能证明了这一设想。

本文通过气液界面限域动态酰腙缩合成功制备了结构完整、柔韧性突出，面积可达 3000 cm^2 的金属卟啉基 COF 纳米膜，系统研究了钴卟啉 COF 膜的电催化性能。实验表明，该膜可同时高效催化析氧反应（OER）和氧还原反应（ORR）。利用该膜组装了全固态柔性锌空电池，在充放电电流密度 1 mA/cm^2 和充放电间隙电压 0.88 V 条件下，大幅度弯曲操作并不影响电池性能。相关研究不仅提供了一种大面积、无缺陷、自支撑 COF 膜制备策略，也展现了 COF 膜在柔性电子学等领域的巨大应用潜力。

第一作者：陕西师范大学博士研究生唐嘉琪、副研究员梁作中
通讯作者：陕西师范大学房喻院士、曹睿教授、新南威尔士大学赵川教授
全文链接：https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.202214449

Covalent organic frameworks (COFs) have attracted increasing interests due to their periodic latticed and porous structures and their potential applications in catalysis, separation, sensing, and others. Compared to powders, films are more processable and applicable to film-based technologies. However, synthesizing large-area free-standing COF films is a big challenge. Most reported COFs were produced as powders using solvothermal methods. Recently, polymerizing amines and aldehydes at liquid-liquid interfaces was reported to fabricate COF films, where amines and acid catalysts are added in aqueous media, while aldehydes are dissolved in water-immiscible organic solvents. However, the initially formed films at the interface will impede substrate monomer diffusion from one phase to the other, therefore hindering the subsequent film growth. Moreover, films fabricated using this method are usually size-limited because of the use of long and thin vessels to enable stable liquid-liquid interface when adding one phase over the other. Polycrystalline nuclei that formed upon mixing the two phases will also affect the homogeneity and roughness of the films.



Metal porphyrins have been studied as electrocatalysts for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), the two important reactions involved in many clean energy devices, such as metal-air batteries, fuel cells, and water electrolysers. The commercial viability of these technologies depends on the efficiency of the two reactions. Integrating metal porphyrins into frameworks often enables improved catalysis as the framework porous structures can lead to large surface areas and easy mass transportations. Thus, developing COF films with integrated active metal porphyrin units for ORR and OER is desired for energy conversion devices, particularly for flexible metal-air batteries. However, few metalloporphyrin-based COF films are reported because of the challenges in synthesizing proper metal porphyrin monomers and also high-quality films.

Herein, we reported on a liquid-air interfacial polymerization method for fabricating large-area free-standing metalloporphyrin-based COF films and demonstrated their applications for oxygen electrocatalysis. We developed a strategy to polymerize meso-benzohydrazide-substituted metal porphyrins with tris-aldehyde linkers at a liquid-air interface. Compared to typical imine bonds formed between amines and aldehydes, the acylhydrazone bonds, formed between benzohydrazide and aldehydes, enable the COFs to have higher hydrolytic stability. The resulted free-standing films, which can be scaled up to 3000 cm^2 in area, are defect free and display mechanical stability and structural integrity. By using Co porphyrins, the formed films are efficient for electrocatalytic ORR and OER. Flexible all-solid-state Zn-air batteries assembled using these films showed remarkable performance and stability under harsh bent conditions.

First Authors: doctoral candidate Tang Jiaqi and Assoc. Prof. Liang Zuozhong, Shaanxi Normal University
Corresponding Authors: Prof. Fang Yu and Prof. Cao Rui, Shaanxi Normal University; Prof. Zhao Chuan, The University of New South Wales
Full Text Link: https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.202214449

ACS APPLIED MATERIALS & INTERFACES
www.acsami.org Research Article

Dual-Mode Optical Sensor Array for Detecting and Identifying Perillaldehyde in Solution Phase and Plant Leaf with Smartphone

Jiayin Zhao, Ke Liu, Ruitong Wang, Taihong Liu,* Zhenfeng Wu,* Liping Ding, and Yu Fang

