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工具助手

编者按：

美国 Science(《科学》)、英国 Nature(《自然》)及美国 Cell(《细胞》)是国际公认的三大享有最高学术声誉的科技期刊，发表在这三大期刊上的论文简称 CNS 论文。

本期梳理 10 月 Nature、Science 期刊上材料科学领域的最新论文。



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[1] Highly flexible and superhydrophobic MOF nanosheet membrane for ultrafast alcohol-water separation

用于超快醇-水分离的高柔性超疏水 MOF 纳米片膜

出版信息: Science, 21 OCT 2022, VOL 378, ISSUE 6617

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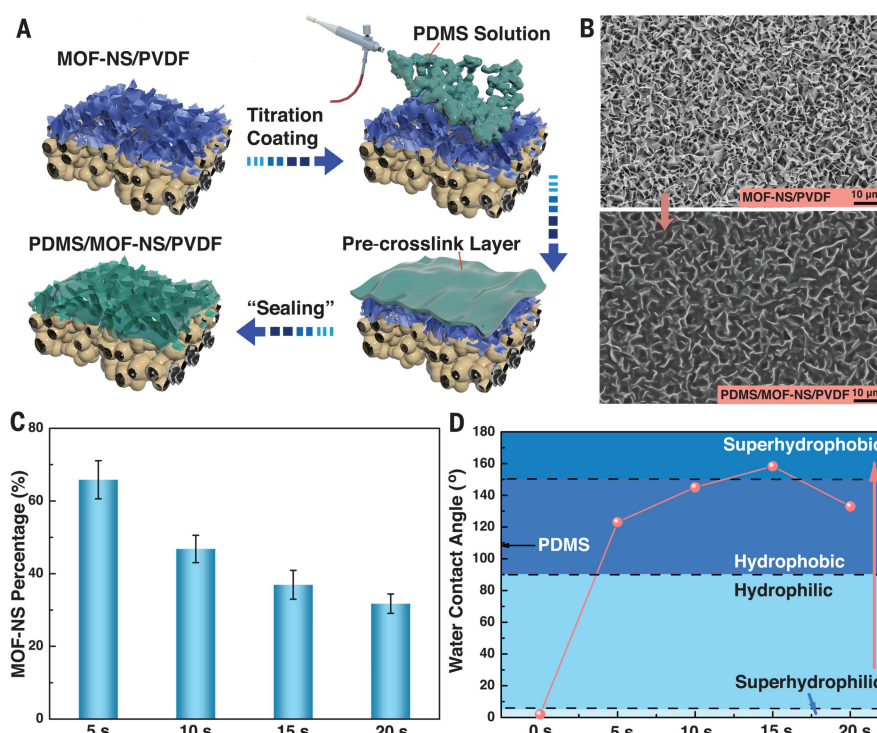
国内相关报道: <https://bit.edu.cn/xww/xzw/xsj11/0cab6174b44342029d85f9cd6d2a2c5c.htm>

全文链接: <https://www.science.org/doi/10.1126/science.abo5680>

Abstract: High-performance pervaporation membranes have potential in industrial separation applications, but overcoming the permeability-selectivity trade-off is a challenge. We report a strategy to create highly flexible metal-organic framework nanosheet (MOF-NS) membranes with a faveolate structure on polymer substrates for alcohol-water separation. The controlled growth followed by a surface-coating method effectively produced flexible and defect-free superhydrophobic MOF-NS membranes. The reversible deformation of the flexible MOF-NS and the vertical interlamellar pathways were captured with electron microscopy. Molecular simulations confirmed the structure and revealed transport mechanism. The ultrafast transport channels in MOF-NS exhibited an ultrahigh flux and a separation factor of 8.9 in the pervaporation of 5 weight % ethanol-water at 40° C, which can be used for biofuel recovery. MOF-NS and polydimethylsiloxane synergistically contribute to the separation performance.

