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D26-智能分子材料

D26-Smart Molecular Materials

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D26 智能分子材料

分会主席：彭孝军、刘冬生、俞燕蕾、浦侃裔、Juyoung Yoon、樊江莉、Sanjay Mathur

最终交流类型：邀请报告

光开关分子介导的光响应高分子材料

李闯*
中国科学技术大学

能量耗散的非平衡过程对于生命体系动态可逆结构的形成、维持乃至功能发挥起着至关重要的作用，设计合成人工非平衡体系进而开发新型动态功能材料是当前化学和材料科学研究的重要前沿领域之一。光作为一种无接触式、可快速开关和具备高时空分辨率的能量形式，可用来调控聚合物微观结构变化，进而改变聚合物溶液和凝胶的宏观动态性能。我们设计合成了一系列基于螺吡喃分子开关的光响应聚合物（图1），能够在外界光能的持续输入下，实现光能-化学能-机械能的转化。在此基础上，我们构筑了光能耗散的高分子相态转变、溶胶凝胶转变以及水凝胶体积变化等，我们揭示螺吡喃分子异构化影响聚合物溶液发生相变的机理和规律，阐明了溶液相变和凝胶体积变化之间的关系。最后，我们探索了这些体系在信息加密、仿生形变和软体机器人等方面的应用。

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最终交流类型: 邀请报告

Digital design, synthesis, and manufacturing of functional materials and reactors

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In recent years, digital technologies such as artificial intelligence and automatic control have played a significant role in compound design and synthesis, greatly accelerating the discovery and synthesis of new compounds. Based on this, our research group has established a fully automated robotic chemical synthesis platform and conducted a series of research on the intersection of digital technology and chemistry. We have obtained potentially high-performance energetic molecules through intelligent molecular design, designed iron-based electrocatalysts using high-throughput computation combined with graph neural networks, optimized the synthesis formulations of pharmaceutical intermediates using big data obtained from high-throughput experimental screening, rapidly optimized molecular synthesis processes using continuous flow synthesis combined with multi-core Bayesian algorithms, and developed a series of structured reactors using digital design and processing.

最终交流类型：邀请报告

功能性蓝相液晶

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蓝相液晶因其独特的三维自组装超结构、多重外界刺激响应性、实时可重构性和优异的光学性能等吸

引了研究者的广泛关注，在柔性光电器件中具有重大应用潜力。然而迄今为止，仍然缺乏对蓝相液晶多级结构和相变过程的实时观测，对功能特性的发掘仍然不足，从而限制了其实际应用发展。我们通过对蓝相液晶自组装过程的研究，引入可聚合液晶单体和非液晶性单体，实现了大面积、高质量、自支撑的多色单畴蓝相液晶光子晶体薄膜的制备；进一步通过合适的聚合物稳定体系扩宽了蓝相液晶的温域（-190~310 ℃），并结合同步辐射、透射电镜等多手段详细研究了其相转变过程；利用蓝相液晶的刺激响应性研究了蓝相液晶光子晶体薄膜在形状记忆聚合物方面的应用；结合喷墨打印技术，发展了多色精美的蓝相液晶“活”图案；基于蓝相液晶谐振腔实现了高品质蓝相液晶激光，并进一步将其激光温域扩宽至超过 400 ℃（-180~240 ℃）。这些工作极大的促进了功能性蓝相液晶在显示、防伪、激光等领域的应用拓展。

最终交流类型：邀请报告

光动诊疗新策略

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光动诊疗（PDT）在医学领域展现了日益引人注目的潜力，其时空可控性、非侵入性等优势突破了传统治疗的局限性。本次报告将从“光动诊疗新策略”的全新视角，阐述 PDT 的基本原理、应用场景以及产业化前景，进一步详细探讨 PDT 领域近年来新兴的研究范式：光动诊疗新方向（如低氧依赖 Type-I PDT）、光动诊疗新作用机制（如光催化生物分子转换）、光动诊疗新应用范畴（如光控细胞焦亡激活用于抗肿瘤免疫），并讨论相关光敏染料分子的设计理念、功能强化以及激发态性能调控的方法。这一系列新策略的提出不仅提高了治疗的针对性和安全性，同时也拓展了 PDT 的应用领域，涉及癌症治疗、自身免疫性疾病等多个医学领域，将为未来医学研究和临床实践提供崭新的视角和可能性。

最终交流类型：口头报告

功能调控芳香化合物用于水系电化学储能的研究

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水系锌基储能器件因其安全、低成本和环境友好性而成为颇具吸引力的储能系统；然而，锌金属阳极面临枝晶生长和界面副反应的问题，进而阻碍了锌基储能器件的实际应用。为了解决上述问题，课题研究了具有不同配体的芳香有机分子数据库，考察了 40 余种电解液添加剂的分子结构对“电极-电解液”界面性质的影响，包含具有羧基、羟基、醛基和磺酸基官能团的芳香化合物。基于此，通过电化学测试研究了的分子结构、电荷状态和螯合基团对金属锌电化学稳定性的影响。测试结果表明，羧基和羟基在锌阳极上产生螯合键，实现了“电极-电解液”界面的保护作用，水杨酸盐和儿茶酚酸盐螯合配体能促进水合 Zn2+的脱溶；而芳醛则通过吸附作用在“电极-电解液”界面形成双电层，匀化界面电场，通过静电屏蔽效应抑制枝晶生长，同时使界面减少自由水，从而减少水分解和副产物产生。此外，界面双电层导致成核过电位变大，从而细化了锌镀层的晶粒，提高了锌阳极表面力学性能，减少了裂纹源产生和裂纹扩展；磺酸基由于极性基团的作用具有去溶剂化效应和形成双电层效应，有效重构了电解液氢键网络，降低了自由水的电化学反应活性。芳香族化合物与电解液离子发生螯合配位产生了具有浓度梯度的钝化层，从而阻碍了在电极表层由于氧化应力引起的裂纹。Zn//Zn 对称电池稳定性测试表明，磺酸盐添加剂在 2 mA cm-2 和 1 mAh cm−2 条件下的使用寿命从 50 次提高到 3000 次。在 1000 次循环后，制备含有间苯二甲醛和 1,3-苯二磺酸二钠添加剂的锌离子电池放电容量分别为 98.8 mAh g−1 和 88.6 mAh g−1，容量保持率分别为 97.71%和 61.16%。

最终交流类型：口头报告

多功能形状记忆高分子复合材料及其应用探索

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上海交通大学

形状记忆聚合物及其复合材料因其合成简单、成本低，可设计实现自修复、多重刺激响应等性能而成为研究热点，在柔性机器人、人工肌肉、信息识别等新型领域内展现出了独特的应用潜力。然而，形状记忆聚合物及其复合材料在应变能力，响应速度，能量密度以及多刺激响应等方面仍存在亟待攻克的问题，限制了其进一步的发展与应用。针对上述问题，本工作结合了半结晶聚氨酯与液晶网络的优势，并通过将体系的特征转变与多种光响应基团，金纳米棒、破碎八面体 Fe3O4 等颗粒有机结合，制备了一系列兼具优异力学性能与不同功能的热响应和光响应柔性器件，具有优越的热响应驱动能量密度、功率密度和双向可逆驱动应变，挖掘了热致和光致形状记忆聚合物的应用深度。以形状记忆聚合物为基体制备的抓手可以实现热驱动双向抓取与释放，也可以制备人工韧带应用于生物医疗领域。光致形状记忆聚合物纸在点光源和泛光源的辐射下，分别具有远程、精准的光控“书写”和“擦写”的能力，能够在多环境（空气、酸/碱溶液、冰）中得以表达并长期保存。基于氨基甲酸酯基团的可逆动态键交换反应的形状记忆聚合物可实现双重编程和可重构功能，在信息识别、4D 打印等领域表现出良好的应用潜力。

最终交流类型：邀请报告

聚噻吩基声敏剂的设计合成及其应用

蓝敏焕*

central south university

声动力疗法具有非侵入性、无耐药性、组织穿透能力强、治疗选择性高等优点，在深部肿瘤治疗中具有独特优势，制备高性能声敏剂是推动其临床应用的关键。我们设计合成了系列聚噻吩衍生物，在超声照射下可以产生 ROS，用于声动力治疗。通过与 化疗药物、siRNA 进行组装，制备了具有化疗或者免疫治疗功能的多功能声敏剂，用于肿瘤的联合治疗。

