陕西师范大学 SHAANXI NORMAL UNIVERSITY

化学化工学院 School of Chemistry & Chemical Engineering

07 / 2023

光子鼻与分子材料团队 简 报

Photonic Nose and Molecular Materials Group Newsletter

PNAS RESEARCH ARTICLE | CHEMISTRY BIOCHEMISTRY OPEN ACCESS

Wrapping anisotropic microgel particles in lipid membranes: Effects of particle shape and membrane rigidity

Xiaoyan Liu[a,b,1], Thorsten Auth[c,1], Nabanita Hazra[d], Morten Frendø Ebbesen[e], Jonathan Brewer[e], Gerhard Gompper[c], Jérôme J. Crasso and Emma Sparr[b]

Edited by Monica Olvera de la Cruz, Northwestern University, Evanston, IL; received October 13, 2022; accepted April 13, 2023

目 录 Contents

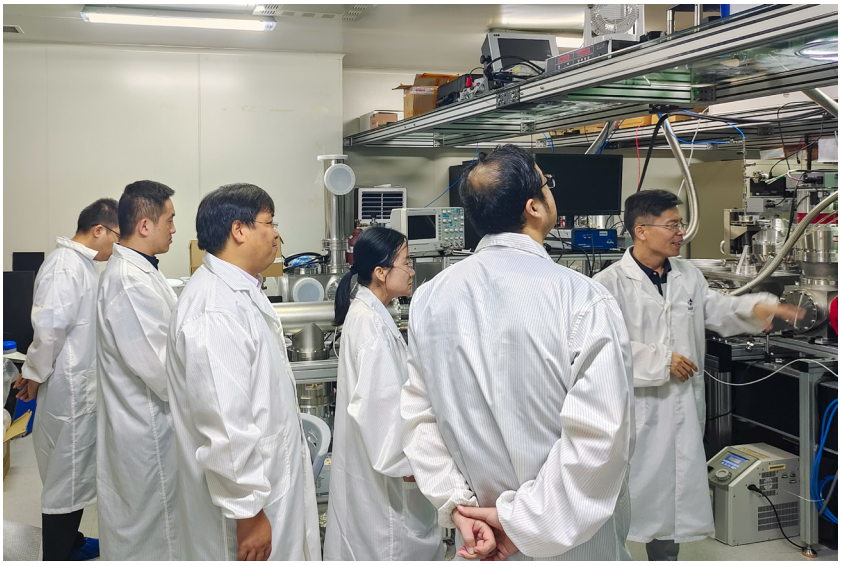
团队应邀赴西安光学精密机械研究所交流

Fang Group visit Xi'an Institute of Optics and Precision Mechanics

2023 年 7 月 6 日上午，新概念传感器与分子材料研究院副院长丁立平教授一行应邀赴中国科学院西安光学精密机械研究所座谈交流。

研究院一行参观了西安光机所瞬态室，并与光机所就共建联合实验室协议内容，联合实验室名称，双方互聘人员，职工、师生科研交流等事项进行了座谈交流。

参加座谈交流的有西安光机所基础科研部、阿秒科学与技术中心副部长、常务副主任付玉喜研究员，基础科研处处长王博研究员，基础科研处主管杨秉青，阿秒科学与技术中心慧丹丹、薛冰研究员，李加林副研究员；陕西师范大学化学化工学院副院长刘成辉教授，科学技术处副处长曹晓仪，化学化工学院刘太宏副教授，新概念传感器与分子材料研究院办公室主任杨小刚。



On July 6, 2023, Prof. Ding Liping, vice dean of the Institute of New Concept Sensors and Molecular Materials, and her colleagues were invited to visit the Xi'an Institute of Optics and Precision Mechanics of Chinese Academy of Sciences.

INCSMM visitors visited XIOPM's transient room, and had a discussion with XIOPM on the issues including the contents of the joint laboratory agreement, the name of the joint laboratory, the dual employment of personnel, and the exchange of staff, faculty and students.

Participating in the discussion were Fu Yuxi, XIOPM executive deputy director, vice director of Basic Research Department and Attosecond Science and Technology Center, Wang Bo, director of XIOPM Basic Research Department, Yang Bingqing, chief of XIOPM Basic Research Department, and Hui Dandan, Xue Bing, and Li Jialin of Attosecond Science and Technology Center; and Prof. Liu Chenghui, vice Dean of School of Chemistry and Chemical Engineering of Shaanxi Normal University, Cao Xiaoyi, vice director of SNNU's Department of Science and Technology, Liu Taihong, Associate Professor of the School of Chemistry and Chemical Engineering, Yang Xiaogang, director of the Administrative Office of the Institute of New Concept Sensors and Molecular Materials.

陕西省化学会物理化学专业委员会暨第九届陕西省物理化学发展研讨会协调会在我院召开

Coordination meeting of SCS Physical Chemistry Committee held at INCSMM

2023 年 7 月 18 日下午，陕西省化学会物理化学专业委员会暨第九届陕西省物理化学发展研讨会协调会在陕西师范大学新概念传感器与分子材料研究院一层会议室召开。

陕西省化学会物理专业委员会主任委员房喻院士、新一届委员会委员西安科技大学刘向荣教授、西北大学马海霞教授、陕西师范大学丁立平教授以及上一届委员西安交通大学赵翔教授、陕西师范大学王文亮教授参加了会议。

会议还邀请了第九届陕西省物理化学发展研讨会承办单位陕西理工大学季晓晖教授和靳玲霞教授、陕西师范大学刘峰毅教授和边红涛教授参加了会议。

会上，房喻院士向新一届委员介绍了陕西省物理化学专业委员会的发展历史和建设情况，肯定了上一届委员对陕西省物理化学学科发展做出的卓越贡献，并希望新一届委员继承好的传统，创新性开展工作，为陕西省物理化学发展建言献策。

季晓晖院长就第九届陕西省物理化学发展研讨会的前期准备情况进行了介绍，会议代表就会议举办时间、会议规模、会议报告安排等进行了讨论和商定，并就后期的筹备工作进行了初步安排。

会议决定，要充分发挥陕西省物理化学发展研讨会的平台作用，为陕西省物理化学工作者提供交流的机会，为优秀的青年学者提供展示的舞台。

On July 18, 2023, the Coordination Meeting of the Physical Chemistry Committee of Shaanxi Chemical Society and the Ninth Shaanxi Physical Chemistry Development Symposium was held in the conference room of the Institute of New Concept Sensors and Molecular Materials, Shaanxi Normal University.

Prof. Fang Yu, chairman of SCS Physical Committee, new members Prof. Liu Xiangrong of Xi'an University of Science and Technology, Prof. Ma Haixia of Northwestern University, Prof. Ding Liping of Shaanxi Normal University, as well as previous members Prof. Zhao Xiang of Xi'an Jiaotong University, and Prof. Wang Wenliang of Shaanxi Normal University, attended the meeting.

Prof. Ji Xiaohui and Prof. Jin Lingxia of Shaanxi University of Science

and Technology, the organizer of the 9th Shaanxi Physical Chemistry Development Symposium, and Prof. Liu Fengyi and Prof. Bian Hongtao of Shaanxi Normal University were also invited to the meeting.

At the meeting, Fang Yu briefed the new members of the history and construction of the committee, affirmed the contribution of the previous members to the development of physical chemistry in Shaanxi Province, and hoped that the new members would inherit the good tradition, carry out their work innovatively, and offer advice and suggestions for the development of physical chemistry in Shaanxi Province.

