



金属有机框架: 定义化学新空间

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金属有机框架的突破性价值, 在于它为化学领域定义了独特的“新空间”——既包括其有序结构内部开放的物理空间, 也涵盖它为科学研究拓展的新思路与新平台。这一兼具结构与学术维度的创新, 让金属有机框架成为推动化学、材料及相关学科发展的重要力量, 也使其获得了今年诺贝尔化学奖的认可。

2025年10月8日, 瑞典皇家科学院宣布, 日本京都大学北川进(Susumu Kitagawa)、澳大利亚墨尔本大学理查德·罗布森(Richard Robson)和美国加利福尼亚大学伯克利分校奥马尔·亚吉(Omar M. Yaghi)三人获得2025年诺贝尔化学奖, 以表彰他们对金属有机框架发展的贡献(for the development of metal-organic frameworks)。诺贝尔奖委员会指出, 金属有机框架具有巨大潜力, 为定制具有新功能的材料带来了前所未有的机遇。

作为一门中心科学, 化学研究物质的组成、结构、性质及其变化规律。通过精准连接原子, 科学家成功设计并合成了无数结构精妙的分子——从维系神经健康的维生素B₁₂, 到用于癌症治疗的顺铂, 再到可传递遗传信息的DNA片段。但要将这种原子级精准构建分子的逻辑, 拓展到可无限延展的二维或三维空间, 人们面临的挑战远比操控孤立分子大得多^[1]。随着20世纪晶体学等领域的发展, 对新合成物质的结构分析逐渐摆脱了早期的高难度限制。但与之相对, 二维或三维结构的理性预测与可控合成却远非易事, 甚至一度成为学界的“固有认知”——人们普遍认为, 固相材料的结构预测和精准合成难以实现^[2]。

1989年, 罗布森提出了一项突破性思路: 可依据给定构造单元的几何形状与连接特征“预测”配位产物结构。他以具有四面体配位构型的Cu(I)与四面体形状的有机膦为研究对象, 成功制备出网络结构, 不仅证实了特定配位网络的可设计性, 还发现该结构是具有较大空腔的类金刚石拓展结构^[3]。尽管罗布森构建的结构稳定性较差, 网络容易解体, 但是它无疑为基于配位键的拓展结构研究奠定了重要基础。

亚吉与北川进各自取得的一系列开创性发现实现了从



李巧伟 复旦大学教授, 从事金属有机框架的设计、合成, 以及应用研究, 主要聚焦于框架材料缺位化学、多组分框架和跨键合框架的合成及结构, 以及框架在电化学储能方面的应用。

“晶体工程”到“框架化学”的跨越。这些发现不仅让金属有机框架实现了结构高稳定性、永久多孔性、可修饰性等独特优异性能——这些性能是其他材料难以同时具备的; 同时还诞生了“次级构造单元”“同网格设计”“软多孔晶体”等关键概念的突破, 为领域发展提供了全新思路。

1995年, 亚吉在报道加热至350°C结构依然保持的二维配位材料时, 首次使用了金属有机框架(简称MOF)一词^[4]。随后, 他提出以多金属的次级构造单元为顶点的构筑原理^[5], 创制出结构稳定的多孔框架材料, 为晶态多孔材料的设计提供了关键理论基础。1999年, 他报道了具有超高孔隙率的MOF-5结构, 打破了由活性炭长期保持的比表面积纪录, 迅速引起了科学界的极大兴趣和公众的广泛关注^[6]。2002年, 他开创性提出同网格功能化概念, 建立了合成具有不同官能团与孔道尺寸的同网格MOF材料的普适方法^[7]。这些研究成果确立了MOF作为孔隙率最高的晶态材料的地位, 发展的合成方法也成为制备MOF材料的主流方法。

1997年, 北川进以钴、镍或锌离子为金属中心, 以联吡啶为有机分子, 成功构建出具有类似“榫卯”结构的三维配位聚合物^[8,9]。这类框架内部贯穿有开放通道, 在去除客体分子后, 内部空间甚至可吸附并释放甲烷、氮气与氧气, 生动地诠释了材料的多孔性。1998年, 基于此类材料潜在的柔性与结构动态性, 他预测这一全新的基本性质将为固态化学开辟

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一种新范式^[10]。为此,他提出了框架材料的“四代”概念,将 MOF 领域从永久多孔材料进一步拓展至柔性 MOF、软多孔晶体等新型态,并引入了缺陷、非对称、杂化、多级、无序等新内容。