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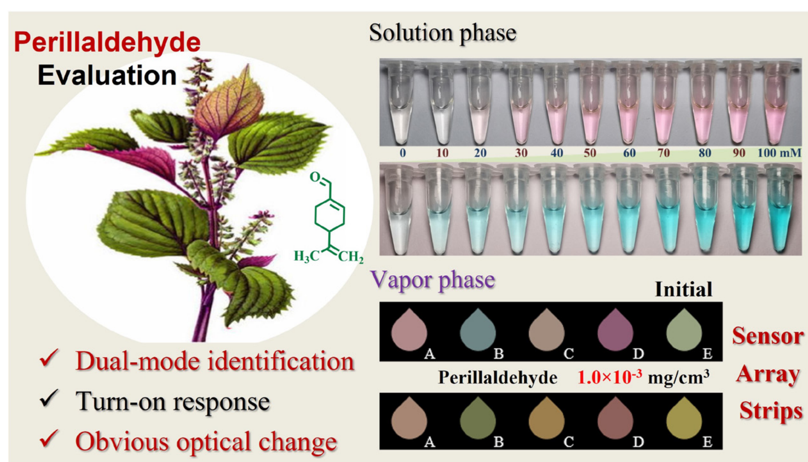
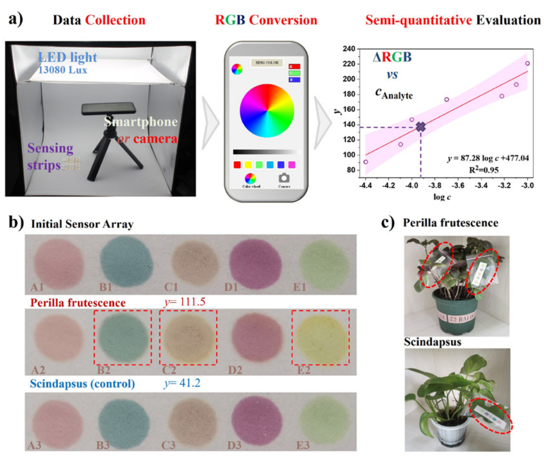
基于智能手机的双模传感器阵列对液态和植物中紫苏醛的识别与检测

近年来，植物性食品中活性成分定量检测技术在全球智能农业领域备受关注，研究快速、灵敏区分监测方法对未来高品质健康生活具有重大意义。紫苏具有解表散寒、行气和胃之功效，用于风寒感冒，咳嗽呕恶等。根据主要成分紫苏属植物有多种类别，2020 版《中国药典》中规定了紫苏醛型紫苏为主要类别。而紫苏醛的含量决定了紫苏叶的质量，其含量测定多通过提取挥发油的方法，这种方法耗时久，耗材也相对较大，不利于快速检测。



双模比色传感器阵列检测液相和植株中紫苏醛含量结果对比图
TOC figure for dual-mode optical sensor array for detecting and identifying perillaldehyde in solution phase and plant leaf with smartphone

本文利用闭环结构罗丹明–肼、方酸–肼和 2, 4– 二硝基苯肼三种衍生物体系，构建了快速准确评估紫苏醛(Perillaldehyde)的 Turn–On 型比色传感器阵列。通过伯胺 / 肼与紫苏醛中活性醛基发生特异性反应引发紫外吸收–荧光发射双模信号变化，实现了对紫苏醛的快速、灵敏传感响应；同时体系中荧光特征信号显著增强也表明了该研究体系对紫苏醛良好的选择性和较高的灵敏度，计算检出限为 20.0 μM。另外我们基于自搭建 RGB 识别系统，开发了阵列化纸基传感试纸条，可在 15 min 内对紫苏醛含量进行半定量评价。测试结果表明，该方法的 RGB 变化值与紫苏醛含量间具有良好的线性相关性，有助于实现紫苏类植物性食品的质量检测和品质控制。该方法首次使用阵列化纸基传感试纸条用于定性和半定量评估紫苏醛含量，具有肉眼可识别、快速简便、溶液态和气相均可使用等优点，有望在未来智能农业领域具



(a) 利用自搭建RGB识别系统对气态紫苏醛含量进行评价，误差范围由至少三次平行测量确定。(b) 以紫苏为真实样品，以绿萝为对照的传感试纸条响应效果。(c) 附有传感试纸条的植物图片。
(a) Evaluation of the gaseous perillaldehyde content using the established calibration equation, error bars were determined from at least three parallel measurements. (b) Testing trials of perilla frutescence as the real samples and scindapsus as a control. (c) Pictures of the plants attached with sensing array strips.