Ji Xiaohui gave a presentation on the preliminary preparations for the 9th Shaanxi Physical Chemistry Development Symposium, and the participants discussed and agreed on the time, scale of the conference, and the arrangement of the conference reports, and made initial arrangements for the preparations in the later stage.

The meeting suggested that the platform of Shaanxi Physical Chemistry Development Symposium should be fully utilized to provide opportunities for physical chemists in Shaanxi Province to communicate with each other and a stage for excellent young scholars to show their talents.

砺剑防卫智能安检设备标准获国家邮政行业科学技术二等奖

SRED equipment standard awarded second prize of National Postal Industry S&T Award

2023 年 7 月 28 日，快递绿色科技发展大会暨第三届邮政行业科学技术奖颁奖仪式在北京举行，深圳砺剑防卫防卫技术有限公司“邮政快件智能安检设备标准体系研究应用”项目获科学技术二等奖。

砺剑防卫依靠房喻院士团队深耕荧光技术，在荧光敏感材料及传感器结构设计构建了全链条知识产权，打破国外技术壁垒，并于 2018 年作为七家成员单位唯一一家荧光传感技术解决方案提供商获邀参与国家邮政局新一代智能安检系统的联合研发，为快递物流行业定制开发了国内最轻便的爆炸物探测设备。2020 年砺剑防卫牵头并组织五家单位共同完成了《邮政行业基于荧光聚合物传感技术的手持式痕量炸药探测仪技术要求》（YZ/T 0176–2020）标准的起草制定工作。

邮政行业科学技术奖由中国快递协会主办，国家科学技术奖励工作办公室批准，于 2018 年正式设立，旨在表彰在邮政、快递科学技术活动中做出突出贡献的组织或个人。

On July 28, 2023, Shenzhen SRED Security and Surveillance Technology's project of "Research and Application in Postal Express Smart Security Inspection Equipment Standard System" was awarded the second prize of Science and Technology Award at Green Express Technology Development Conference and the third Postal Industry Science and Technology Awards Ceremony held in Beijing.

Relying on the fluorescent technology developed by Prof. Fang Yu's group, SRED Security has cultivated and built a full chain of intellectual property rights in fluorescent sensitive materials and sensor structure design, breaking foreign technical barriers. In 2018, as the only fluorescent sensing technology solution provider of the seven member units, SRED Security was invited to participate in the joint research and development of the State Postal Bureau's new-generation smart security inspection system, and developed a customized explosive detection equipment for the courier and logistics industry, which is the lightest in China. In 2020, SRED Security led and organized five units to complete the drafting and formulation of the standard "Technical Requirements for Handheld Trace Explosives Detectors Based on Fluorescent Polymer Sensing Technology in the Postal Industry" (YZ/T 0176-2020).

The Postal Industry Science and Technology Award, sponsored by the China Express Association and approved by the State Office for Science and Technology Awards, was formally established in 2018 to recognize organizations or individuals who have made outstanding contributions to postal and express science and technology activities.

房喻院士出席全国高师第 24 届物理化学教学研讨会并作报告

Fang Yu speaks at 24th National Normal University Physical Chemistry Teaching Seminar

2023 年 7 月 7 日至 10 日，房喻院士应邀赴兰州出席全国高师第二十四届物理化学（含实验）教学研讨会并作题为“基础科学的重要性—以化学科学为例”的大会报告。此次研讨会由全国高师物理化学教学中心组主办，西北师范大学、甘肃农业大学、师范院校物理化学课程虚拟教研室和西部高校化学专业（师范）虚拟教研室共同承办。

From July 7 to 10, 2023, Prof. Fang Yu attended and gave a conference report titled “The Significance of Basic Science - Taking Chemical Science as an Example” at the 24th Physical Chemistry (including Experimental) Teaching Seminar held in Lanzhou. The seminar was sponsored by the Physical Chemistry Teaching Center Group of National Normal Universities and Colleges, and jointly hosted by Northwest Normal University, Gansu Agricultural University, Virtual Teaching and Research Department of Physical Chemistry Courses of Normal Universities and Colleges, and the Virtual Teaching and Research Department of Physical Chemistry (Teacher Training) in Western Universities and Colleges.

房喻院士受邀访问中国石油兰州石化公司

Fang Yu visits PetroChina Lanzhou Petrochemical Company

2023 年 7 月 8 日，房喻院士和团队刘太宏、彭浩南两位老师受邀参观了中国石油兰州石化公司，走进石油精神教育基地，感受兰州石化的厚重文化及发展理念。作为“共和国长子”和石油化工的“摇篮”，兰州石化是新中国第一个现代化炼油化工生产基地，已累计加工原油 2.87 亿吨、上缴税费 1674 亿元。

On July 8, 2023, Prof. Fang Yu and Photonic Nose and Molecular Materials Group members Dr. Liu Taihong and Prof. Peng Haonan visited PetroChina Lanzhou Petrochemical Company. They toured the Petroleum Spirit Educational Base to experience Lanzhou Petrochemical’s rich culture and development concept.

As the “Eldest Son of the Republic” and the “Cradle” of China’s petrochemical industry, Lanzhou Petrochemical Company is the first modernized refining and chemical production base in China after founding of the republic, with a total of 287 million tons of crude oil processed and 167.4 billion yuan of taxes and fees contributed.

团队教师参加第九届全国高等学校物理化学课程教学研讨会

Fang Group teachers attend 9th National College Physical Chemistry Course Teaching Symposium

2023 年 7 月 7 日至 10 日，光子鼻与分子材料团队刘静教授、丁立平教授和边红涛教授参加了在北京理工大学良乡校区举行的“第九届全国高等学校物理化学（含实验）课程教学研讨会”。此次研讨会由教育部高等学校化学类专业教学指导委员会、南开大学、北京理工大学、科学出版社联合主办。

From July 7 to 10, 2023, Prof. LiuJing, Prof. Ding Liping and Prof. Bian Hongtao from Photonic Nose and Molecular Materials Group attended the Ninth National Symposium on Teaching of Physical Chemistry (Including Experiments) in Colleges and Universities in the Liangxiang Campus of Beijing Institute of Technology. The Symposium was jointly organized by the Steering Committee for Teaching Chemistry in Colleges and Universities of the Ministry of Education, Nankai University, Beijing Institute of Technology and Science Publishing House.

刘凯强教授参加中国材料大会水凝胶材料分会并作报告

Liu Kaiqiang presents at Hydrogel Material Session of China Materials Conference

2023 年 7 月 8 日至 11 日，刘凯强教授参加了在深圳举办的 2022–2023 中国材料大会水凝胶材料分会并作题为“功能软物质及其应用：限域结晶与界面粘合”的邀请报告。此次大会由中国材料研究学会主办，水凝胶材料分会由上海交通大学、中山大学、浙江大学和国科温州研究院承办。

From July 8 to 11, 2023, Prof. Liu Kaiqiang attended the Hydrogel Materials Session of 2022-2023 China Materials Conference held in Shenzhen and gave an invited report titled "Functional Soft Matter and Its Applications: Confined Crystallization and Interfacial Adhesion". The conference was sponsored by the Chinese Society for Materials Research, and the Hydrogel Materials Session was hosted by Shanghai Jiaotong University, Sun Yat-sen University, Zhejiang University and Wenzhou Institute UCAS.