摘要翻译: 高性能渗透汽化膜在工业分离应用中具有潜力, 但克服渗透-选择性权衡是一个挑战。我们报告了一种在聚合物基质上具有偏好形结构的高柔性金属-有机框架纳米片 (MOF-NS) 膜用于醇-水分离的策略。控制成长速度后, 我们采用表面涂层方法有效地生产出柔性和无缺陷的超疏水 MOF-NS 膜。电子显微镜捕捉到了柔性 MOF-NS 的可逆变形和垂直层间通路。同时, 通过分子模拟证实了其结构, 揭示了传递机制。MOF-NS 的超快输运通道在 40° C 条件下, 在乙醇-水渗透汽化过程中具有极高的通量和 8.9 的分离因子, 可用于生物燃料回收。MOF-NS 和聚二甲基硅氧烷在分离性能上具有协同作用。

文中插图:



[2]

Hallucinating symmetric protein assemblies

“幻觉法”生成对称蛋白质组合

出版信息: Science, 7 OCTOBER 2022, VOL 378, ISSUE 6615

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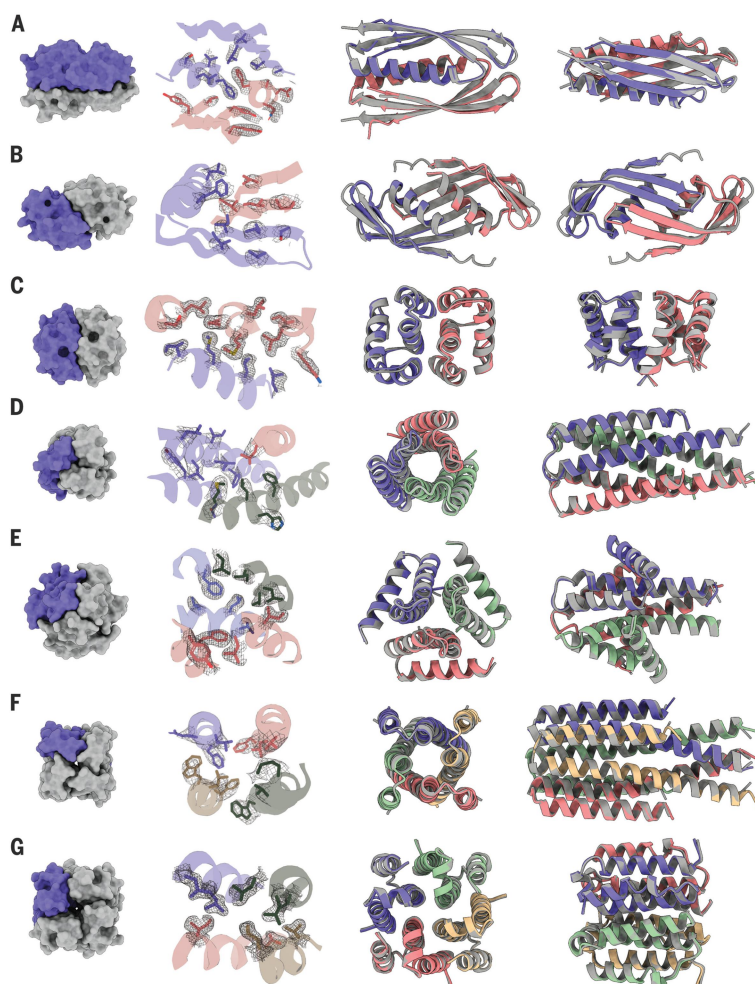
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全文链接: <https://www.science.org/doi/10.1126/science.add1964>

Abstract: Deep learning generative approaches provide an opportunity to broadly explore protein structure space beyond the sequences and structures of natural proteins. Here, we use deep network hallucination to generate a wide range of symmetric protein homo-oligomers given only a specification of the number of protomers and the protomer length. Crystal structures of seven designs are very similar to the computational models (median root mean square deviation: 0.6 angstroms), as are three cryo-electron microscopy structures of giant 10-nanometer rings with up to 1550 residues and C33 symmetry; all differ considerably from previously solved structures. Our results highlight the rich diversity of new protein structures that can be generated using deep learning and pave the way for the design of increasingly complex components for nanomachines and biomaterials.