有潜在应用。

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Promising techniques for detecting and quantifying active components in the plants and foods have received global concern in smart agriculture. Perilla frutescence was widely used as spices and preservatives in Asian food. As an active ingredient as in traditional medicine, its extracted essential oil has the virtue of vasodilative, anti-inflammatory, antimicrobial, antiseptic effects, etc. Several different chemotypes of perilla frutescens were classified corresponding to the main constituents, and importantly, perillaldehyde chemotype is qualified for perilla folium source in the 2020 edition of “Chinese Pharmacopoeia”. The volatile oil was normally extracted by the solvent-assisted steam distillation followed by the traditional determination methods which require sophisticated instruments, professional trained personnel, and complex processing procedures. These limitations result in a certain gap in the detection efficiency, portable and on-site analysis.

We herein unveil a novel turn-on and dual-mode sensor array comprising three kinds of reactive indicators including ring-closed rhodamine-hydrazine, squaraine-hydrazine, and 2,4-dinitrophenylhydrazine for evaluating perillaldehyde. Significant colorimetric and fluorescent changes were triggered through reacting primary amine/hydrazine with the active aldehyde group in perillaldehyde, thus turn on the chromogenic responses of all the indicators. Optimal colorimetric sensing showed good responses to perillaldehyde ranged up to 100 mM in ethanol solution. Dramatic fluorescence enhancement was also exhibited, illustrating good selectivity as well as high sensitivity (detection limit ~ 20.0 μM). Inspired by rapid chemical reactions and distinct optical changes, distinct sensor array strips loaded with the optimal solid-state reactive indicators were developed for evaluating the perillaldehyde content in the perilla frutescence leaves. Smartphone-enabled readout system and digital data processing were further performed for chemometric analysis. A good correlation was obtained and the semi-quantitative evaluation of the perillaldehyde content could be achieved within 15 min, possessing the significant features of naked-eye recognition, easy operation, and disposability. To the best of our knowledge, present work demonstrated the use of chromogenic sensing strips to evaluate the active perillaldehyde content in solution and vapor phases for the first time. Taken together, these characteristics also indicate that present turn-on sensor array has great potential applications in precise detection and evaluation of perillaldehyde in the forthcoming smart agriculture.

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Distinct Hydrogen Bonding Dynamics Underlies the Microheterogeneity in DMF–Water Mixtures

Published as part of The Journal of Physical Chemistry virtual special issue "Early-Career and Emerging Researchers in Physical Chemistry Volume 2".

Yimin Bai, Dexia Zhou, Somnath Mukherjee, Jing Liu, Hongtao Bian,* and Yu Fang

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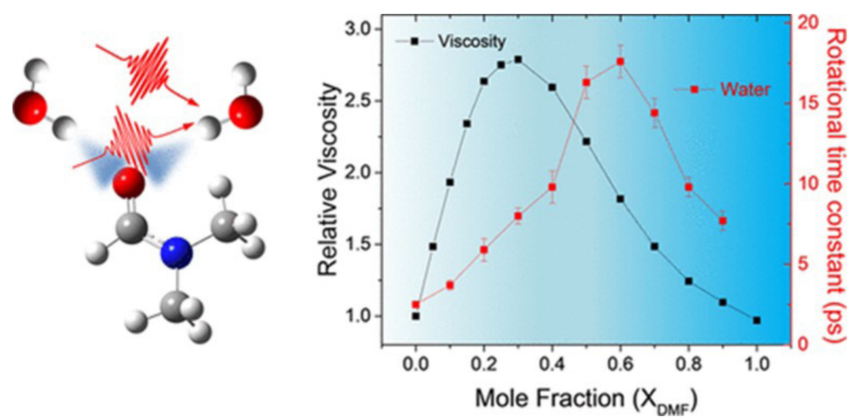
DMF –水二元混合物中氢键动力学研究