薄鑫老师指导学生团队获第九届互联网 + 大赛校内选拔赛铜奖

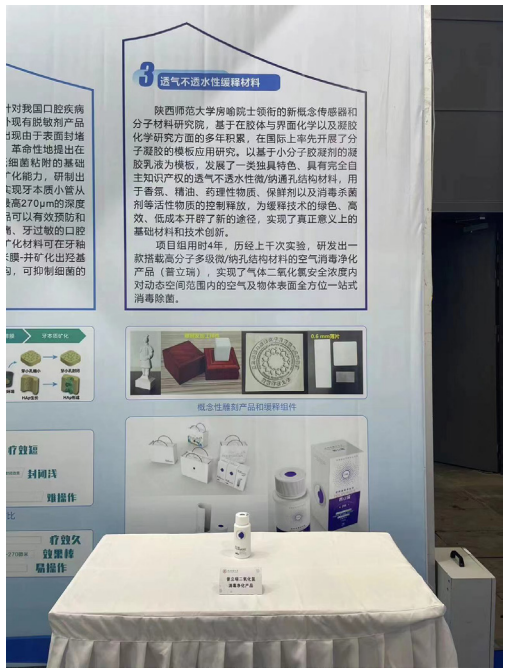
Bo Xin coaches student team to win bronze prize at 9th Internet+ Competition Intramural Tryout

2023 年 7 月 15 日，在第九届中国国际“互联网 +”大学生创新创业大赛陕西师范大学校内选拔决赛上，由新概念传感器与分子材料研究院薄鑫老师指导的、由 2022 级化学专业本科生闫禹彤、猴雅宁、陈晓钻组成的“墨希”团队获本科生创意组校级铜奖。

On July 15, 2023, at the Shaanxi Normal University intramural tryout of the 9th China International Internet Plus Student Innovation and Entrepreneurship Competition, the team Moxi, which is composed of Class 2026 undergraduates of Chemistry major students Yan Yutong, Gou Yaning and Chen Xiaodrang, and coached by Dr. Bo Xin of the Institute of New Concept Sensors and Molecular Materials, won the Bronze Prize of Undergraduates Creative Group.

团队成果亮相第 17 届中国西安国际科学技术产业博览会

Fang Group achievements exhibited at 17th China Xi'an Int'l S&T Industry Expo



2023 年 7 月 14 至 16 日，由光子鼻与分子材料团队研发的透气不透水性缓释材料和隐藏爆炸物超灵敏探测仪等成果，在西安国际会展中心举行的“2023 第 17 届中国西安国际科学技术产业博览会暨硬科技产业博览会”上亮相展出。

From July 14th to 16th, 2023, the breathable and impermeable sustained-release materials and the ultra-sensitive hidden explosives detector developed by the Photonic Nose and Molecular Materials Group were exhibited at the 17th Xi'an International Science and Technology Industry Expo and Key & Core Tech Industry Expo held at the Xi'an International Convention and Exhibition Center in Xi'an, China.

房喻院士应邀出席 2023 亚太肉类科技大会

Fang Yu attends 2023 Asia-Pacific Meat Science and Technology Conference

2023 年 7 月 20 日，房喻院士应邀赴西安市临潼区出席 2023 亚太肉类科技大会暨第二十届中国肉类科技大会暨第七届肉类加工与新产品开发技术研讨会，并与王鹏副区长为 20 个研究生论坛汇报优秀奖获奖者颁奖并合影留念。此次会议由中国畜产品加工研究会、食品伙伴网、陕西师范大学、临潼区人民政府联合举办。

On July 20, 2023, Prof. Fang Yu attended the 2023 Asia-Pacific Meat Science and Technology Conference and the 20th China Meat Science and Technology Conference and the 7th Symposium on Meat Processing Technology and New Product Development in Lintong District, Xi'an, China, and presented awards to the 20 winning presenters of Postgraduate Forum and took a group photo together with deputy head of district Wang Peng. The conference was jointly organized by the China Livestock Product Processing Research Association, Food Partner Network, Shaanxi Normal University, and Lintong District Government.

房喻院士应邀出席第二届全国精细化工大会并作报告

Fang Yu speaks at Second National Fine Chemical Industry Conference

2023 年 7 月 23 日，房喻院士应邀赴大连出席第二届全国精细化工大会暨 2023 大连市科协年会开幕式，并作题为“薄膜荧光传感器——从敏感材料创新到器件结构研制”的大会报告。此次会议由中国化工学会精细化工专业委员会、大连市科协、《精细化工》编辑部主办，会议主题为“新时代中国精细化工前沿与行业发展”。

On July 23, 2023, Prof. Fang Yu was invited to Dalian to attend the opening ceremony of the Second National Fine Chemical Conference and the 2023 Annual Meeting of Dalian Association of Science and Technology, and gave a report titled “Film-based Fluorescent Sensors - From Innovation of Sensitive Materials to Development of Device Structure”. The conference was organized by the Fine Chemical Committee of the Chinese Chemical Society, Dalian Science and Technology Association, and the editorial department of Fine Chemical Industry, with the theme of “Frontier and Development of China’s Fine Chemical Industry in the New Era”.

马佳妮教授参加微纳结构表征创新论坛并作报告

Ma Jiani presents at Micro-Nano Structure Characterization Innovation Forum

2023 年 7 月 24 日至 26 日，光子鼻与分子材料团队马佳妮教授参加了由中国微米纳米技术学会主办、兰州理工大学承办，在兰州举办的“微纳结构表征创新论坛”，并在微纳体系表征技术发展及其应用分会场做了题为“薄膜荧光传感分子激发态行为研究”的邀请报告。

From July 24 to 26, 2023, Prof. Ma Jiani of the Photonic Nose and Molecular Materials Group participated in the Micro-Nano Structure Characterization Innovation Forum sponsored by the Chinese Society of Micro-Nano Technology and hosted by Lanzhou University of Technology in Lanzhou, and made an invited presentation titled Research on Excited State Behavior of Film Fluorescence Sensing Molecules at the parallel session on the development and application of micro-nano system characterization technology.

团队物理化学类研究生培养模式获国家级教学成果二等奖

Fang Group Physical Chemistry Graduate Student Cultivation Model awarded Second Prize of National Teaching Achievements


中华人民共和国教育部
Ministry of Education of the People's Republic of China

信息名称： 教育部关于批准2022年国家级教学成果奖获奖项目的决定
信息索引： 360A10-04-2023-0009-1 生成日期： 2023-07-24 发文机构： 中华人民共和国教育部
发文字号： 教师〔2023〕4号 信息类别： 教育综合管理
内容概述： 教育部关于批准2022年国家级教学成果奖获奖项目的决定

教育部关于批准2022年国家级教学成果奖
获奖项目的决定

教师〔2023〕4号

国家级教学成果奖评审委员会评审确定的2022年国家级教学成果奖项目，已经公示并完成异议处理，共计1998项成果获得国家级教学成果奖。

2023 年 7 月 24 日，教育部发布关于批准 2022 年国家级教学成果奖获奖项目的决定，房喻院士主持的项目“‘素养为要 能力为本’物理化学类研究生五维一体培养模式的探索与实践”荣获高等教育（研究生）国家级教学成果二等奖。项目完成人为房喻、丁立平、刘静、 杨鹏、彭军霞、边红涛、刘凯强、刘太宏、彭浩南、苗荣和刘忠山。此次共计 1998 项成果获得国家级教学成果奖，其中特等奖 7 项，一等奖 245 项，二等奖 1746 项。

On July 24, 2023, the Ministry of Education released a decision on the approval of the winning projects of 2022 National Teaching Achievement Award, and Fang Group project “Exploration and Practice of Literacy-focused and Capacity-based Five-dimensional Integrated Cultivation Model for Physical Chemistry Graduate Student” headed by Prof. Fang Yu was awarded the Second Prize of National Teaching Achievement Award in Higher Education (Graduate Students). The participants of the project are Fang Yu, Ding Liping, Liu Jing, Yang Peng, Peng Junxia, Bian Hongtao, Liu Kaiqiang, Liu Taihong, Peng Haonan, Miao Rong and Liu Zhongshan. A total of 1998 projects have been awarded the national teaching achievement awards, including 7 grand prizes, 245 first prizes and 1746 second prizes.