最终交流类型：邀请报告

S 原子促进碳酸氢根解离加速单原子 Zn 位点电还原 CO2 动力学

侯阳*

浙江大学

提高质子耦合电子转移(PCET)过程中的质子转移速率是加快 CO_2 电还原(CO_2ER)反应动力学的关键。然而，在单一的活性位点上很难实现对于质子供给和 CO_2 活化的同步增强，这使得 CO_2 还原制备高选择性产物的快速转化成为一个相当大的挑战。在此，我们开发了一种负载孤立单原子 Zn 位点的 N、S 共掺杂分层多孔碳(Zn-NS-C)电催化剂用于 CO_2ER，X 射线吸收光谱拟合结果表明 Zn-N_4 活性位点及其相邻的 S 原子（Zn-N_4-S）是 Zn-NS-C 中的一种具有代表性的配位结构。动力学实验结合原位红外光谱揭示了邻位辅助性 S 位点促进了碳酸氢根离子解离的动力学，进而提高活性位点周围的质子补给，而原子级分散的 Zn-N_4 位点是 CO_2ER 的活性中心。理论计算辅助证明，掺杂 S 原子为体系引入了更多的亲电中心，使得碳酸氢根在材料表面的吸附在热力学上变得更有利；而碳酸氢根的解离为催化活性位点提供了质子源，显著促进了*CO_2质子化生成*COOH 的反应动力学。实验结果表明，Zn-NS-C 具有优异的 CO_2ER 性能，在 200 mA cm^{-2} 的工业级电流密度下具有近乎 100%的 CO 选择性，并且展现了超高的转化频率（11,419 h^{-1}）；此外，通过构建 Zn-NS-C 和 Cu/PTFE 组装的串联催化剂，将 Zn-NS-C 上还原得到的 CO 在 Cu 上进一步还原为 C_2H_4，其中 C_2H_4 部分电流密度比纯 Cu/PTFE 催化得到的值高 1.7 倍，证明了 Zn-NS-C 催化 CO_2-CO 转化的高活性。

最终交流类型：主题报告

智能激活型药物控释体系

易涛*

Donghua University

响应型荧光分子材料在人工智能、信息存储、分子探针、生物医用等领域具有重要的应用价值。小分子控释体系具有组成单一、功能明确、易于调控的特点，在智能前药制备方面具有独特的优势。近年来，我们基于外场和化学调控相结合的响应激活策略，利用化学合成及组装手段，设计针对靶标驱动力高特异性、高灵敏的分子或超分子体系，发展多重响应的荧光材料和高效的激活型分子控释工具。特别是发现新的活性氧响应机制，发展了针对活性氧相关疾病的智能型激活控释体系应用于活体成像和诊疗一体化。

最终交流类型: 主题报告

Intrinsically Dynamic Covalent Poly(disulfide)s

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The rise of supramolecular and dynamic covalent chemistry offers many approaches to the construction of dynamic polymers and materials that can adapt, respond, repair, and recycle. Within this toolbox, the building blocks based on 1,2-dithiolanes have become an important scaffold, featuring their reversible polymerization mediated by dynamic covalent disulfide bonds and supramolecular noncovalent interactions tuned by molecular engineering strategy, which enables a unique class of dynamic materials at the intersection of supramolecular polymers and adaptable covalent networks. This presentation aims to explore the dynamic chemistry of 1,2-dithiolanes as a versatile structural unit for the design of intrinsically dynamic covalent materials.

最终交流类型: 口头报告

ESIPT-Inspired Dual-Mode Photoswitches with Fast Molecular Isomerization in the Solid State

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Photoswitchable materials have attracted considerable attention in various fields. Developing excellent solid state dual-mode photoswitches is an important but challenging task. Herein, we propose a new strategy to construct an excited-state intramolecular proton transfer (ESIPT) inspired photoswitch (DiAH-pht) that possesses aggregation-induced emission (AIE) features and displays a fast molecular isomerization process characterized by dual-mode behavior in the solid state. Mechanistic studies indicate that introduction of a bulky group can create a folded molecular conformation that provides adequate volume to facilitate photoisomerization and the enhanced ESIPT effect can boost the isomerization process. The feasibility of our strategy was further demonstrated by the activated photoisomerization performance of the Schiff base derivatives. Furthermore, DiAH-pht shows good performance in the fields of dual-mode information encryption and high-density data storage.

最终交流类型：口头报告

基于白蛋白的智能荧光识别

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近年来，基于主客体复合物的超分子荧光探针引发大家的格外关注，该类探针以具有内腔结构的大环作为主体，嵌套与其尺寸匹配的客体分子组成主客体复合物，利用待测物与主体内腔的次价键相互作用，实现对目标检测物的高效识别。超分子荧光探针的优势在于，其识别过程依赖主体与客体的结构适配，而不依赖特定的化学反应，从而能够对无化学反应活性的“惰性”目标分子实施检测。

然而，由于现有的大环主体通常是刚性或半刚性的空间对称结构，且空腔内部的次价键种类比较单一，而从头设计合成具有复杂空间拓扑学结构的分子大环的实施难度非常高，因此，目前超分子荧光探针能够检测的目标物种类仍然十分有限。白蛋白是哺乳动物血清中含量最为丰富的蛋白质，其内部含有多个空间拓扑结构的半柔性非对称空腔，包括三个药物位点和多个脂肪酸位点，空腔内部含有丰富的氨基酸残基，能够与配体形成多种类型的次价键相互作用。白蛋白的以上结构特征，克服了常见合成大环类主体的固有缺点，理论上可以突破传统的超分子荧光探针的设计与应用局限。

因此，基于天然或功能化修饰的白蛋白主体，以亲白蛋白的荧光染料为客体，通过精确调控主客体的结构适配，可以系统的构筑基于白蛋白-染料复合物的超分子荧光识别体系。基于指示剂取代、共存、反应等多种响应策略，开发具备交叉响应特征的荧光探针阵列，以实现对复杂目标物的特异性检测，并充分地探索该体系在环境、食品、安全、健康、医疗领域的应用潜力

最终交流类型：主题报告

液晶分子材料的制备与性能研究

杨洪*
东南大学

液晶分子对热、光、电、磁等外源物理刺激都能产生响应，是极为重要的一类智能软物质材料，在光电显示、非线性光学、弹性体材料、光反射屏蔽材料、手性分离、微流体控制等研究领域有广阔的应用前景。本报告将汇报课题组在液晶分子材料，特别是液晶弹性体研究领域，聚焦“功能基团与液晶网络的协同机制”科学问题，取得的三个阶段性成果：1、提出了化学键合网络功能增强构筑策略，实现了液晶弹性材料形变速度和力学性能的显著提升；2、发展了液晶基元多层次梯度取向方法，实现了对液晶弹性体的高自由度连续性驱动；3、构建了空间几何网络结构协同驱动机制，发展了多维度复杂形变液晶弹性体驱动器。

最终交流类型: 主题报告

4D printing liquid crystal elastomer soft robots and light-controlled movement behavior

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Soft robots achieve lifelike mechanical intelligence by mimicking the asymmetric contraction of muscles, playing an irreplaceable role in specific applications such as wearable devices and exploration in extreme environments. Liquid crystal elastomers (LCE) combine the entropic elasticity of polymer networks with the anisotropy of liquid crystals, capable of reversible deformation under external stimuli such as heat and light. By controlling the gradient orientation of mesogens, gradient deformation can be achieved, thereby imitating the asymmetric contraction of muscles to construct soft robots. In the manufacturing technology of LCE, 4D printing can program liquid crystal orientation while designing structures through the application of shear forces. However, due to the uniform shear action within the nozzle during printing, achieving gradient orientation poses a challenge. In this report, we present a new strategy for constructing gradient deformation LCE soft robots based on exterior nozzle tip shearing and progressive printing. First, on the basis of the interior nozzle shearing, we introduced the non-uniform exterior nozzle tip shearing to induce the mesogens forming gradient orientation in the thickness direction, achieving large curvature bending deformation. Further imitating the alternating arrangement of caterpillar’s muscle fibers and exoskeleton, we constructed a hinged soft robot through multi-material 4D printing and achieved multi-mode motion via photodeformation. Secondly, we introduced local orientation changes in LCE by combining interior nozzle shearing and progressive printing, controlling the spatial distribution of shrinkage to achieve gradient deformation. Further, by simulating the annular arrangement of the pupil sphincter muscle through 4D printing, we managed a gradient reduction in mesogens alignment from the inside out, achieving a

light-controlled adaptive flattening contraction similar to an iris. This work provides new insights into 4D printing LCE soft robots.

最终交流类型: 口头报告

Supramolecular delivery of hydrogen sulfide

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Hydrogen sulfide (H_2S) is the third gasotransmitter, which plays a vital role in many biological processes. It has been unraveled that the therapeutic effect is highly dependent on its concentration. In this regard, on-demand delivery of H_2S is of great importance. In the presentation, we will introduce the supramolecular delivery strategies developed in our lab. By these, we could not only transport H_2S to the lesion site, but also tune the release rate through the modulation of nanocarriers' morphologies. Both in vitro and in vivo studies demonstrated that H_2S-based gas therapy or H_2S synergized combination therapy had a satisfactory therapeutic outcome for disease treatment. We would like to highlight in the presentation that our recent contribution on supramolecular delivery of H_2S by biomineralized nanocarriers from natural materials such as protein.