微观尺度下的相分离是一种广泛存在于水溶液中的现象。目前，研究者们普遍认为水溶液系统的微观不均性是导致二元溶液中反常的热力学和运输性质的原因。水分子可以在凝聚相中形成独特的三维氢键网络，理解复杂体系中的微观不均一性需要了解溶剂化结构和溶质与溶剂之间的氢键动力学。



酰胺官能团是多肽和蛋白质的基本重复单元，它和水份子之间的氢键相互作用是理解生物系统中液–液不均一性的基础。N,N–二甲基甲酰胺 (DMF) 是一种最简单的含有酰胺键的有机分子，具有相对较高的介电常数，可与水混溶。DMF 和水的二元混合物表现出强烈的非理想行为，表明在 DMF–水混合物中可能形成特定的复杂结构。然而，实验上获得在超快时间尺度下发生的氢键重组过程，并理解混合溶液中微观不均匀性的潜在机制仍是一个挑战。

本工作中，我们结合傅里叶变换红外光谱和超快红外光谱，以 SCN^- 和 OD 作为探针，分别研究了 DMF–水二元溶液在整个组成范围内的氢键动力学。SCN^- 的浓度依赖性转动动力学定性地遵循溶液粘度变化的趋势，转动各向异性显示 SCN^- 转动动力学在 X_{DMF}=0.3 时最慢。而 OD 的转动动力学显示出与外源性探针 SCN^- 不同的显著差异，OD 最慢的转动动力学出现在 X_{DMF}=0.6，OD 的转动各向异性衰减表现出双指数行为，可以用锥摆模型来解释。在 DMF–水混合物中观察到的明显氢键动力学是溶液中微观不均一性的显著证据，独特的结构动力学有望为液–液相分离的潜在机制提供微观层次的认识。

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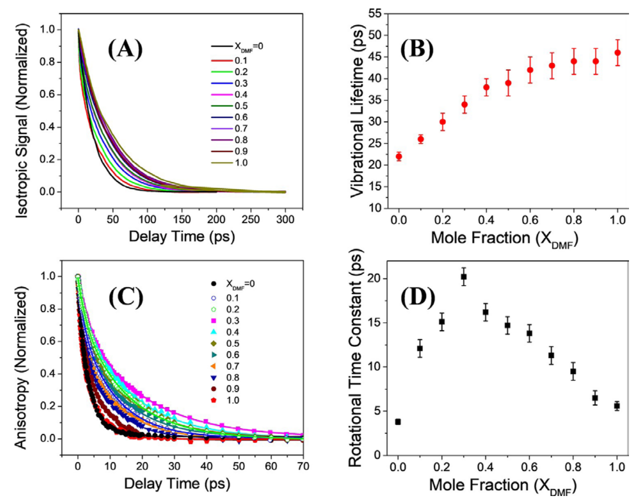
Microscopic phase segregation has been demonstrated as a general phenomenon in aqueous mixtures, ranging from aqueous electrolyte solutions to binary combinations of water and organic solvents. The anomalous thermodynamic and transport properties of binary mixtures are believed to be caused by the microheterogeneity in those systems. Water molecules can form unique three-dimensional hydrogen bonded networks in the condensed phases. Understanding the microscopic heterogeneity in complex systems requires knowledge about solvation structure and hydrogen bond dynamics between solute and solvent.



SCN^- 在不同浓度 DMF 水溶液中 (A) 反对称伸缩振动的归一化振动布局弛豫曲线；(B) 浓度依赖性振动寿命（慢组分）；(C) 归一化各向异性衰减，实线是用双指数函数拟合的数据；(D) 浓度依赖的转动时间常数（慢组分）

(A) Normalized vibrational population relaxation curves for the antisymmetric stretch of SCN− in DMF aqueous solutions with different concentrations. (B) Concentration-dependent vibrational lifetime (slow component) of SCN− stretch in the DMF aqueous solutions. (C) Anisotropy decay of SCN− probe in the DMF aqueous solutions. All the anisotropy decay curves are normalized to 1 at the delay time of zero. The solid lines are the fitting data using biexponential decay function. (D) Concentration-dependent rotational time constants (slow component) of SCN− stretch in the DMF aqueous solutions.