研究院参赛项目获第九届互联网 + 大学生创新创业大赛陕西省金奖

INCSMM project wins Shaanxi Gold Award in 9th Internet+ Innovation and Entrepreneurship Competition for College Students

2023 年 7 月 28 日，新概念传感器与分子材料研究院参赛项目“‘膜’法控释消毒除菌——空间安全守护者”在第九届中国国际“互联网 +”大学生创新创业大赛陕西赛区省级复赛上获得金奖。

参赛学生团队由化学化工学院本科生李重洋、曾嘉琪、彭旭阳、马岩婷、董芯如和国际商学院本科生周文、张怡、杨可欣等八名同学组成，指导教师为彭军霞副教授。房喻院士对团队进行了多次指导。

On July 28, 2023, the project of the Institute of New Concept Sensors and Molecular Materials, “Membrane Controlled-Release Disinfectant - Guardian of Environment Safety”, won the Gold Prize at the Shaanxi Provincial Competition of the Ninth China International Internet+ Innovation and Entrepreneurship Competition for College Students.

The student team consist of eight undergraduates, including Li Chongyang, Zeng Jiaqi, Peng Xuyang, Ma Yanting, Dong Xinru from the School of Chemistry and Chemical Engineering, and Zhou Wen, Zhang Yi, and Yang Kexin from the International Business School. Associate Professor Peng Junxia is their coach, and Prof. Fang Yu also instructed the team.

PNAS RESEARCH ARTICLE | CHEMISTRY BIOCHEMISTRY OPEN ACCESS

Wrapping anisotropic microgel particles in lipid membranes: Effects of particle shape and membrane rigidity

Xiaoyan Liu[a,b,1], Thorsten Auth[c,1], Nabanita Hazra[d], Morten Frendø Ebbesen[e], Jonathan Brewer[e], Gerhard Gompper[c], Jérôme J. Crassous[d], and Emma Sparr[b]

Edited by Monica Olvera de la Cruz, Northwestern University, Evanston, IL; received October 13, 2022; accepted April 13, 2023

各向异性纳米颗粒的形状和细胞膜的刚性对胞吞作用的影响

细胞通过胞吞作用吞噬和摄取大分子组装体或胶体纳米颗粒与药物递送、医学诊疗、以及纳米颗粒的潜在毒性密切相关。胞吞作用受到体系的物理和化学属性影响，附着在细胞膜上的纳米颗粒可能稳定吸附在膜表面、或者被膜包裹、也可能穿过细胞膜进入细胞内部。此研究通过设计合成各向异性的纳米颗粒和合成细胞膜研究了胶体颗粒与脂质膜的相互作用，致力于揭示胞吞作用受纳米颗粒和细胞膜物理和化学属性影响的规律。

研究发现体积相近的各向异性软物质纳米颗粒更容易进入细胞内部，并且发现细胞膜在具有较高流动性时更有利于胞吞作用发生。同时通过理论计算预测了纳米颗粒的粘附强度对胞吞作用的影响，阐明了细胞膜和各向异性纳米颗粒的物理属性、以及颗粒与细胞膜之间的粘附强度对胞吞作用的影响，并且发展了制备二维胶体晶体组装结构的新方法。

第一作者：陕西师范大学刘小燕副研究员
通讯作者：陕西师范大学刘小燕副研究员，德国于利希研究中心 Thorsten Auth 研究员
全文链接：https://doi.org/10.1073/pnas.2217534120

The cellular uptake of colloidal-sized particles of biological or synthetic origin has important implications for cellular function, and for the design of particles for diagnostic and therapeutic applications in nanomedicine. Here, we present experimental data combined with theoretical modeling showing how anisotropic microgels wrap at the lipid membrane depending on the physicochemical properties of the particles and the membrane. Important properties are the bending rigidity of the membrane,

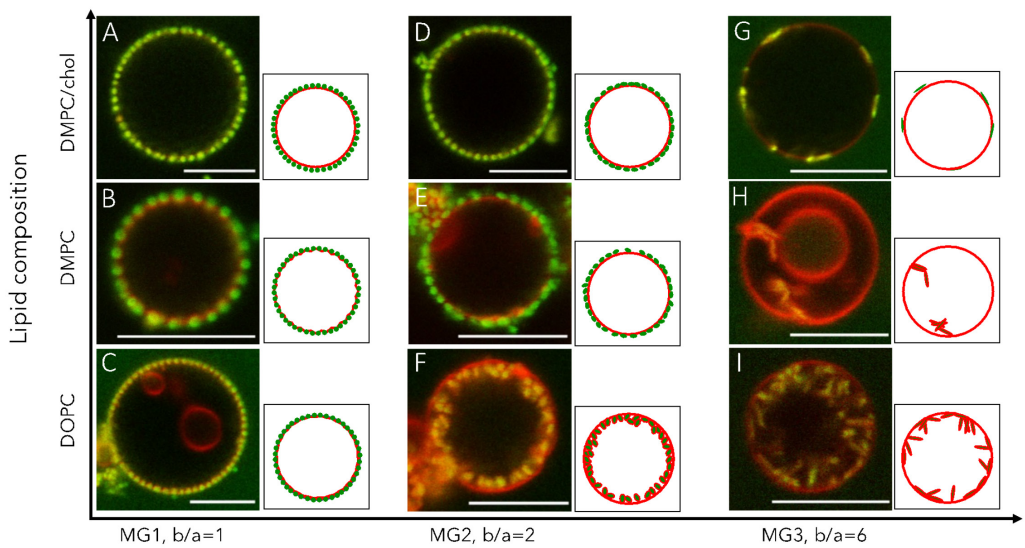


图 1. 不同形状的软物质纳米颗粒与合成细胞膜的相互作用。
Figure 1. 2D CLSM images of adsorption and wrapping of microgel particles (green) on lipid membrane (red) in GUVs.