最终交流类型：邀请报告

高对比荧光成像材料的设计和应用

赵征*
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荧光成像技术在生命科学基础研究中具有广泛应用，并在生物医学应用等领域展现出良好的应用前景。近年来爆炸式增长的临床前和临床试验项目足以体现生物医学荧光成像的重要性。由于生物体自发荧光的存在，可能对目标荧光信号的检测产生干扰，严重时甚至淹没目标荧光信号。因此，如何最大限度的降低生物体的自发荧光，提高成像的对比度和信噪比，是荧光成像领域最为重要的科学问题之一。基于成像的原理和方法，有不同的策略来实现成像对比度的提高。例如，基于磷光材料的余辉成像，可以通过时间门控完全消除背景的自发荧光，目前已成为一个热门的研究领域。相比于可见光，近红外荧光(NIR, 700-1700 nm)成像具有更强的光学组织穿透能力和更低的生物自发背景荧光干扰，因而能够提供更高的活体成像对比度，实现更灵敏、更准确的活体检测，也是目前的热点研究方向。此外，手性材料可以发出圆偏振光，在偏振片的辅助下，可以选择性的接受成像部位的圆偏振发光，同时虑掉部分活体自发荧光的信号，理论上也可将对比度提高约一倍。目前由于圆偏振发光材料的研究尚在起步阶段，该策略进展缓慢。

本次报告将介绍申请人在高对比度成像材料设计方面的研究进展，尤其是近红外发光材料的设计和应用探索，包括其在于肿瘤诊断、动态成像、手术导航领域的应用。

最终交流类型：主题报告

DNA 超分子水凝胶

刘冬生*
清华大学

由于高分子链熵弹性的存在，高分子交联网络的有效孔径呈正态分布，使人工合成水凝胶体系的分子通透性不能与细胞外基质相比拟。利用核酸双链分子刚性大且水溶的特点，我们制备了纯核酸超分子水凝胶，在其分子网络中避免了高分子链熵卷曲的产生，具有类似细胞外基质的高通透性。在此基础上，我们发展了多种拓扑构型的核酸超分子组件，可以在生理条件下快速形成并具有较好的强度；利用其快速形成

和良好的生物相容性，此系列水凝胶还在单细胞培养与操控、活细胞的三维打印等方面获得了良好的应用。

最终交流类型：主题报告

DNA Supramolecular Hydrogels

Dongsheng Liu*
Tsinghua University

Based on the excellent rigidity of DNA duplexes, we designed and prepared kinds of pure DNA supramolecular hydrogels, which possess an ‘all-rigid’ molecular network. Based on experimental results and theoretical studies, we also demonstrate these hydrogels have extraordinary permeability of macromolecules such as proteins. Due to their supramolecular nature, these hydrogels also retain extraordinary self-healing and fast-responding thixotropic properties, which make them injectable and writable.

Holding all these advantages, the DNA supramolecular hydrogels are excellent mimics of extra-cellular matrix (ECM). We will show its application in server spinal-cord injury repairing, where implanted stem cells only respond to in-situ signals generated by the injured animals.

Through DNA sequence design, we enabled the univariant mechanical strength of materials based on DNA supramolecular hydrogel platform, and demonstrate that ‘Univariate mechanical strength does not influence neural progenitor cell fate in 3D matrix’ for the first time.

最终交流类型：闪报

Biomolecule-targeted functional dyes for imaging and therapy

Beidou Feng,Li Zhong,Hua Zhang*
Henan Normal University

Mitochondria are the center of energy metabolism and cell death regulation in cells, playing a crucial role in the regulation of cell survival and death. Therefore, by targeting mitochondria and modulating the expression of relevant active substances, triggering mitochondrial dysfunction and thus inducing cell death, it may become an effective strategy for the treatment of cancer. Based on this, this work developed a targeted photo-sensitizing dye PAT-Cy-I for hypoxic tumor treatment that is specific to mtDNA. PAT-Cy-I accumulates in mitochondria through insertion of mtDNA and causes mtDNA destabilisation via PDT, leading to mitochondrial dysfunction and subsequent cell death. UV absorption and circular dichroism spectra show good binding of PAT-Cy-I to mtDNA. Solution and cellular experiments verified that PAT-Cy-I was capable of generating large amounts of ROS as well as inducing mtDNA damage under both hypoxia and normoxia. Tumour therapy experiments in mice showed that PAT-Cy-I was able to generate large amounts of ROS and inhibit tumour growth under specific light exposure. In conclusion, the present work provides a targeted photosensitive dye, which is capable of target binding to mtDNA to achieve in situ induction of mitochondrial dysfunction, and is an effective tool for cancer therapy.

最终交流类型：主题报告

From Fluorescent Probes to Phototherapy

Juyoung Yoon*
Ewha Womans University

The development of fluorescent probes for various analytes has been actively pursued by chemists. Since

their inception, these efforts have led to many new sensors that have found wide applications in the fields of chemistry, biology, environmental science, and physiology.

Recently, a near-infrared two-photon fluorescent probe was developed to not only specially image carboxylesterase (CE) activity in vivo and in situ but also target orthotopic liver tumor after systemic administration.1

On the other hand, photodynamic therapy (PDT) and photothermal therapy (PTT) have attracted considerable interest as a noninvasive treatment method.2 We devised a novel molecular design approach to create heavy-atom-free photosensitizers for thionapthalimides.3 The in vivo specific binding between albumin and PcS, arising from the disassembly of injected NanoPcS, was also confirmed using an inducible transgenic mouse system.4 We recently reported a viscosity-sensitive, endoplasmic reticulum (ER)-targeting fluorescent probe, ER-ZS, which can monitor ER stress-induced viscosity changes in real time. ER-ZS is also an excellent anti-hypoxia type I photosensitizer that activates tumor cell pyroptosis by damaging the ER pathway.5

Photodynamic antibacterial therapy is regarded as an innovative and promising antibacterial approach due to its minor side effects and lack of drug resistance.6 Recently, we suggested that reactive differences may pave a general way to design selective photodynamic agents for ablating Gram-positive bacteria-infected diseases.7

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最终交流类型：口头报告

近红外二区染料氟硼吡咯的构建及应用

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沈阳化工大学

近红外二区染料有利于降低生物体内物质的自吸收和自发荧光的干扰，可以穿透深层组织，因而功能化的近红外二区荧光染料氮杂氟硼二吡咯(aza-BODIPY)备受关注及富有挑战的构建。在此，本报告通过延伸共轭体系，在 aza-BODIPY 的 1,7 或 3,5 位引入强的推电子基团久洛尼定，合成了 1,7 或 3,5 位久洛尼定取代的染料 aza-BODIPY 并解析其单晶结构（Fig. 1）。考察 aza-BODIPY 体系的 1,7-或 3,5-位久洛尼定基对光谱性能、构效关系等影响 1，重在脑胶质瘤的近红外二区的光线治疗的探索与应用。

最终交流类型: 口头报告

Precise Theranostic Technology for Diseases Based on Small Molecular Probes

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Hainan Medical University

There are urgent demands that targeting anti-tumor drugs with reliable efficacy and clear pharmacokinetics for non-small-cell lung cancer (NSCLC) therapy. We designed and synthesized an active tumor-targeting prodrug for the precision therapy of NSCLC. The prodrug polyamine analog Gefitinib (PPG) was derived from the conjugation between a tumor-targeting ligand polyamine analog (PA) and an epidermal growth factor receptor tyrosine kinase inhibitor Gefitinib via a cleavable disulfide linker. Furthermore, the integration of the near-infrared αzo-BODIPY fluorophore into the structure of the prodrug PPG yielded an activatable fluorescent theranostics (TPG), which could be used to monitor the in real-time delivery of prodrug PPG and initiate precise medicine in vivo. PPG efficiently delivered the anti-tumor drug to cancer cells. We provided a new evidence that the tumor-targeting PA ligand could inhibit the Akt pathway in H1650 cells, and had a synergistic effect with Gefitinib for anticancer efficacy. The in vivo results on nude mice bearing tumors of NSCLC cell lines demonstrated that PPG could target tumor lesions and had the expected therapeutic effects. Finally, we used TPG for fluorescent labeling of transbronchial lung biopsy (TBLB) specimens. Our work had identified that PPG could be effectively used for the treatment of Gefitinib-resistance NSCLC in cells and in mice models. The theranostic TPG emerged as a promising fluorescent imaging tool for the application in the therapy and diagnosis of NSCLC.