The interaction between water and the amide functional group, serving as the basic repeating unit of peptides and proteins, can represent a model system to investigate the dynamical heterogeneity in complex systems. N, N-Dimethylformamide (DMF), one of the simplest amides, is a polar aprotic solvent with a relatively high dielectric constant and miscible with water. Binary mixtures of DMF and water can exhibit strong nonideal behavior, indicates that the specific complex structure may be formed in the DMF–water mixtures. However, getting a complete picture of liquid reorganization specifically occurring on the ultrafast time scale to understand the underlying mechanism of the microheterogeneity in the mixture solution remain challenging.

In this work, we used OD and SCN^- probes to investigate the hydrogen bond dynamics of DMF–water mixtures over the entire composition range by the combination of Fourier transform infrared (FT-IR) spectroscopy and ultrafast IR spectroscopy. Rotational anisotropy measurement shows that the slowest orientational dynamics of SCN- probe is observed at X_{DMF} = 0.3, and the concentration-dependent orientational dynamics of SCN^- qualitatively follows the trend of viscosity change in the mixture solution. The reorientational dynamics of OD shows a remarkable difference from the extrinsic probe of SCN^-, and the slowest rotational dynamics of water is observed at X_{DMF} = 0.6. The rotational anisotropy decay of the OD stretch shows biexponential decay behavior, which can be explained by the wobbling-in-a-cone model. The distinct hydrogen bond dynamics observed in the DMF–water mixtures shows striking evidence of the local heterogeneity in the solution. The unique structural dynamics reported here is expected to provide significant insights into the underlying mechanism of liquid–liquid phase separation.

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国家毒品实验室陕西分中心来访

Meeting held with National Narcotics Laboratory Shaanxi Branch visitors

11月10日下午，国家毒品实验室陕西分中心主任姚震一行4人来访，与房喻院士及团队成员进行座谈交流。

姚震介绍了陕西分中心成立的背景、承担提升西北地区禁毒科技化水平的职能，希望与房喻院士团队在攻克关键技术难题、人才共育、技术共研、平台共建、资源共享方面展开交流合作。

房喻院士肯定了陕西分中心在禁毒科技化、高质量发展的重要作用，介绍了团队在毒品技术研究方面的核心成员和技术储备，希望能够与陕西分中心加强交流合作，为西北地区禁毒工作贡献力量。

团队成员刘静、刘太宏、刘科、左振男，国家毒品实验室陕西分中心杨春、黄欣菁、周潇警官参加了座谈。

On November 10, National Narcotics Laboratory Shaanxi Branch director Yao Zhen and his three colleagues visited the Institute of New Concept Sensors and Molecular Materials and had a discussion with Prof. Fang Yu and his group members.

Yao Zhen briefed about the background of the Shaanxi Branch and its functions of improving drug control technologies in Northwest China, and hoped to carry out exchanges and cooperation with the institute in tackling key technological problems, talent cultivation, technological development, platform construction, and resource sharing.

Fang Yu affirmed the important role of the Shaanxi Branch in the technological and high-quality development of drug control, briefed about the core members and technological reserves of the institute in drug control technology research, and hoped to strengthen exchanges and cooperation with the Shaanxi Branch,so as to contribute to the drug control work in Northwest China.

INCSMM faculty and staff members Liu Jing, Liu Taihong, Liu Ke and Zuo Zhennan, NNL Shaanxi Branch officers Yang Chun, Huang Xinjing and Zhou Xiao attended the meeting.

《化学与创新中国》书稿节选

Excerpt from the manuscript of "Chemistry and Innovation in China"

文 / 房 喻 by Fang Yu

传感器是一类具有信息感知和物理量转换功能的有形器件，在工农业生产、社会管理、公共安全、国防建设等领域具有广泛应用。在当今，传感器是实现万物互联的基础，是发展人工智能的必须。传感器技术发展备受重视。

不同于普通工业产品，传感器技术密集、种类繁多。传感器研发门槛高、周期长，而且具有突出的跨学科特点。传感器研发能力在一定程度上反映了一个国家、一个地区科技创新能力和科技发展水平。