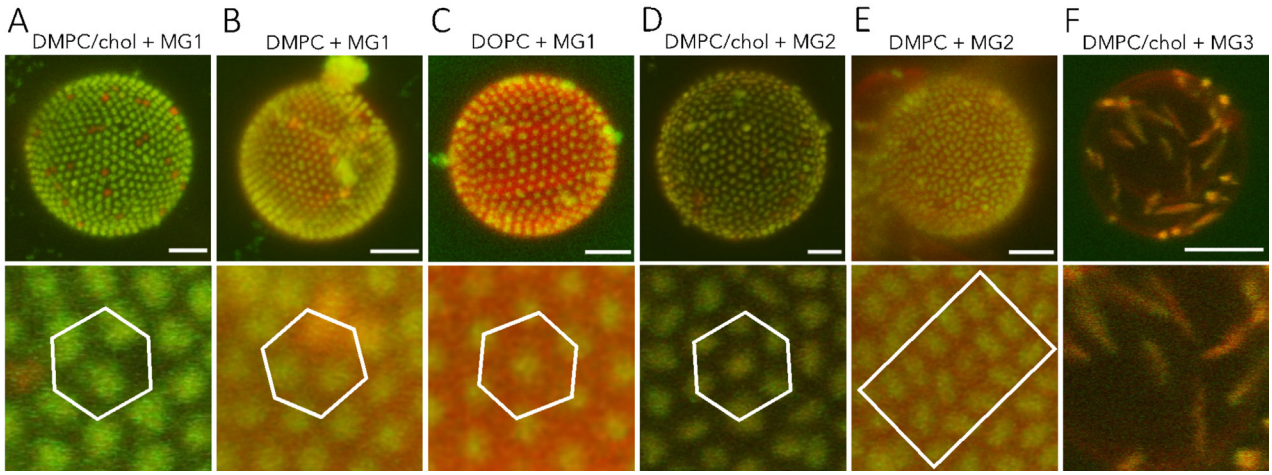


图 2. 不同形状的软物质纳米颗粒在合成细胞膜上的组装结构。

Figure 2. 3D CLSM images of the adsorbed spherical and ellipsoidal microgels on the GUVs.

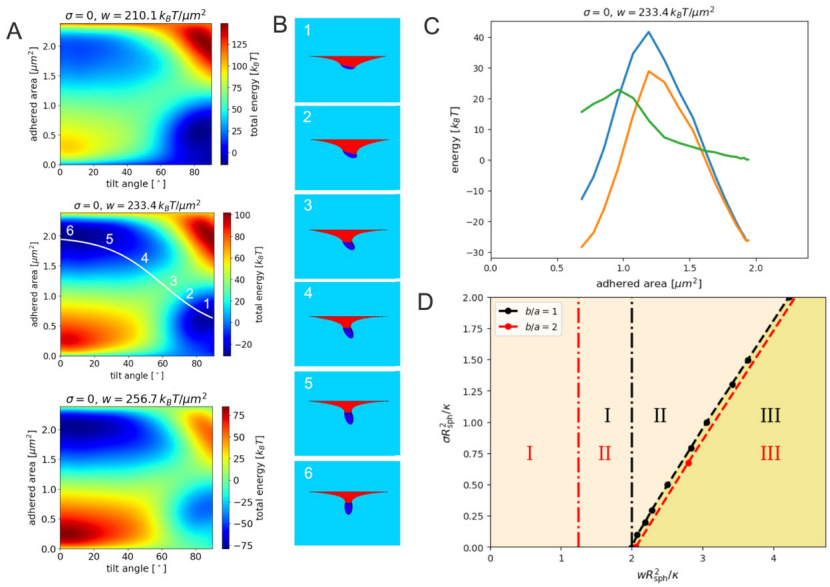


图 3. b/a=2 的椭圆形纳米颗粒与 DOPC 细胞膜相互作用的体系能量。

Figure 3. Wrapping energies for ellipsoidal particles with DOPC GUV.

the particle shape, and the adhesion energy between the particles and the membrane. Accounting for the possibility offered by microgel systems to be custom-designed, it further opens up opportunities for future fundamental studies, therapeutic applications, and self-assembly strategies which involve nanoparticle–membrane interactions.

We have demonstrated in this study that microgel particles wrapping in lipid membranes can be affected by particle shape and membrane rigidity. The general trend is that deep wrapping of the microgels occurs for the lipid membranes with the lowest bending rigidity, and for the microgels with the largest aspect ratio. 2D colloidal crystals with hexagonal structure is formed at the membranes by the spherical microgels. For the shallow wrapped ellipsoidal MG2 microgel local side to side "smectic-like" ordering was observed at DMPC membrane and they also possess some hexagonal positional ordering at more rigid DMPC/chol membrane. While the ellipsoidal microgels of the highest aspect ratio show random distribution and orientation at DMPC/chol membrane. The microgels strongly prefer to adsorb to the liquid disordered membrane. The calculations predict the same behavior with respect to shallow and deep wrapping as observed in the experimental studies under the conditions when the adhesion strength is slightly higher for the ellipsoidal microgels compared with the spherical ones. We believe that the observations of microgel particle wrapping in the model systems add new understandings to how particle shape and membrane properties engulfment and endocytic processes in living cells and provide new strategies to the future design of novel self-assembling structures on fluid templates by employing nonspherical particles.

First Author: Dr. Liu Xiaoyan, Shaanxi Normal University

Corresponding Authors: Dr. Liu Xiaoyan, Shaanxi Normal University; Dr. Thorsten Auth, Forschungszentrum Jülich, Germany

Full Text Link: https://doi.org/10.1073/pnas.2217534120

THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCL Letter

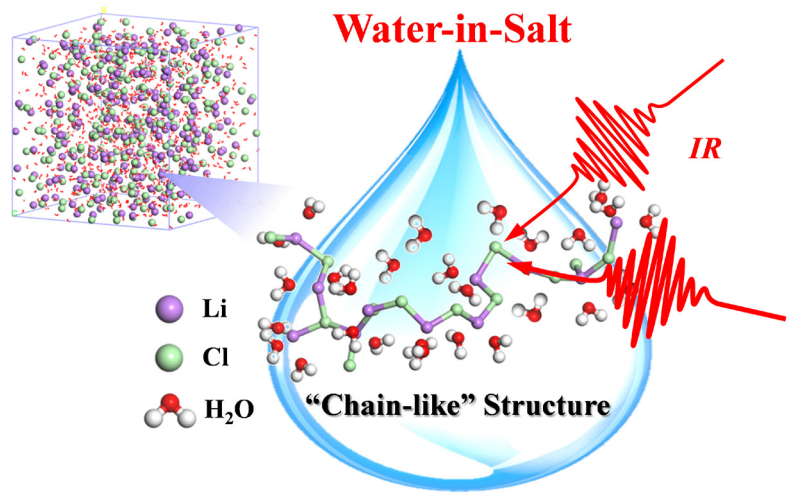
Chain-like Structures Facilitate Li^+ Transport in Concentrated Aqueous Electrolytes: Insights from Ultrafast Infrared Spectroscopy and Molecular Dynamics Simulations

Miaomiao Zhang, Yuting Gao, Lanya Fu, Yimin Bai, Somnath Mukherjee, Cheng-Lung Chen, Jing Liu,* Hongtao Bian,* and Yu Fang