最终交流类型：口头报告

新型杂芳烃大环主体的合成与性能研究

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东北大学

大环主体是超分子化学研究的重要工具，开发具有结构和功能特色的新型大环主体是超分子化学领域的一个永恒的主题。尽管这些年来，基于相同重复单元组成的大环主体的研究取得了巨大的进展，然而如何有效设计合成具有不同类型的重复单元的功能性新型大环主体仍然存在很大的挑战。另一方面，碳氢化合物分离广泛应用于能源、化工、环保等领域。现有的碳氢化合物吸附分离技术通常是基于多孔材料（如金属有机骨架、共价有机骨架、多孔有机笼）来实现的。这些多孔材料具有比表面积大、孔道有序等优点，但也存在合成复杂、稳定性差、可重复使用性低等缺点。非多孔自适应晶体作为一种新型的吸附分离材料，在碳氢化合物分离纯化领域具有广阔的应用前景。相较于传统的大环主体柱芳烃，杂芳烃在吸附分离方面具有独特的优点。本研究将重点介绍一种使用杂[3]芳烃非多孔自适应晶体的环保节能吸附分离策略。自适应杂[3]芳烃晶体从等摩尔苯/环己烷混合物中分离苯，纯度为 97.5%。选择性来自于捕获首选客体苯时新晶体结构的稳定性和可变性。此外，非多孔客体结构和含客体结构之间的可逆转换使杂[3]芳烃具有很高的可回收性。由于杂[3]芳烃的合成简单、分离效率高、回收性能好，在化工领域具有巨大的应用潜力。此外，本研究还将讨论杂[4]芳烃非多孔自适应晶体材料在碳氢化合物吸附分离中的应用。

最终交流类型：邀请报告

AI for Smart Molecules- 智能分子材料的智能设计与合成

王笑楠*

清华大学

本文探讨了人工智能在智能分子材料发现、设计与合成中的应用及相应智能算法的开发。基于 机器学习和深度学习算法设计分子结构和性能，可以显著加速新材料的发现和优化。AI 驱动的高通量理论计算和自动化合成平台进一步提高了科学发现效率，缩短了研发周期。智能技术的突破不仅推动了分子和材料科学的发展，也为新型功能材料尤其是智能分子材料的创新提供了前所未有的机遇。

最终交流类型：邀请报告

智能荧光高分子凝胶

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智能荧光高分子凝胶是材料化学的前沿研究领域之一，在智能显示、变色伪装、仿生驱动等方面具有潜在应用价值。荧光性能（颜色、强度等）的动态精准调控是其功能发挥和应用拓展的关键，但依然存在很多困难。然而，自然界中发光水母可通过 Ca2+可逆配位等实现绿色荧光蛋白发光强度在有无之间的动态精准调控；在颜色调控方面，发光章鱼进化出多层色素细胞有序排列多层结构，可通过不同层色素细胞的差异化响应呈现出丰富多彩的皮肤颜色。受此启发，近年来聚焦荧光高分子凝胶研究，取得如下成果：(1) 仿水母荧光蛋白的发光强度调控原理，提出了构筑动态交联荧光高分子凝胶的仿生新思路，获得了一系列发光性能动态可调的荧光高分子水凝胶新材料；(2) 仿发光章鱼皮肤多层结构，发展了多层动态交联网络的仿生新结构，实现三原色荧光团的多层独立分布及其荧光强度的正交调控，获得了宽范围荧光变色高分子凝胶。本次报告将具体汇报以上成果。

最终交流类型：口头报告

Chemical signals-triggered dynamic self-assembly of molecular hydrogels

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Supramolecular self-assembly is ubiquitous in nature and is usually dictated by complex biochemical signals, giving rise to various spatiotemporally controlled supramolecular structures that underpin many vital biological functionalities. In this context, the development of synthetic counterparts would not only accelerate the development of new smart molecular materials but also further our understanding of the self-assembly process in living systems. In recent years, we have realized spatiotemporal control over the self-assembly of molecular hydrogels using chemical reactions. First, a hydrazone-based molecular hydrogel system has been developed, by which spatially controlled molecular hydrogels have been achieved by controlling the distribution of catalysts. This methodology has also been extended to the case of living cells, leading to intracellular self-assembly of the hydrogel that significantly influences the fate of the cell. Second, chemically fueled dissipative self-assembly of molecular hydrogels has been constructed, resulting in out-of-equilibrium hydrogels bearing time-dependent structures and properties. These efforts may not only contribute to the development of new lifelike smart molecular materials.

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最终交流类型: 口头报告

Development of gas signaling molecular donors based on molecular fluorescent probes

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Nitric oxide (NO) and nitroxyl (HNO) have unique chemical, biochemical, and pharmacological activities. Due to their instability, it is necessary to use NO and HNO donor compounds to achieve in situ release of NO and HNO. Therefore, NO and HNO donor molecules play an extremely critical role in the current chemical, biological, and physiological activities and clinical studies of NO and HNO. Currently, the NO and HNO release cannot be monitored in situ. Herein, we have developed a series of functional donor molecules that can be used to release NO and HNO under physiological conditions. They can efficiently release NO or HNO and fluorescent probes simultaneously, specifically, these fluorescent probes can be used to successfully monitor NO and HNO in situ.

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最终交流类型：邀请报告

基于动态共价力敏团的力诱导发光高分子材料

陈于蓝*
吉林大学

高分子力化学主要研究高分子在机械力作用下化学键形成与断裂、分子间相互作用的变化，是连接化学（微观分子水平）与力学（宏观材料性能）研究的桥梁。在微观分子层面上大多数力响应的高分子体系都基于共价键的轴向拉伸来实现激活，并伴随着高分子主链的断裂。突破共价高分子力化学的研究范畴，发展新兴的力学响应体系，将机械力的破坏作用转变为增效作用，不仅将丰富力响应高分子的种类和功能，也将推动高强韧高分子新材料的发展。我们近期研究发现，二硒基团和蒽-炔 Diels-Alder 环加成基团这两类重要的含动态共价键的官能团还具有灵敏的力响应特性。机械力能诱导高分子链中心二硒键的高选择性断裂和交换，是调控含硒高分子动态响应性能的新手段，利用机械力诱导的硒自由基引发单体聚合与自由基转移反应，得到了具有自增强特性的原位应力指示弹性体。此外，蒽-炔 Diels-Alder 环加成力敏团 FA 可以通过“柔性活化”机制实现力诱导荧光小分子的释放。与传统的基于拉伸断键的可视化力敏基团相比，FA 的活化过程保证了高分子主体结构的完整性，使材料实现多次连续活化，为新型光学应力探针的开发开辟了新思路。这些结果拓展了动态共价键在机械力响应材料方面的应用。

最终交流类型：口头报告

结构明确的硫配位铜(I)单原子纳米酶级联催化增强协同铁死亡/铜死亡免疫治疗

张斌*
深圳大学第一附属医院

虽然免疫原性细胞死亡(ICD)在三阴性乳腺癌(TNBC)免疫治疗中显示出了巨大的潜力，但有效诱导强免疫反应且副作用最小的 ICD 诱导剂仍有待开发。在这里，我们报告了一种结构明确且功能强大的单位点铜(I)纳米调节剂，称为 CuNTD，通过将原子分散的自组装 S-Cu(I)-S 位点锚定在二维 Ti3C2 表面而巧妙地构建。与 Cu2+相比，CuNTD 具有更高的催化效率，通过光热增强级联催化产生活性氧簇(ROS)风暴，进一步诱导线粒体功能障碍、铁死亡和铜死亡。多功能 CuNTD 通过光热放大的 ROS 风暴、铜死亡和铁死亡的级联调节通路触发强 ICD，有效促进树突状细胞成熟，同时减少单药治疗的副作用和耐药性。体内实验中，CuNTD 联合免疫佐剂 R848 显著延长小鼠生存期。鉴于 CuNTD 作为 ICD 诱导剂的生物安全性和有效性，本研究为增强型 TNBC 免疫治疗提供了一种有很高前景的方案。

最终交流类型: 墙报

D26-P01

An Innovative High-Performance, Ultra-Stretchable, and Flexible Moist-Electric Hydrogel Initiated by LM-MMt