需要指出的是，敏感材料的研制是传感器研发的关键所在。以创造新物质为己任的化学学科在传感器，特别是高端传感器研制中扮演的角色越来越重要。在过去的二十多年里，我国科学家房喻教授团队围绕薄膜荧光传感器（Film-based Fluorescent Sensors, FFSs）核心技术，坚持开展“敏感薄膜传感器探测装备”全链条研究，实现了爆炸物、毒品探测技术和装备研制的重大突破，形成了具有完全自主知识产权的薄膜荧光传感技术体系。

在敏感材料创制方面，房喻教授团队通过敏感单元分子结构、薄膜态敏感单元聚集结构和敏感单元激发态性质的精细调控，发展了以化学键合、凝胶介导、 组合设计和界面限域动态聚合等策略为特色的荧光敏感薄膜制备技术，创制了高性能爆炸物、毒品敏感薄膜材料，创造了爆炸物 10^{-15} 摩尔量级气相探测纪录，首次实现了冰毒等多种毒品和“撒旦之母”等液体爆炸物的高灵敏快速可逆探测。

在 FFSs 和探测装备研制方面，房喻教授团队首创了叠层式薄膜荧光传感器结构，打破了国外公司对波导管技术的垄断，实现了 FFSs 底层技术的突破。

在敏感材料和传感器硬件结构创新基础上，发明了新型爆炸物传感器、毒品传感器、爆炸物 / 毒品阵列型传感器，研制了 SRED 系列爆炸物单模，首创了 SRED 毒品单模和 SRED 爆炸物 / 毒品双模荧光探测装备，创造了响应速度最快、灵敏度最高、薄膜器件使用次数最多的爆炸物和毒品探测纪录，实现了 FFSs 类高端传感器和探测装备的中国制造。

相关装备在众多领域获得了应用并销往国外，2019 年开始列装部队。涉及化学战剂、神经毒剂、病原体等高危物质超灵敏探测的 FFSs 和装备研制也在有序推进中。基于原创研究，房喻教授出版了国际首部《薄膜基荧光传感技术与应用》专著。

经遴选与严格评审，世界最大、最权威的化学组织，国际纯粹与应用化学联合会（IUPAC）于 2022 年 10 月 17 日宣布，房喻教授团队提出的 FFSs 以第四名入选 IUPAC 2022 年度化学十大新兴技术（Top Ten Emerging Technologies in Chemistry 2022）。

作为一个新的传感器细分领域，FFSs 已经成为继离子迁移谱技术之后，最具发展潜力的微痕量物质探测技术。有理由相信，FFSs 将在服务国家建设、保障人民生命财产安全、提高疾病诊断能力等方面发挥日益重要的作用。

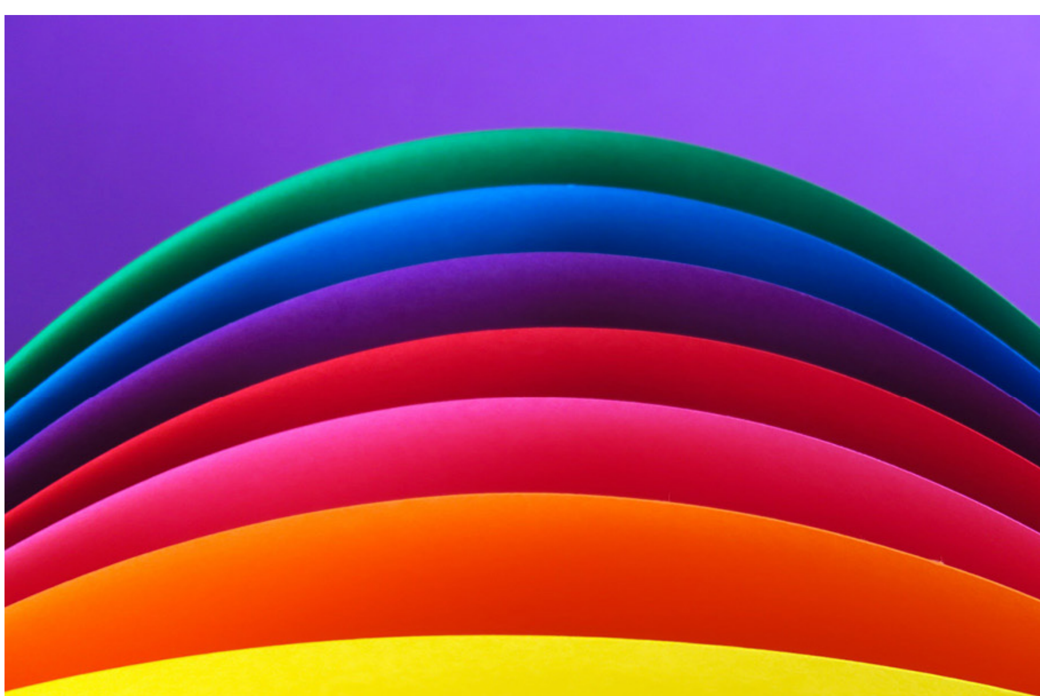
Sensors are a kind of tangible devices with the functions of information perception and physical quantity conversion, and are widely used in industrial and agricultural production, social management, public security, national defense and other fields. Today, sensors are the foundation for the realization of the Internet of Everything and a must for the development of artificial intelligence. The development of sensor technology is highly valued.