Cite This: *J. Phys. Chem. Lett.* 2023, 14, 6968−6976 Read Online

链状结构促进超浓水系电解质中的 Li^+ 传输：超快红外光谱和分子动力学模拟研究

在锂离子电池（LIBs）领域，水系电解质因其优越的安全性和离子导电性引起了广泛关注。这些水系电解质具有较长的循环寿命和可观的能量密度，因此在能量储存系统和设备的大规模应用中具有极高的应用潜力。然而，水的较窄电化学稳定性窗口长期以来一直是该领域的一个挑战。"盐包水"（Water−in−salt，浓度一般高于 10 m）电解质的出现为解决这个问题提供了可能，它通过扩大水的电化学稳定性窗口来提高能量密度，极大的推动了水系电解质的发展。然而，在高浓度水溶液中，Li^+ 的传导和其局部溶剂结构仍未完全了解。Li^+ 的溶剂化结构和特定离子 – 离子相互作用对于理解其迁移行为以及确定宏观粘度和电导率至关重要。溶液中的离子扩散通常通过两种迁移模式进行：集体迁移和跳跃传输。集体迁移是指离子及其紧密结合的溶剂化层作为一个整体扩散。相反，跳跃传输是一种通过溶剂化层之间的连续解离或结合交换来进行离子扩散的过程。有关水系电解质溶液中 Li^+ 传导机制目前仍不清楚，前期研究表明，氢键网络重新排列有助于实现集体迁移。然而，由于氢键网络的重新排列在超快时间尺度上（快于 1 纳秒）发生，目前尚未就水系电解质中 Li^+ 的传导机制达成共识。



为了深入研究这一问题，本文采用了超快红外光谱和分子动力学模拟来研究超浓 LiCl 水溶液中 Li^+ 的结构和动力学。本文采用超快红外光谱和硫氰酸根（SCN^-）作为局部阴离子振动探针，研究 LiCl 水溶液中 Li+ 的结构动力学。实验发现外部探针的红外

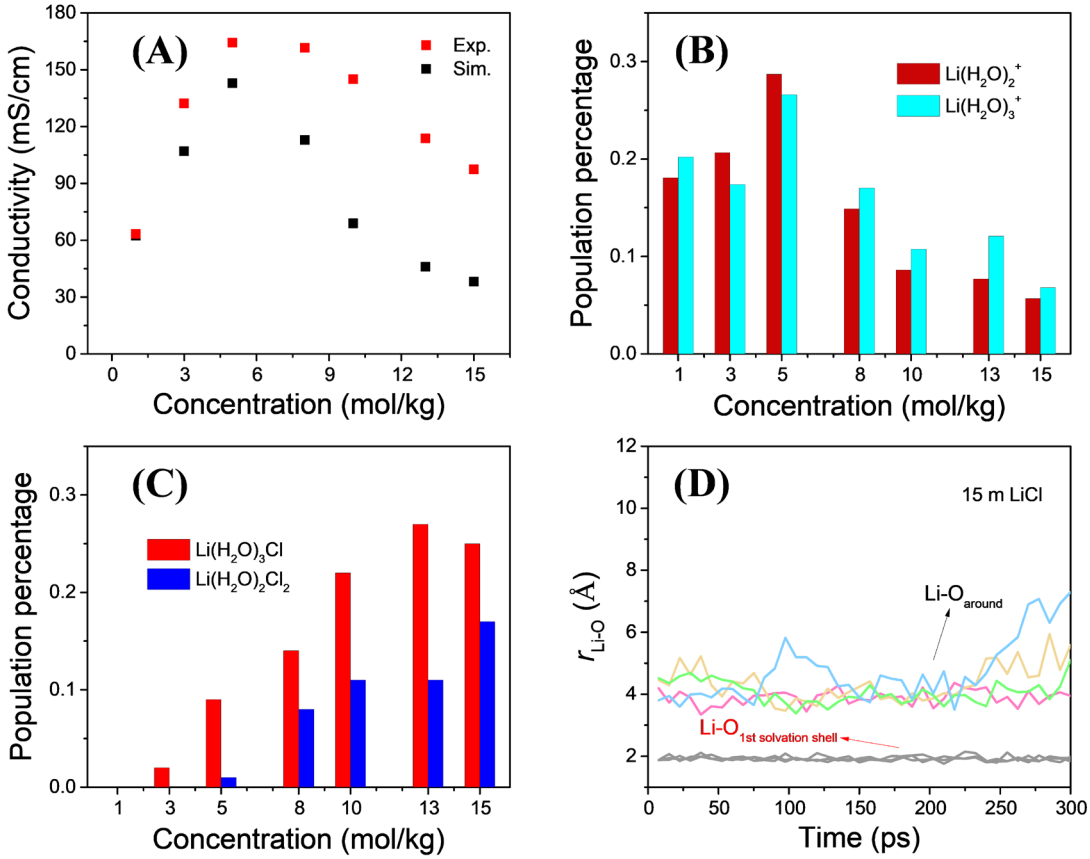


图 . (A) 不同浓度下 LiCl 溶液的实验和分子动力学模拟计算电导率。(B) LiCl 溶液中 $Li(H_2O)_2^+$ 和 $Li(H_2O)_3^+$ 物种随浓度的变化趋势。(C) LiCl 溶液中 $Li(H_2O)_3Cl$ 和 $Li(H_2O)_2Cl_2$ 物种随浓度的变化趋势。(D) 15 m LiCl 水溶液中，在 300 ps 时间范围内指定 Li^+ 和氧原子的轨迹 (r(Li−O))。

Figure . (A) Experimental and calculated conductivity of LiCl solutions at different concentrations. (B) Population trends of $Li(H_2O)_3Cl$ and $Li(H_2O)_2Cl_2$ complexes in aqueous LiCl solutions as a function of concentration. (C) Population trends of $Li(H_2O)_3Cl$ and $Li(H_2O)_2Cl_2$ complexes in aqueous LiCl solutions as a function of concentration. (D) Trajectories of selected Li^+ and oxygen atoms in water molecules (r (Li-O)) over 300 ps time range in LiCl aqueous solutions.

频率和振动弛豫动力学强烈依赖于体相浓度，可以有效探测 Li+ 的局部环境和结构动力学，同时弥补了以往文献中使用 OD 伸缩振动作为探针的局限性。通过使用 Stokes–Einstein–Debye（SED）方程，分析了 LiCl 水溶液中外部探针的取向转动时间常数与宏观粘度的关联性，揭示了离子 – 水络合物的形成和动态非均匀结构。为了获得 LiCl 水溶液中的空间结构非均匀性，进行了分子动力学（MD）模拟。这些模拟揭示了 Cl^- 和 Li^+ 通过静电相互作用在高浓度下形成链状结构。这些扩展的链状结构强烈限制了水分子在其周围的运动，影响了 Li^+ 的动力学和传输。通过分子动力学模拟，我们可以获得与实验相当吻合的 LiCl 水溶液浓度依赖的电导率。进一步分析发现，$Li(H_2O)_2^+$ 和 $Li(H_2O)_3^+$ 是主要的离子物种，对 Li+ 的传导起着主要的贡献。作者还对 15 m LiCl 溶液中选定锂离子和水分子氧原子的轨迹（r(Li–O)）进行了长达 300 ps 的动力学分析。轨迹分析支持锂离子通过溶剂和离子之间形成的动态链状结构进行集体迁移。锂离子的笛卡尔坐标分析显示，Li^+ 与第一层溶剂化水分子之间的 r(Li–O) 距离保持在约 2.0 Å，表明与相邻三个水分子形成了稳定的络合物。然而，在给定时间范围内，周围的水分子会靠近然后再远离，但从未突破溶剂化层进入更内部的溶剂化层，表明 Li^+ 扩散主要通过集体迁移传输而非跳跃传输。实验和 MD 模拟表明，$Li(H_2O)_3Cl$ 和 $Li(H_2O)_2Cl_2$ 则主要决定 LiCl 溶液的粘度。离子 – 水络合物和链状结构能够促进 Li+ 通过水系电解质的集体迁移，这些结果有望深入解析高浓度电解质水溶液中黏度和电导率的起源。