摘要翻译: 深度学习生成方法提供了一个机会, 可广泛探索超越天然蛋白质序列和结构的蛋白质结构空间。研究组使用深度神经网络“幻觉法”生成了广泛的对称蛋白质同源寡聚体, 只需给定原聚体的数量和长度。七种设计的晶体结构与计算模型非常相似(中位均方根偏差: 0.6 埃), 具有高达 1550 个残基和 C33 对称性的巨型 10 纳米环的三种冷冻电子显微镜结构; 所有这些都与先前解析的结构有很大不同。该研究结果突出了利用深度学习可生成新蛋白质结构的丰富多样性, 并为纳米机器人和生物材料越来越复杂的组件设计铺平了道路。

文中插图:



[3]

Plastic deformation in silicon nitride ceramics via bond switching at coherent interfaces

氮化硅陶瓷在共格界面上通过键切换产生塑性变形

出版信息: Science, 28 OCTOBER 2022, VOL 378, ISSUE 6618

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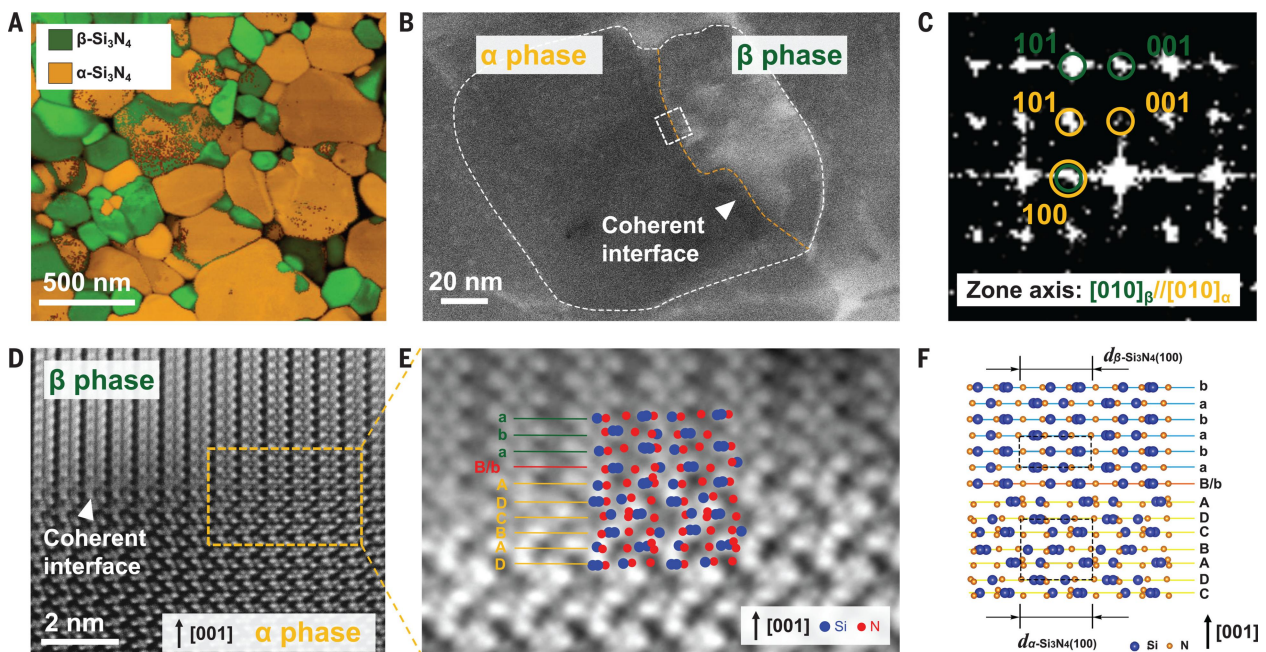
国内相关报道: <https://www.tsinghua.edu.cn/info/1175/99464.htm>

全文链接: <https://www.science.org/doi/10.1126/science.abq7490>

Abstract: Covalently bonded ceramics exhibit preminent properties—including hardness, strength, chemical inertness, and resistance against heat and corrosion—yet their wider application is challenging because of their room-temperature brittleness. In contrast to the atoms in metals that can slide along slip planes to accommodate strains, the atoms in covalently bonded ceramics require bond breaking because of the strong and directional characteristics of covalent bonds. This eventually leads to catastrophic failure on loading. We present an approach for designing deformable covalently bonded silicon nitride (Si_3N_4) ceramics that feature a dual-phase structure with coherent interfaces. Successive bond switching is realized at the coherent interfaces, which facilitates a stress-induced phase transformation and, eventually, generates plastic deformability.