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Guangzhou University

Air humidity is a huge and sustainable energy source that can be used continuously, unlike solar energy and wind energy. However, the previous technologies for collecting energy from air humidity were either greatly influenced by humidity or required unique material synthesis or processing, which hindered the large-scale application and popularization of energy technologies. Here, we have successfully created a unique gel material with simple preparation and sustainable power supply in various humidity environments by mixing highly conductive gallium-indium alloy with montmorillonite with high water absorption capacity to induce acrylamide organic gel. We evenly disperse the gallium-indium alloy in montmorillonite through simple mechanical stirring, and the dispersed powder has a good initiating effect that can rapidly polymerize acrylamide organic gel at room temperature. The good conductivity of gallium-indium alloy effectively reduces the resistance of organic gel, while the layered structure of montmorillonite provides a channel for rapid ion transport. At the same time, acrylamide organic gel has excellent moisture absorption and water retention properties, which can spontaneously adsorb moisture from the air and maintain the internal moisture gradient, thus achieving stable power output in a wide range of environments. Due to the synergistic effect of significant asymmetric moisture absorption capacity and rapid ion transport capacity in the ionic hydrogel network, a single 0.25 cm^2 LM-MMT organic gel unit can continuously generate direct current, with an open-circuit voltage of 1.02 V, duration exceeding 1400 hours, short-circuit current density of 1mA cm^{-2}, and a power density up to 70μW cm^{-2}. The LM-MMT gel generator is flexible, sustainable, biocompatible, and environmentally friendly, and can obtain electricity from humid airflows in nature and industry (such as wind, breathing, and sweat). It can also be used in wearable and miniaturized power devices to directly drive many commercial electronic products, including electronic ink screens, metal electrodeposition devices, and LED arrays (as we will demonstrate later). Organic hydrogels have the characteristics of environmental protection, easy scaling-up, and high power output, opening a new perspective for developing green, multifunctional, and efficient power sources for the Internet of Things and wearable electronic products.

最终交流类型: 闪报

Regulation of excited state and enhancement of dye function

Yafu Wang*

Henan Normal University

Photosensitive dye is one of the key factors to regulate the efficacy of photodynamic therapy (PDT), the structure design and function strengthening have become the research focus at home and abroad. However, most of the existing photosensitive dyes still have some limitations in tumor cell lethality and efficacy monitoring, which greatly limits the clinical therapeutic efficacy. In view of this, based on the biological characteristics of mitochondrial DNA (mtDNA), which is easy to damage, sensitive, and can indicate the process of apoptosis [1, 2], this work takes mtDNA as the target and constructs a series of mtDNA target photosensitive dyes (DSs) through the molecular excited state regulation strategy. It is expected to improve tumor lethality by rapidly inducing mtDNA damage, and adjust treatment process with accurate feedback based on real-time monitoring of mtDNA damage, so as to maximize therapeutic efficacy. In this work, through a series of optical and biological properties tests, the dye molecule DSs can be highly bound to DNA through small grooves based on a special conjugated structure. At the same time, the molecular conformation changes significantly, which causes changes in the distribution and transfer of electrons within the molecule, triggering obvious fluorescence signals, and realizing specific and highly sensitive monitoring of mtDNA damage. In addition, the introduction of heavy atoms in the dye molecules enables them to induce photodynamic therapy when activated by light and exhibit high tumor cell lethality. Based on the above characteristics, further verified by living tumor model, dye molecules have high tumor cell lethality, and can monitor and feedback their PDT process in real-time to adjust relevant therapeutic parameters, and successfully achieve efficient treatment of living tumors.

最终交流类型：口头报告

力致发光材料与触觉传感器件

王春枫*
深圳大学

仿生触觉传感器作为未来人工智能系统的核心部件，是一切触觉信息采集的入口以及智能感知的前端，随着人工智能技术不断的发展和成熟，其重要性将日益凸显。报告人主要从事光电功能材料及触觉传感器件方面的研究。以力-电-光耦合效应为基础，以光电功能材料为载体，以构建智能触觉传感器件及系统为目标，从材料出发，结合结构设计，构筑了一系列发光、显示、传感等光电功能器件，探究器件力-电-光耦合作用，发展触觉刺激调控器件光电性能的新方法，实现触觉信息的超高空间分辨率、自驱动、可视化、多模态传感及显示，研究触觉传感器件与电子电路的集成，实现触觉传感器件在人机交互、智能机器人、可穿戴电子领域的应用。

最终交流类型: 主题报告

Fluorescent chemosensors and imaging agents

Tony James*
University of Bath

Sensors and imaging agents can be used to monitor analytes within physiological, environmental, and industrial scenarios. The interactions between the “chemosensor” and an analyte of choice occurs on a molecular level and as such gathering and processing the information is challenging. Therefore, I will outline the trials and challenges encountered in the development of several robust chemical molecular sensors “chemosensors” able to detect such analytes selectively and signal or map their concentration in a biological or environmental scenario. During the talk you will be introduced to a variety of fluorescent probes designed for diols (D-glucose), and redox imbalance. With the goal being the development of chemosensors capable of determining the concentration (and

location) of a target species in any medium. Particular attention will be paid to the underlying chemistry associated with the construction of practical chemosensors for both sensing and imaging applications.

最终交流类型: 主题报告

Publishing with Wiley Chemistry Journals

Juan Jin*
Wiley

The speaker will introduce in-house Wiley chemistry journals, including Angewandte Chemie, a journal of the German Chemical Society (GDCh), and journals published on behalf of Chemistry Europe and Asian Chemical Editorial Society (ACES). The main focus will be the recent developments at Angewandte Chemie, which would make Angewandte Chemie an inclusive home for excellent chemistry. Some practical tips on scientific writing and publishing from the aspect of editors will also be covered. some practical tips will be given on how to avoid ethical problems, how to select an appropriate journal, what aspects of preparation and presentation to focus on from an editor's and referee's perspective, and hints for increasing the discoverability of your paper after publication.

最终交流类型：邀请报告

动态响应有机光电材料

陶冶*
南京邮电大学

静态和动态有机光电材料相辅相成，发展具有动态响应特性的光电材料，有望赋予光电器件独特的性能，开拓器件应用研究领域的新视野，为研制高性能和新功能器件提供新途径。近年来我们围绕动态响应有机光电材料理性设计和激发态性质动态调控的关键科学问题展开研究，以功能导向的合成化学为基础，综合利用和发展了化学与物理调控方法，建立其分子设计、材料结构和激发态性质之间的内在关联性，为开发高性能和新功能动态响应光电材料奠定了理论基础。针对动态响应光电材料的理性设计问题，我们开发了动态响应结构单元—“共振结构”，提出了理性设计动态响应光电材料的新方法，研制了新型“动态共振有机光电材料”，提升了磷光器件效率及稳定性，解决了余辉效率和寿命不能同时提高的矛盾问题；针对激发态性质动态调控的难题，利用外部物理调控方法，通过凝聚态结构和能量传递的有效调控，实现了激发态性质的动态调控，构建了高性能新功能动态响应有机长余辉材料，开发了多级信息加密、显示和多彩安全打印新应用。

最终交流类型: 口头报告

Multifunctional Sensing Systems for the Effective Detection of Bacteria

Kai-Cheng Yan[1],Tony D. James*[1],A. Toby A. Jenkins[1],Xiao-Peng He[2],Yuan Wang[3],Wei-Na Wu[3],Zhi-Hong Xu[4]
1. University of Bath
2. East China University of Science and Technology
3. Henan Polytechnic University
4. Xuchang University

As a major pathogen, bacteria have caused significant threats to human health, and as such has been a major biological target for therapeutics over the past several decades. In the area of chemistry, biochemistry, chemical biology, and biomedicine, fluorescence spectroscopy using advanced fluorescence chemosensors has enabled the detection, sensing, and treatment of a wide range diseases including cancer, inflammation, neurodegenerative diseases, etc., for understanding of disease processes and the development of new therapeutics. The use of

long-wavelength or even NIR fluorophores for fluorescence based chemosensors is of particular significance since it enables several advantages including effective penetration through tissues, minimal interference from background fluorescence, lowered tissue damage etc. As such clinic-based use for in situ evaluation is particularly adventitious. Herein, I will introduce several recent examples including long-wavelength red-emitting fluorophores to construct smart sensors for detecting nitroreductase (NTR) in a wide range of bacteria. As well as, the construction of a novel ferrocene-chalcone-based molecular probe enabling the detection of Carboxylesterases (CEs) in bacteria. Finally, a green-emitting indene-chalcone-based fluorescent “turn-on” probe and a merocyanine-based probe will be introduced for the detection of CEs in planktonic form and also in chronic biofilms.