本文为我们深入理解高浓度水系电解质中 Li^+ 的结构动力学和传输机制提供了重要的见解。理解链状结构和离子 – 水络合物在 Li^+ 传导中的作用，有可能为开发新的水系电解质指明方向，并用于锂离子电池中。通过建立离子对结构与宏观性质之间的相关性，可推动设计更安全、更高效的锂离子电池，实现水系电解质在能源存储领域的广泛应用。

第一作者：陕西师范大学博士研究生张苗苗
通讯作者：陕西师范大学边红涛教授、刘静教授

全文链接：https://pubs.acs.org/doi/10.1021/acs.jpclett.3c01494

In the field of lithium-ion batteries (LIBs), aqueous electrolytes have garnered extensive attention due to their superior safety and ionic conductivity. These aqueous electrolytes exhibit long cycling life and significant energy density, making them highly promising for large-scale applications in energy storage systems and devices. However, the narrow electrochemical stability window of water has been a persistent challenge in this field. The emergence of "Water-in-salt" (WIS) electrolytes offers a potential solution by expanding the electrochemical stability window of water, thus significantly advancing the development of aqueous electrolytes. However, in highly concentrated aqueous solutions, the conduction of Li^+ and their local solvation structure remain not fully understood. Understanding the solvation structure of Li^+ and specific ion-ion interactions is crucial for understanding their migration behavior and determining macroscopic viscosity and conductivity. Ion diffusion in solution generally occurs through two modes: vehicular migration and hopping transport. Vehicular migration involves the diffusion of ions and their tightly bound solvated layer as a whole, while hopping transport is a process of ion diffusion through successive dissociation/association exchanges between solvation layers. The mechanism of Li^+ ion conduction in aqueous electrolyte solutions is currently unclear. Some previous studies suggest that rearrangement of hydrogen bonding networks plays a role in achieving vehicular migration. However, due to the rapid timescale (faster than 1 nanosecond) of hydrogen bonding network rearrangement, a consensus on the conduction mechanism of Li^+ in aqueous electrolytes has not been reached.

To solve this issue, we used ultrafast infrared spectroscopy and molecular dynamics simulations to investigate the structure and dynamics of Li^+ in highly concentrated LiCl water solutions. Ultrafast infrared spectroscopy and thiocyanate (SCN) were used as local anionic vibrational probes to study the structural dynamics of Li^+ in LiCl water solutions. The experimental results indicated that the infrared frequencies and vibrational relaxation dynamics of the external probe strongly depend on the bulk concentration, effectively probing the local environment and structural dynamics of Li^+, while overcoming the limitations of using OD stretching vibrations as probes in previous literature. By using the Stokes-Einstein-Debye (SED) equation, the coupling between the reorientational dynamics of the external probe in LiCl water solutions and the macroscopic viscosity was analyzed, revealing the formation and structural dynamics of ion-water complexes. To obtain the spatial structural heterogeneity of LiCl water solutions, molecular dynamics (MD) simulations were performed. These simulations revealed the formation of chain-like structures consisting of chloride ions and Li^+ through electrostatic interactions at high concentrations. These extended chain-like structures strongly constrained the reorientation of water molecules around them, impacting the dynamics and transport of Li^+. Through MD simulations, the concentration-dependent conductivity of LiCl water solutions, which is in good agreement with experimental results, was obtained. Further analysis revealed that $Li(H_2O)_2^+$ and $Li(H_2O)_3^+$ were the main ion species contributing to Li^+ ion conduction. The study also performed a detailed analysis of selected lithium ions and oxygen atoms in water molecules (r(Li-O)) in 15 m LiCl solutions over a time range of 300 ps. The trajectory analysis supported the vehicular migration of Li^+ through the dynamic chain-like structure formed between solvents and ions. The Cartesian coordinates analysis of Li^+ indicated that the r(Li-O) distance between Li+ and water molecules in the first solvation shell remained constant at about 2.0 Å, indicating stable complex formation with the adjacent three waters. However, the surrounding water molecules moved closer and then further away within a given time range but never penetrated the solvated shell to enter the inner solvation sheath, suggesting that Li^+ ion diffusion mainly occurs through vehicular transport rather than hopping. The experimental and MD simulation results indicate that $Li(H_2O)_3Cl$ and $Li(H_2O)_2Cl_2$ are the major determinants of the viscosity of LiCl solutions. These specific Ion-water complexes and chain-like structures facilitate the vehicular migration of Li^+ through the aqueous electrolytes, providing a deeper understanding of the origin of viscosity and conductivity in highly concentrated electrolyte aqueous solutions.

This study provides important insights into the structural dynamics and transport mechanism of Li^+ in highly concentrated aqueous electrolytes. Understanding the role of chain-like structures and ion-water complexes in Li^+ ion conduction may guide the development of novel aqueous electrolytes for use in lithium-ion batteries. Establishing correlations between ion pair structures and macroscopic properties can also facilitate the design of safer and more efficient lithium-ion batteries, promoting the widespread application of aqueous electrolytes in the field of energy storage.

First Author: Zhang Miaomiao, Doctoral candidate, Shaanxi Normal University
Corresponding Authors: Prof. Bian Hongtao, Prof. Liu Jing, Shaanxi Normal University
Full Text Link: https://pubs.acs.org/doi/10.1021/acs.jpclett.3c01494

深圳砺剑防卫公司来院商讨项目合作推进

Shenzhen SRED Security and Surveillance visitors received for promotion of cooperation

2023 年 7 月 4 日，深圳砺剑防卫技术科技有限公司董事长蔡文斌、总经理许 亮一行到访新概念传感器与分子材料研究院，并与房喻院士等召开项目合作推进会。

在参观了研究院成果展厅和实验室之后，蔡文斌董事长一行与房喻院士、辛云宏教授、丁立平副院长等就项目合作推进进行了商讨。双方同意从可实施落地项目、应用研发类项目、基础研发（探索）类项目三个维度加深合作，按照“三步走”的方式推进合作，针对砺剑防卫现有产品存在的技术短板、痛点持续优化提升，借力深圳市政府产业资金扶持共同申报课题，择机设立专项研发课题组，并确定了可实施落地项目、应用研发类项目、基础研发（探索）类项目及负责人。

砺剑防卫公司副总经理胡冬寒、发展部经理崔红、研发部经理吴哲、实验室副主任王莉；研究院刘静教授、彭浩南教授、彭军霞副教授、刘太宏副教授，化学化工学院专职组织员闫永昌，研究院办公室主任杨小刚参加了会议。西安交通大学何刚教授应邀参加了会议。

On July 4, 2023, Shenzhen SRED Security and Surveillance Technology Co., Ltd. president Cai Wenbin and General Manager Xu Liang visited the Institute of New Concept Sensors and Molecular Materials (INCSMM) and held a meeting with Prof. Fang Yu to promote the project cooperation.

After visiting the exhibition room and laboratories of the institute, Cai Wenbin and his colleagues discussed the promotion of project cooperation with Prof. Fang, Prof. Xin Yunhong and Vice dean Prof. Ding Liping. The two sides agreed to deepen cooperation from the three aspects of project implementation, applied research projects and basic research and exploration projects, promote cooperation in accordance with the "three-step" approach, continue to optimize and improve the technical shortcomings and pain points of the existing SRED products, apply for the industrial funds of the Shenzhen municipal government through joint projects, and set up special research and development group, and determined the three projects and the persons in charge.