Unlike ordinary industrial products, sensors are technology intensive and versatile. The threshold of sensor research and development is high and its cycle is long, and it has outstanding interdisciplinary characteristics. To a certain extent, the sensor research and development capability reflects the scientific and technological innovation ability and development level of a country or region.

It should be pointed out that the development of sensitive materials is the key to sensor research and development. The discipline of chemistry, which is committed to creating new substances, plays an increasingly important role in the development of sensors, especially high-end sensors. In the past two decades, Chinese scientist Prof. Fang Yu has led his team in carrying out the whole chain research of “sensitive film sensor detection device” around the core technology of film-based fluorescent sensors (FFSs), achieved major breakthroughs in explosives and narcotics detection technologies and device development, and formed a film fluorescence sensing technology system with completely independent intellectual property rights.

In terms of the creation of sensitive materials, Prof. Fang Yu’s group has developed fluorescent sensitive film preparation technology featuring strategies such as chemical bonding, gel mediation, combination design and interface-limited dynamic polymerization, through the fine regulation of sensitive unit molecular structure, thin film sensitive unit aggregation structure and excited state properties of sensitive units, developed high-performance explosives and narcotics-sensitive film materials, creating a gaseous phase detection record of 10-15 molar magnitude, and realizing the highly sensitive, fast and reversible detection of a variety of drugs such as methamphetamine and liquid explosives such as Mother of Satan (Triacetone triperoxide, TATP) for the first time.

In the development of FFSs and detection devices,



they pioneered the structure of laminated thin-film fluorescent sensors, breaking the monopoly of foreign companies on waveguide technology and achieving a breakthrough in the underlying technology of FFSs.

On the basis of the innovation of sensitive materials and sensor hardware structure, they invented new explosives sensors, narcotics sensors, explosives/narcotics array sensors, developed SRED series explosives single-module, created SRED drug single-module and SRED explosives/narcotics dual-module fluorescence detection devices, creating explosives and narcotics detection records with the fastest response, highest sensitivity and the most number of uses of thin-film devices, and realized the created-in-China manufacture of high-end FFSs sensors and detection devices.

These devices and equipment have been applied in many fields and sold abroad, and began to be used by the Chinese military in 2019. The development of FFSs and devices for ultra-sensitive detection of high-risk substances such as chemical warfare agents, nerve agents, and pathogens is also in progress. Based on his original research, Prof. Fang Yu published the world's first monograph on "Film-based Fluorescence Sensing Technology and Application".

After selection and rigorous review, the world's largest and most authoritative chemical organization, the International Union of Pure and Applied Chemistry (IUPAC), announced on October 17, 2022 that the FFSs proposed by Prof. Fang Yu's group were selected as the fourth place in the IUPAC Top Ten Emerging Technologies in Chemistry 2022.

As a new segment in sensors, FFSs have become the most promising microtrace material detection technology after ion mobility spectroscopy. There is reason to believe that FFSs will play an increasingly important role in many areas such as serving national construction, safeguarding people's lives and properties, and improving disease diagnosis capabilities.

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