最终交流类型：主题报告

动态超分辨成像荧光染料

徐兆超*
中国科学院大连化学物理研究所

超分辨荧光成像突破衍射极限，在纳米尺度至单分子水平可视化生物分子，以前所未有的时空分辨率研究活细胞结构和动态过程，已成为生命科学研究的有力工具。然而，如何获得更高空间分辨率（低至 0.1 nm），如何在保障空间分辨率前提下获得更高时间分辨率（低至微秒），最终实现细胞内生物分子全景时空超分辨成像，依然面临巨大挑战。荧光团是超分辨荧光成像的关键，荧光团通过结构的改造获得性能的巨大提高，可望解决以上问题。报告从荧光团的发光原理和分子结构关系讨论开始，介绍我们近期在荧光染料的结构改造和在亚细胞器动态超分辨成像中的进展。

最终交流类型：邀请报告

基于可交联聚芳醚的光功能化耐溶剂纳滤膜设计与膜污染机制研究

贾坤*、冉启蒙、许小玲
电子科技大学

聚芳醚是一类具有耐高温、高强度、耐辐照等综合优异性能的高性能高分子材料，在膜分离工程领域具有重要应用价值。特别是以聚醚砜为代表的聚芳醚高性能膜材料，得益于其良好的生物相容性、易于调控的孔道结构及较高的性价比，已在生物医用分离领域获得广泛应用。但聚醚砜仍然存在本征疏水、易污染及不耐溶剂等不足，致使其在耐溶剂纳滤膜领域的应用受限。基于上述背景，我们设计合成了不同分子结构与分子量的腈基化聚芳醚，进一步通过大分子化学反应合成一系列侧链含有氨基、羧基、磺酸基等活性官能团的可交联聚芳醚，再借助原位化学反应在其膜表界面可控生长光学纳米探针，最终制备了一类具有耐有机溶剂及光学传感功能的分离膜材料，并通过表面增强拉曼散射及微区荧光光谱研究了耐溶剂纳滤膜的膜污染过程，为设计制备抗污染高性能耐溶剂纳滤膜提供了新思路。

最终交流类型：主题报告

聚集诱导发光特性药物

秦安军*
South China University of Technology, China

疾病给人们带来极大的痛苦。靶向药物的出现可为患者带来生存的希望。因此，科学家们从未停止对新药的研发。在药物研发过程中，研究人员普遍关注药物的构效关系以不断提高药物活性，而对药物的其他功能如光学性质关注较少。大多数药物，例如紫杉醇、青蒿素和阿司匹林等 因其没有大的共轭体系，使其发射光很弱或者在紫外区域发光，难以用肉眼观察到。然而，药物的发光性质研究是了解其工作机制

的理想途径之一，可以说明药物分子结构的差异对其光学性质的影响，也可以利用药物的发光性质监测药物浓度和位置的变化，以更好地了解代谢过程，减少毒副作用，实现精准化治疗。因此，对药物的光学性质的研究，对于其实现原位可视化，有效提高对药物的代谢认知具有重要意义。

本报告将汇报我们最近在基于氟代喹诺酮类抗生素的 AIE 药物。改造后的药物不仅能够进行微生物的荧光成像，而且可以进行光疗和化疗的联合治疗。此外，所得 AIE 药物还可实现对真菌液泡膜的特异性识别，并可在真菌增殖过程中液泡形成过程的原位可视化。此外，AIE 药物强的 ROS 产生能力被用于对真菌的高效杀伤，其效果要明显优于商业药物氟康唑。

因此，我们制备的 AIE 药物不仅是一种具有多重功能的分子荧光探针，而且有望用作微生物的快速诊断和治疗的试剂。

最终交流类型: 闪报

Targeted peptide-functionalized reduction-responsive polyamide amine as vaccine adjuvants against Streptococcus pneumoniae infections

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Department of Bioengineering,Zunyi Medical University

The iron uptake ABC transporter proteins PiaA and PiuA have been reported as candidate protein antigens for Streptococcus pneumoniae vaccines. However, protein vaccines alone suffer from weak immunogenicity and limited level of immune response elicited. Therefore, we designed a reduction-responsive cationic polymer: bisulfide-bonded polyamide amine (PAA) and modified 30 amino acids at the C-terminal end of the peptide-Clostridium perfringens enterotoxin protein (CPE30) at the end of the polymer by an amide reaction, to obtain the cationic polymer PAA-CPE30, which has the function of targeting the antigen-presenting cells (M-cells) in the mucosal tissues.PAA- CPE30 was used as an adjuvant, and the fusion protein PiuA-PiaA was used as an antigen to prepare the Streptococcus pneumoniae protein vaccine PAA-CPE30@PiuA-PiaA by electrostatic interactions. The level and type of antigen-specific immune response induced by this vaccine preparation in mice immunised by nasal drops, as well as the immune protective effect against Streptococcus pneumoniae in the attacking mice, were further investigated. The results showed that in the presence of the vaccine adjuvant PAA-CPE30, the protein antigen PiuA-PiaA induced stronger antigen-specific humoral and cellular immune responses, and induced stronger resistance to bacterial infection. Mechanistic studies revealed that the vaccine adjuvant PAA-CPE30 prolonged the retention time of the vaccine in the nasal cavity, promoted the uptake efficiency of antigenic proteins by antigen-presenting cells, and mediated the lysosomal escape of antigenic proteins, which may be the mechanisms by which the vaccine adjuvant enhances the immune effect.

最终交流类型：邀请报告

近红外二区生物医用光功能纳米材料

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2. 香港中文大学（深圳）

得益于其生物安全性好、光物理性质可调、易于合成和功能化修饰、出色的荧光和光敏性能、以及可便于构筑多模态诊疗试剂等优势，聚集诱导发光（AIE）材料在光学成像和诊疗领域取得了重大突破进展。我们依托材料学和生物医学的学科交叉，构建了一系列性能优异的近红外二区生物医用光功能聚集体探针；揭示了材料结构与光敏性能之间的构效关系；实现了对动物活体的肿瘤靶向成像、细菌区分检测、生理环境变化的体内示踪、生物活性分子检测，以及疾病的多模态光学治疗。在这些工作的基础上，提出了“聚集增强诊疗”新概念。

最终交流类型：口头报告

生物成像用荧光染料及功能调控

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北京理工大学

有机荧光染料被广泛应用于生物体系中重要生物组分和过程的可视化成像，逐渐成为生命信息解读与重大疾病诊断不可或缺的强大工具。随着先进荧光成像技术的快速发展，特别是多通道、超分辨、高保真动态生物成像的需求，对染料的发光强度、光稳定性等关键性能参数提出了更高的要求。在复杂的生物体系和动态的生理环境中，针对特定组分以及多组分的特异性靶标识别是荧光染料面临的重要挑战。近年来，围绕染料分子结构与性能调控之间的科学问题，比如荧光量子产率、光稳定性、靶向性等，本人聚焦基于芳基乙烯骨架生物成像用荧光染料的创制，取得了系列研究成果：（1）提出“多重分子内作用”机制，促进染料亮度和光稳定性的协同提升；（2）揭示转子型染料的“限域工程”响应机理，实现同工酶的特异性区分；（3）调控分子结构异构化，开发智能响应型染料，取得双靶标双色成像的应用突破。

最终交流类型：口头报告

具有高葡萄糖选择性的硼酸荧光探针的合成与活体应用研究

王凯、姚庆强*
山东第一医科大学

Synthesis and application of boronic acid-based fluorescent probes for selective detection of glucose in vivo

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Glucose homeostasis is one of the most important research areas in life sciences. In the field of molecular recognition, there is an urgent need to develop a molecular probe with high selectivity, high sensitivity and reversible recognition for glucose to dynamically track changes in glucose levels and elucidate their regulation in complex metabolic networks with spatiotemporal resolution.

To crack this hard nut, we designed and synthesized reversible recognition mechanism-based boronic acid probes Mc-CDBA and Ca-CDBA for glucose: First, the water-soluble group cyano (-CN) was introduced on the para-position of phenylboronic acid in the prototype PDBA to improve the biocompatibility of the molecular probe. At the same time, the pKa of the probe is decreased due to the electron-absorbing induction effect of -CN, and the affinity for glucose is improved. Secondly, by introducing conjugated effect groups methoxyl (-COOCH3) and carboxyl (-COOH) at the β position of anthracene in PDBA (λex/em = 370/423 nm), the overall conjugation degree of the molecule is increased, and the fluorescence of the probe is redshifted (Mc-CDBA, λex/em = 393/457 nm; Ca-CDBA, λex/em = 382/438 nm), successfully applied the probe to multi-dimensional imaging of cells and zebrafish at the same time, providing a technical tool for clinical medical research on glucose homeostasis in vivo and the study and diagnosis of metabolic diseases.

References:

[1] Wang K. et al. J. Am. Chem. Soc., 2023, 145: 8408.
[2] Wang K. et al. ACS Sensors, 2021, 6: 1543.