今年恰逢“金属有机框架”这一概念进入科学家研究视野 30 周年。金属有机框架把有机化学和配位化学的细致精妙和错综复杂带入到固相材料领域。围绕 MOF 的研究活力比以往任何时期都更为强劲。在 MOF 的结构设计和合成化学方面,新的网络拓扑理论(合并网络^[11]、相关网络、衍生网络、网络裁剪^[12]等)层出不穷,配位键与其他键合(共价、氢键)等融合的构筑方法发展迅速^[13,14]。框架组分单元不断多元化,激发了人们对各向异性材料、多级孔材料、编织材料^[15]、互锁结构、框架中的基元序列^[16]等方向的探索 and 追求。原位电子显微技术^[17](如缺位、掺杂的原位表征)与电子晶体学^[18](结构确定、框架动态行为分析)等手段的发展,正助力人们在不同时空维度下,逐步明晰 MOF 的清晰结构。MOF 的网络拓扑概念与结构有序性,为计算化学和机器学习辅助的新材料结构预测、合成及性质研究提供了极佳切入点,人工智能与金属有机框架的深度融合更成为科学研究范式变革的典型范例^[19,20]。

多孔的 MOF 不仅提供了在分子层次之上控制物质的手段,还提供了可进一步操控分子的空旷空间。可达性、响应性、自适应性已成为科学家频繁讨论的关键词。基于框架上或孔道内有序分布的活性位点,MOF 不仅成为研究催化反应的绝佳载体,同时提供了其他材料难以比拟的精准可控的催化微环境^[21]。这些新空间内展现了独特的粒子传递行为及规律,使得电子、质子、光子等的传递过程呈现出以往未见的新现象,导电框架、导质子框架、电催化框架、光催化框架等的研究也随之层出不穷^[22-25]。框架与其他化学物质(石墨烯等二维材料、纳米粒子、聚合物、金属等)或者与生物物质(酶、DNA、蛋白、抗体、细胞)之间^[26],能形成怎样的独特界面?在这类界面上,物质传递与能量转化涌现出哪些过去未被察觉的突破性规律?对这些问题的探索,正极大地吸引着科研工作者的兴趣。

MOF 超高的气体吸附容量、高选择性的气体分离能力正助力实现“碳达峰碳中和”目标(图 1)。在水的吸附(低湿度空气集水、吸附驱动热泵、室内环境控制)^[27]、碳捕集与利用(直接空气捕集 DAC 技术、工况下二氧化碳吸附与转化一体化)^[28]、天然气存储^[29]、高附加值及生物代谢气体吸附分离(稀有气体、电子特气、同位素、呼气)^[30,31]等领域,MOF 的应用正加速走向市场。世界经济论坛在 2017 年将“从空气中提取饮用水”评为“改变世界的十大新兴技术”之一^[32]。此外,MOF 在环境污染物去除、药物缓释方面也展现出极具应用价值的潜力。通过与其他类型材料的复合,MOF 既能保留自身核心特性,又能融合对方的优势性能,从而突破单一材料的功能局限。科学家与工程师通过跨学科合作,实现了颗粒



图 1 (网络版彩色)诺贝尔奖基金会网站用一幅卡通图,将金属有机框架提供的化学新空间,形象描绘成专为“水分子”定制的宽敞公寓楼。此类独特空间的用途远不止于此,还可用于二氧化碳捕集、水处理、气体分离与转化等多个领域。图片来源: www.nobelprize.org
Figure 1 (Color online) The official website of the Nobel Prize uses a cartoon to vividly depict the new chemical spaces offered by MOFs as spacious apartment buildings tailored specifically for “water molecules”. The applications of such unique spaces extend far beyond this—they can also be used in CO₂ capture, water treatment, gas separation and conversion, and various other fields. Image source: www.nobelprize.org

尺寸的精准调控,并成功开发出玻璃态、薄膜态、纤维态及成型造粒等多种形态的 MOF 材料,使 MOF 在传感、储能、微电子等前沿领域的器件研发与实际应用不再遥远。

这些成果不仅拓展了人类对物质科学的认知边界,更为应对全球性挑战提供了切实可行的技术路径,展现了基础研究驱动社会进步的典范价值。MOF 已被纳入多个全球性计划,包括中国科技部的国家重点研发计划、“欧洲绿色协议”、“地平线欧洲”及美国能源部的温室气体减排、资源效率和水安全相关项目。各国政府已开始将 MOF 视为实现长期气候与可持续发展目标的关键技术。已有 BASF、Svante、Atoco、NuMat、乐帝化学、Atomis、Framergy 等多家企业致力于 MOF 材料的规模化生产,推动其在气体分离、环境治理、能源存储及医疗载体等领域的商业应用落地^[33]。尽管复杂 MOF 结构的精准预测、苛刻工况下材料的持久稳定性等技术瓶颈仍需业界持续攻克,但这些商业化实践不仅证明了框架材料能够具备满足不同应用场景需求的功能性,也验证了其制备工艺可实现规模化放大,且符合经济性要求。根据 2023 年的 Global Market Insights 报告,到 2034 年网格材料市场预计将达 292 亿美元,显示其强大的工业前景^[34]。