SRED deputy general manager Hu Donghan, Development Dept manager Cui Hong, Research and Development Dept manager Wu Zhe, Laboratory vice director Wang Li; INCSMM Prof. Liu Jing, Prof. Peng Haonan, Assoc. Prof. Peng Junxia, Assoc. Prof. Liu Taihong, School of Chemistry and Chemical Engineering organizer Yan Yongchang, and Administrative Office director Yang Xiaogang attended the meeting. Prof. He Gang from Xi’an Jiaotong University was invited to attend the meeting.

西安市科协来院调研科普教育基地建设

Xi'an S&T Association visitors received for survey in science education base construction

7月6日上午，西安市科协党组书记、常务副主席耿占军，市科协党组成员、副主席张传时一行前来新概念传感器与分子材料研究院，就科普基地建设情况进行调研，并召开座谈会。

在参观了研究院成果展厅和实验室之后，调研组与中国科学院院士、西安市科协主席房喻教授、陕西师范大学科技处处长薛东教授等进行了座谈，听取了陕西师范大学科研、产学研、科普教育基地建设情况汇报。

长安区副区长梁文辉、区投资商务局相关负责同志陪同调研，陕西师范大学科技处副处长屈新运、肖辉等参加座谈。

On July 6, Geng Zhanjun, secretary of the Party Group and executive vice chairman of Xi'an Science and Technology Association, and Zhang Chuanshi, member of the Party group of and vice chairman of Xi'an Science and Technology Association visited the Institute of New Concept Sensors and Molecular Materials to survey the construction of the science popularization base.

After visiting the exhibition hall and laboratories of the Institute, the visitors had a discussion with Prof. Fang Yu, academician of the Chinese Academy of Sciences and chairman of Xi'an Science and Technology Association, and Prof. Xue Dong, director of Science and Technology Department of Shaanxi Normal University, and listened to the report on the scientific research, industry-university-research cooperation and popular science education base of the university.

Chang'an District deputy mayo Liang Wenhui and officials of the District Investment and Business Bureau accompanied the visit, and SNNU Science and Technology Department vice directors Qu Xinyun, Xiao Hui participated in the discussion.

西安创美集团总裁杨劲辉一行来访

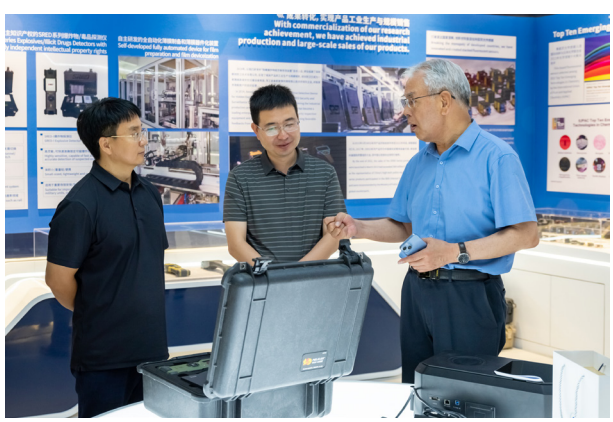
Meeting held with Xi'an Chuangmei Group visitors

2023 年 7 月 13 日，西安创美集团总裁杨劲辉、西安市科协副主席张传时一行到访新概念传感器与分子材料研究院，并与房喻院士会面商谈合作事宜。

首先，创美集团一行在房喻院士带领下参观了研究院成果展厅，了解了研究院的基本情况、科研成果和成果转化情况。接下来，双方在会议室进行了座谈。创美集团方面对房喻院士团队的最新研究成果进行了深入了解，并与研究院探讨了进行合作的可能性。

创美集团投资总经理岳显著、总裁助理杨鹏、人力资源总监武昕陪同来访；研究院副院长丁立平教授和办公室主任杨小刚参加了会议。

创美集团是一家以健康医疗、美容养生、生物科技、美容产品研发等产业为主的大型民企集团，总部位于西安高新区，员工近 3000 人。



On July 13, 2023, Xi'an Chuangmei Group president Yang Jinhui and Xi'an Association for Science and Technology vice chairman Zhang Chuanshi visited the Institute of New Concept Sensors and Molecular Materials and met with Prof. Fang Yu to discuss cooperation.

Chuangmei Group visitors were first shown the exhibition room of the institute by Prof. Fang Yu, to understand the basic situation, research achievements and achievements transformation of the institute. Then, the two sides held a discussion in the conference room. Chuangmei Group had an in-depth understanding of the latest research results of Fang Group, and discussed the possibility of cooperation with the institute.

Chuangmei Investment general manager Yue Xianzhu, assistant president Yang Peng and of human resources director Wu Xin accompanied Yang Jinhui in the visit. INCSMM vice dean Prof. Ding Liping and Administrative Office director Yang Xiaogang attended the meeting.

Chuangmei Group is a large private enterprise group headquartered in Xi'an Hi-Tech Development Zone, focusing on the industries of healthcare, beauty and wellness, biotechnology, and beauty product research and development, which has nearly 3,000 employees.

澳大利亚新南威尔士大学赵川教授应邀作报告

UNSW Prof. Chuan Zhao invited to give a presentation

2023 年 7 月 17 日下午，澳大利亚新南威尔士大学化学院赵川教授应光子鼻与分子材料团队邀请在新概念传感器与分子材料研究院报告厅为团队成员作报告。报告由刘静教授主持，团队老师和学生参加了本次报告会。

赵川教授为团队做了题为 Challenges and Opportunities for Green Hydrogen Production from Water Electrolysis 的报告，系统的介绍了电化学制氢的意义，研究过程中所遇到的问题和挑战，以及未来的设想和思路。

赵川教授是国际著名电化学家，是澳大利亚八大名校联盟中首位华裔化学终身教授，获澳大利亚电化学会的最高成就奖 R. H. Stokes Medal。其先进的制氢技术多次被包括新华社在内的国际主流新闻媒体报道，并入选首批科技部“火炬创新园”项目。

报告结束后，赵川教授与在场师生就相关问题进行了讨论，并与团队老师合影留念。

On July 17, 2023, Prof. Chuan Zhao from the School of Chemistry at the University of New South Wales, Sydney, Australia, was invited by the Photonic Nose and Molecular Materials Group to give a presentation to the group members in the Lecture Hall of the Institute of New Concept Sensors and Molecular Materials. The presentation was hosted by Prof. Liu Jing and attended by group teachers and students.

In the presentation titled Challenges and Opportunities for Green Hydrogen Production from Water Electrolysis, Prof. Zhao systematically introduced the significance of electrochemical hydrogen production, the problems and challenges encountered in the research process, as well as plans and thoughts for the future.

Prof. Zhao is an internationally renowned electrochemist, the first Chinese-Australian tenured professor of chemistry in Australia’s top eight universities, and the recipient of the R. H. Stokes Medal, the highest achievement award of the Electrochemical Society of Australia, whose advanced hydrogen production technology has been reported by international mainstream news media, including Xinhua News Agency, for multiple times, and has been selected as one of the first batch of the Ministry of Science and Technology’s Torch Innovation Park project.

After the presentation, Prof. Zhao discussed with the teachers and students present on related issues and took a group photo with the teachers.

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

装帧设计：长乐央吉 | 泛象空间
Designed by Changle Yangji, FanForm Art Space

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