最终交流类型：闪报

基于水溶液硫量子点的可调控氧化反应研究

赵静喃、赵国峰、芦悦、孟庆伟*、彭孝军
大连理工大学

氧化反应是化学工业的基石，然而氧化反应存在危险性大、选择性控制难、环境负担重等问题。因此，构建本质绿色、安全、高效的氧化反应是全球学术界和工业界的追求目标，如何实现分子氧的可控活化及催化剂的结构设计是实现绿色、高效氧化反应的关键。

本研究旨开展基于含硫光敏剂的可调控光催化分子氧氧化，前期实现了二硫化物介导的 C-O、C-C、C-N 选择性构建，在连续流光化学条件下，气液两相光催化反应效率大幅度提高。目前正在开展水溶液硫量子点的光催化分子氧氧化反应研究，系统建立可精细调控的水溶液硫量子点构筑方法，揭示硫量子点光催化俄歇效应与水/氧逐级活化的内在规律，重点发展有机化合物碳氢键和碳碳键可见光催化氧化策略，实现硫量子点催化剂的理论设计、可控制备及精准调控，建立硫量子点组成-结构-性质的关联机制。本项目采用非金属纯元素硫量子点为光催化剂，在水溶液中实现以分子氧为终端氧化剂的高效、高选择性氧化反应，为本质绿色、安全、高效的氧化策略开辟一条新方法。

最终交流类型：邀请报告

湿气响应性氧化石墨烯/高分子复合膜

宾月珍*、曲美洁、宋婧怡
大连理工大学

湿度响应可应用于监测皮肤湿度、呼吸状态等生理参数以及仿生和人机交互-非接触式传感与控制等。本研究基于电阻型湿度传感器操作简单、可重复使用、驱动功率低、易于小型化等优点，以氧化石墨烯为主体，纳米纤维素作为填料，研制了具有湿度驱动和湿气传感功能的复合膜。以氧化石墨烯为主体，细菌纤维素作为填料，通过溶剂挥发的方法制备了兼具湿度传感和湿度驱动的复合膜。细菌纤维素(BC)的加入改善了纯氧化石墨烯(GO)薄膜电阻变化率重复性差和力学强度低的问题。当 BC 含量为 20%时复合膜在 80%RH 下的电阻变化率达 74%，偏转角为 175°。并对其进行仿生模拟—捕蝇草和含羞草，发现样条在改变环境的相对湿度后能产生相似的“应激反应”。以 L-抗坏血酸为还原剂，通过浸渍的方法部分还原氧化石墨烯/细菌纤维素(BG)复合膜，大幅提高了 BG 复合膜的湿气灵敏度，通过调节还原条件控制含氧官能团浓度及电导率，进而有效调控湿气传感性能，可实现在 80 %RH 下的最大电阻变化率达 94%，响应/恢复时间为 13 s/47 s。复合膜响应速度快，灵敏度高，并可以区分不同的呼吸状态和湿度源纵向位置，通过构建非接触阵列，可以定位湿度源。这种薄膜在人体健康监测和非接触传感方面具有很大的潜力。

最终交流类型：主题报告

Wiley 合作出版 - 助力中国高品质期刊发展

刘哲*
威力约翰出版集团

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最终交流类型: 主题报告

Addressing Optical Imaging Challenges for Biomedical Research

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Molecular optical imaging plays a crucial role in biology and medicine. However, the strong tissue autofluorescence and shallow tissue penetration of optical imaging compromise not only its sensitivity and specificity but also limit its clinical translation. In this talk, I will introduce our approaches (molecular afterglow imaging and artificial urinary biomarkers) to tackle these challenges. First, I will introduce molecular afterglow probes with long-lasting luminescence after cessation of electromagnetic irradiation by light, ultrasound, or X-ray. Due to the elimination of real-time light excitation, molecular afterglow probes have a signal-to-background ratio more than two orders of magnitude higher than NIR fluorescence, allowing for sensitive detection of tiny peritoneal metastatic tumors and monitoring therapeutic outcomes. Second, I will discuss how to design renal-clearable optical probes as artificial urinary biomarkers for the early diagnosis of acute kidney injury and allograft rejection as well as the profiling of tumor immune microenviroment. Molecular renal probes (MRPs) can specifically activate their NIR fluorescence/chemiluminescence signals toward the biomarkers of interest, followed by rapid renal clearance for urine tests. MRPs can thus act as artificial urinary biomarkers to bypass the tissue penetration issue of optical imaging, permitting optical urinalysis that outperforms typical clinical/preclinical assays. These studies provide the basis for an entirely new class of molecular optical probes with ultrahigh sensitivity and high translational potential for disease diagnosis and prognosis.

最终交流类型：仅发表论文
D26-PO01

水下抗溶胀水凝胶的传感运用及机器学习检测

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在本研究中，我们设计并测试了一种新型的水下抗溶胀水凝胶传感器，专为长时间水下作业和极端环境条件下的监测而开发。这种水凝胶传感器通过在聚合物网络中引入特定的交联剂，成功实现了在水下环境中的高稳定性和低溶胀率。此外，该传感器采用了环境友好材料，确保在海洋生态系统中使用时的安全性和可持续性。为了提升传感器的数据处理能力，我们整合了机器学习技术。通过部署多种机器学习模型，如支持向量机（SVM）和随机森林算法，传感器能够对收集的数据进行实时分析，有效识别复杂的环境变量和模式。这种智能化的数据处理方法不仅提高了监测的准确性，还增强了传感器对环境变化的响应速度。实验阶段，我们将这些传感器部署在不同的水下环境中，包括淡水和咸水体系，以测试其性能和稳定性。初步结果表明，这些传感器能够在各种水质条件下保持良好的功能，无论是低温还是高盐度环境。机器学习算法成功地从传感数据中提取出关键信息，并进行了有效的数据分类和预测。此外，在人体水下运动识别及手势识别所拓展的摩尔斯电码识别能实现精准的水下通信运用。通过这些应用，我们展示了水凝胶传感器在实际环境中的广泛潜力和实用性。最终，本研究不仅推动了水凝胶材料在环境科学领域的应用，也为环境监测技术的发展提供了一种结合传统材料科学和现代信息技术的创新方案。未来，我们计划继续优化这些传感器的设计，并扩展其机器学习功能，以实现更广泛的环境应用和更精确的数据分析。

最终交流类型：口头报告

基于阻滞溶胀过程的相变过程调控

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溶胀指在渗透压驱动下物体吸收液体发生体积亦或质量增大的传质过程。日常生活、工业界以及自然

界，比如尿不湿吸水、粉条泡发，水熊虫复生和药物缓释等，都伴随着溶胀过程。对于具有低临界溶解温度的相变材料，溶胀过程存在一个长期忽视的关键问题：在日常经验的时空下，溶胀体是否处于热力学平衡态？其决定性因素又是什么？如果处于平衡态，则后续升温诱导相分离为可逆相变，否则，则为不可逆过程。本报告利用聚乙烯醇缩醛类聚合物为模型体系，通过调控分子结构，探索明确了玻璃化是阻滞溶胀到达平衡态的关键因素。在此基础上，我们进一步探索可逆相变在智能窗领域，以及不可逆相变在人工角膜等领域的独特应用。

最终交流类型：仅发表论文

D26-PO02

海洋的海洋保护：水下原位防污超疏油涂料的创新设计

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海洋工程和水下作业对水下防污涂料有很高的要求。在水环境中对各种大型基材表面进行原位喷涂是理想的，但极具挑战性。在本文中，我们报道了一种新的方法来实现可直接在水下应用的防污超疏油涂层，其涉及与共价交联互锁的侧链的水解迁移，其可直接粘附到水下的各种湿基材上，而无需任何基材表面预处理，以形成具有水下超疏油性和可持续的基材粘附性的涂层。它同时具有水下涂覆能力、水下超疏水性和对各种基材的附着力。因此，本工作为设计未来的水下直接湿附型防污超疏油涂料提供了一个简单的新范例。

最终交流类型：邀请报告

生物基水凝胶的制备和生命健康检测探索

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上海应用技术大学

生物基材料由于可再生、可降解、环境友好和生物相容性好等优点，受到广泛关注。根据生物基材料结构特点，利用低共熔效应，制备生物基水凝胶，解决水凝胶在电子皮肤应用中的低环境耐受性和抵抗损伤性。分别以动物蛋白和植物多糖为原料，结合绿色低共熔溶剂，通过致密交联形成力学性能强、黏附性能好、自愈合速度快且传感灵敏的生物基水凝胶，实现检测的灵敏性，进一步探究其在脉搏监测的应用。