回望 100 多年前,美国化学家吉尔伯特·路易斯在他开创性的“The atom and the molecule”论文中^[35],搭建了原子成键连接形成分子的核心理论框架,塑造了人类对原子间化学键合的思考方式。在一个多世纪的探索里,人类对微观粒子单元的驾驭从认识键合走向了设计空间。原子以特定的朝向和

空间排布被固定于分子中；同理，分子以特定的朝向和空间排布被固定于框架中。化学既延续着对物质本质的追问，也在历史递进中为材料世界打开了从自然赋予到按需定制的新

维度。“The Atom, the Molecule, the Framework and Beyond”——这正是化学科学的动人轨迹：每一步突破都是对前人智慧的呼应，更是对未来可能的拓展。

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Summary for “金属有机框架: 定义化学新空间”

Metal–organic frameworks: defining new spaces for chemistry

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The 2025 Nobel Prize in Chemistry has been awarded to Susumu Kitagawa from Kyoto University, Richard Robson from the University of Melbourne, and Omar M. Yaghi from the University of California, Berkeley, for the development of metal–organic frameworks (MOFs). The Nobel Committee for Chemistry emphasized that MOFs have enormous potential, bringing previously unforeseen opportunities for custom-made materials with new functions. The groundbreaking significance of MOFs centers on their definition of a unique “new space” in chemistry, which encompasses both the open physical space within their ordered structures and the paradigm-shifting platforms they have unlocked for scientific research. This space spanning structural and academic dimensions has established MOFs as a key engine for developments in chemistry, materials science, and related disciplines, earning them recognition with this year’s Nobel Prize in Chemistry.

As a central science, chemistry has long enabled precise molecular design, but extending atomic-level control to two- and three-dimensional extended structures remained a daunting challenge. Robson’s pioneering concept of predicting coordination network structures based on building units’ geometry laid the important groundwork, while Yaghi and Kitagawa shifted the field from “crystal engineering” to “framework chemistry”. MOFs with high stability, permanent porosity, and tunability were realized through the introduction of key concepts such as secondary building units, isorecticular design, and soft porous crystals. This View article traces the historical development of MOF chemistry, emphasizing key breakthroughs in the structural design and synthesis, adsorption measurements, functionalization, and flexibility and dynamics.

The article further examines the evolving trends in modern MOF synthesis research, distinguished by new topology theories (e. g., merged net, related net, derived net, and net-clipping) and hybrid linkage construction methods. The increasing diversification of building units has spurred exploration of anisotropic materials, interwoven materials, interlocked structures, and frameworks with sequences. Developments in techniques such as *in-situ* electron microscopy and electron crystallography have rendered structural characterization of MOFs more comprehensive and unambiguous, while their integration with artificial intelligence (AI) and machine learning has accelerated material prediction and synthesis.

Porous MOFs not only offer methods to control matter beyond the molecular level, but also provide highly open space for further manipulation, with accessibility, responsiveness, and adaptability as key research focuses. Leveraging ordered active sites on the framework backbones or in the pores, they serve as ideal catalytic centers with unparalleled precision and controllable microenvironments. Electrically conductive, proton-conductive, electrocatalytic, and photocatalytic frameworks have emerged. Additionally, studies exploring the distinct interfaces between MOFs and other chemical or biological entities have garnered substantial research interest.

Highlighting MOFs’ practical value, the article also discusses their role in addressing global challenges: their ultrahigh gas adsorption capacity and selectivity drive applications in carbon capture (including direct air capture), natural gas storage, and water harvesting. MOFs also show promise in pollutant removal, targeted drug delivery, and electronics, with commercialization advancing via leading companies and supported by global research initiatives.

Over a century since Gilbert Lewis’s seminal paper, *The Atom and the Molecule*, human mastery of microscale units has advanced from understanding atomic bonding to designing deliberate spatial architectures. Atoms are fixed in molecules with specific spatial arrangements; similarly, molecules are anchored in frameworks with distinct directional alignments and spatial configurations. Fittingly, the 2025 Nobel Prize in Chemistry honors the pioneering development of MOFs—the epitome of this spatial design philosophy—recognizing their transformative potential to address global challenges in clear energy, clean water, and carbon neutrality.

metal–organic framework, Nobel Prize in Chemistry, reticular chemistry, porous materials

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