最终交流类型：口头报告

超分子驱动的智能响应发光材料

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华中科技大学

智能发光材料是指对外界刺激具有感知，且以发光色彩变化或发光强度变化输出响应的一类材料。超分子调控具有动态可逆性，是构筑诸多智能材料的有效策略。我们课题组利用超分子调控策略，构筑了基于有机发光分子和无机钙钛矿纳晶发光材料的智能响应发光材料，具体为：1）设计了一种具有形致变色功能的发光高分子材料 PGP，PGP 可以在不同环境下自组装形成纳米片、球形胶束、无规则枝状物三种典型形貌，并发射组装形状依赖的荧光色彩，使宏观可观测的荧光色彩和微观组装形貌关联；同时，PGP 还可以作为荧光墨水在纸上实现多次可逆的荧光显色和擦除。2）设计了一种表面带有金刚烷（AD）基团的钙钛矿 AD-CsPbBr3 发光纳晶，利用纳晶表面金刚烷与环糊精的主客体作用，提高了 CsPbBr3 纳晶在极性溶剂中的稳定性，同时实现了基于 AD-CsPbBr3 的四级信息加密。

最终交流类型：主题报告

Direct Synthesis of Two-Dimensional Metal Chalcogenides
Through Molecular Preorganization

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Two-dimensional materials are of substantial interest, due to their unique fundamental characteristics (e.g., non-symmetric conductivity) and the possibility of large-scale processability. Recent progress in the synthesis of two-dimensional (2D) materials has embraced precursor-based methodologies, offering a transformative approach to material fabrication. Notably, the utilization of specific precursors plays a pivotal role in engineering tailored 2D materials. For instance, the controlled manipulation of two bismuth alkyl thiolates, Bi(SR)3, differing only in alkyl substituents (-But versus -Pri), has demonstrated their efficacy as single-source precursors in the chemical vapor deposition (CVD) process. These precursors efficiently supply both Bi and S for the fabrication of targeted 2D structures without the need of any carrier gas or co-reactants.
Moreover, the direct synthesis of tin monoselenide (SnSe) and tin diselenide (SnSe2) materials has been achieved through the thermolysis of molecular compounds utilizing a novel class of seleno-ligands. These advancements underscore the precision and versatility of precursor-driven techniques in harnessing the “power of synthesis” for controlling the layer thickness, crystal structure, and elemental composition, thereby enabling the development of diverse 2D materials. This talk will address the chemically controlled synthesis of 2DMs and demonstrate their superior performance in electrocatalysis, and sensing applications.

最终交流类型：主题报告

面向临床的分子成像新探针与新技术

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基于分子探针的光学成像（包括荧光、化学发光、长余辉和光声成像等）技术因响应速度快、对样本损伤小、可实现实时动态监测等优点，已成为医学检测、临床手术导航和药物开发等领域的强有力研究工具。然而，传统光学探针由于响应特异性有限以及样本背景干扰信号大等问题，难以实现临床病理环境中靶标的精准成像。针对这些关键科学问题，本课题组开展了系列研究工作： 1）为了实现了复杂病理样本中生化信息的高特异性获取，提出分子结构调控开发高选择性荧光探针的策略，发展高选择性生物成像分析新方法，成功实现临床疾病样本的精准分型；2）为了降低临床样本的背景信号干扰并增强传统光学探针的组织成像深度，基于富电子蒽衍生物开发新型高亮度长余辉发光材料，发展有机长余辉发光共振能量转移精准成像分析方法，首次实现清醒动物的长余辉成像；在国际上首次提出超声发光成像技术，降低了临床样本检测中的背景信号干扰，并提升组织成像穿透深度，为实现小动物长时程成像及深层肿瘤 PDT 治疗提供新思路。

关键词：分子成像；光学探针；超声发光；有机余辉发光；精准成像

最终交流类型：口头报告

单线态氧和疾病诊疗

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近些年，以单线态氧（Singlet Oxygen，$^1O_2$）为主体的光动力疗法（Photodynamic Therapy）逐渐兴起，已经在皮肤癌、头颈癌、浅表性膀胱癌等多种癌症的治疗中呈现出较好的效果。但是，肿瘤乏氧和光源有限的穿透能力严重限制了单线态氧的产生，而光动力对氧气的消耗也会加重肿瘤乏氧，导致恶性循环。将单线态氧精准、高效地递送到病灶已成为这一领域的重大挑战。近年来，报告人团队围绕单线态氧载体的设计及应用开展工作，将光动力过程转移到体外，通过构建内过氧类单线态氧载体，实现了不依赖于光源和病灶氧气的单线态氧递送和疾病治疗。

利用肿瘤微环境为响应元素，报告人团队开发了硝基还原酶促发的内过氧结构转化和精准的单线态氧控释机制，实现了不需要外源性刺激的单线态氧自递送和乏氧肿瘤治疗[1]。基于赖氨酸-脲-谷氨酸能够特异性靶向前列腺特异性膜抗原的特点，报告人开发了前列腺癌靶向的萘类内过氧，进一步提高了内过氧化物递送单线态氧的精准性[2]。从单线态氧载体的分子结构出发，报告人团队开发了基于硫黄素T和内过氧的药物协同递送体系，实现了对Aβ淀粉样蛋白聚集的双重抑制剂[3]。设计了基于内过氧化物的三线态氧载体，为肿瘤乏氧提供新工具[4]。于此同时，为解决传统光亲和标记策略[5-6]在靶点鉴定过程中存在的关键问题，报告人首次开发了基于上转化纳米材料的光亲和标记方法，开发的纳米靶点鉴定探针稳定性好，适用于多个亲和力弱蛋白的标记，同时具有标记蛋白分离容易、产率高、安全性好的特点。更为重要的是，该类纳米探针能够进行活体靶点鉴定并具有较好的安全性[7]。利用这一探针探索内过氧药物作用机制的工作正在有序进行。此外，将内过氧类单线态氧载体和上转化纳米材料有机结合，报告人开发了多个近红外光控释的单线态氧递送体系并取得了较好的抗癌效果。

最终交流类型：邀请报告

Interface Engineering of Conductive Polymer Composite for Wearable Electronics

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The application of wearable technologies in personalized health management and medical treatment has attracted significant attention. The rapid progress of personalized health management generates new demands on the multifunctionality of wearable devices, for example, to maintain function under large and frequent deformations when the device is equipped on the human body and to monitor diverse physiological parameters simultaneously with minimum energy supply. To address the abovementioned challenges, our lab has developed a series of polymer composites with well-controlled mechanoelectrical properties and surface properties, making them feasible to be mounted with electronic components for the manufacturing of conformable circuits to be used as artificial skins or on-skin electronics.

最终交流类型：邀请报告

Data-Driven Design of Functional Fluorescent Dyes

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Keywords: Fluorescent dyes; Computational chemistry; Machine learning; Molecular design

Fluorescent probe imaging technology has been widely applied in fields such as biology, medicine, chemistry, and environmental science due to its fast recognition rate, high sensitivity, high selectivity, and biocompatibility. Developing methods for predicting dye properties and constructing molecular design strategies for dyes plays a crucial role in advancing functional fluorescent dyes. Computational chemistry combined with machine learning algorithms has become an effective tool for predicting dye properties and designing dye molecular structures. Using density functional theory calculations, they have developed theoretical descriptors for predicting dye quantum yield[1], spontaneous blinking properties[2], and viscosity response. Additionally, they have proposed the fluorescence quenching mechanism and molecular design strategies for bioorthogonal tetrazine dyes. Employing deep learning methods, they have presented intelligent models for predicting the photophysical properties of mono-benzene ring fluorophores and near-infrared II cyanine dyes. These findings provide new insights and a theoretical foundation for the development of efficient fluorophores.

最终交流类型：口头报告

搭载免疫细胞的光诊疗材料

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关键词：光动力治疗；荧光识别；巨噬细胞；

基于功能染料的光诊疗技术以其灵敏度高的特点在生物医疗领域应用广泛，但受限于病灶靶向性、潜在毒副作用、光穿透深度等问题，其在活体水平的实际应用并不理想。

本研究聚焦诊疗染料响应性及靶向性调控，提出将功能染料搭载于免疫细胞的策略，利用免疫细胞的先天趋化特性，实现对炎症等病灶的精准靶向，大幅降低诊疗染料剂量，提升活体水平光诊疗效率[1-3]。一、恶性细菌感染引发的脓毒症病情发展快，治疗时间窗口期短，我们将 pH 响应型光敏剂搭载于巨噬细胞的溶酶体中，改造后的巨噬细胞会像士兵一样利用其先天趋化特性主动捕获全身游离的细菌，经光照介导光动力治疗，脑膜炎小鼠治愈率达 100%[2]；二、继续构建了一类炎症因子（HClO、NO 等）响应型光敏剂，载于巨噬细胞，用于全身性细菌感染的治疗，病鼠在户外通过日光浴就能彻底清除体内细菌，恢复健康。响应型诊疗染料及搭载免疫细胞的设计让光治疗回归“日光浴”的本源，简化光治疗的操作，提高光治疗的安全性。