摘要翻译: 共价键合陶瓷具有优异的性能（包括硬度、强度、化学惰性、耐热性和耐腐蚀性），但由于其室温脆性，如何实现更广泛的应用颇具挑战。与金属中的原子可以沿着滑移面滑动以变形不同，共价键合陶瓷由于原子间共价键的强定向性，其变形需要断键。这最终会导致加载时发生断裂。研究组提出了一种可变形共价键合氮化硅（ Si_3N_4 ）陶瓷的设计方法，其特点是具有共格界面的双相结构。在共格界面上实现了连续键切换，这有利于应力诱导相变，并最终产生塑性变形能力。

文中插图:



[1]Self-assembly of emulsion droplets through programmable folding
通过可编程折叠实现乳液液滴自组装

出版信息: Nature, 20 October 2022, VOL 610, ISSUE 7932

作者: Angus McMullen, Maitane Muñoz Basagoiti, Zorana Zeravcic & Jasna Brujic

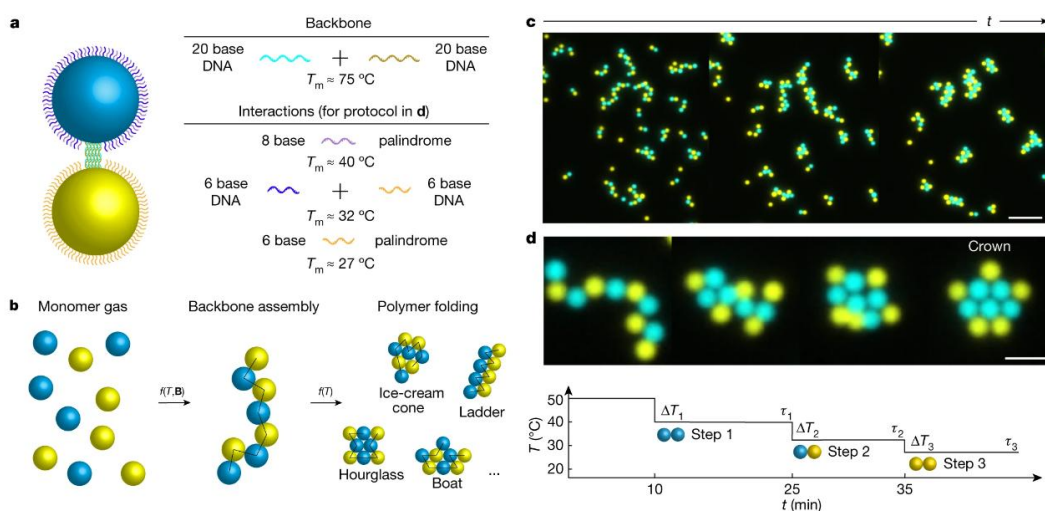
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全文链接: <https://www.nature.com/articles/s41586-022-05198-8>

Abstract: In the realm of particle self-assembly, it is possible to reliably construct nearly arbitrary structures if all the pieces are distinct^{1,2,3}, but systems with fewer flavours of building blocks have so far been limited to the assembly of exotic crystals^{4,5,6}. Here we introduce a minimal model system of colloidal droplet chains⁷, with programmable DNA interactions that guide their downhill folding into specific geometries. Droplets are observed in real space and time, unravelling the rules of folding. Combining experiments, simulations and theory, we show that controlling the order in which interactions are switched on directs folding into unique structures, which we call colloidal foldamers⁸. The simplest alternating sequences (ABAB...) of up to 13 droplets yield 11 foldamers in two dimensions and one in three dimensions. Optimizing the droplet sequence and adding an extra flavour uniquely encodes more than half of the 619 possible two-dimensional geometries. Foldamers consisting of at least 13 droplets exhibit open structures with holes, offering porous design. Numerical simulations show that foldamers can further interact to make complex supracolloidal architectures, such as dimers, ribbons and mosaics. Our results are independent of the dynamics and therefore apply to polymeric materials with hierarchical interactions on all length scales, from organic molecules all the way to Rubik's Snakes. This toolbox enables the encoding of large-scale design into sequences of short polymers, placing folding at the forefront of materials self-assembly.

摘要翻译: 在粒子自组装领域, 如果所有单元都不同, 则有望构建出几乎任意结构, 但迄今为止, 含有较少种类构建块的系统仅限于奇异晶体的组装。研究组介绍了一种胶体液滴链的最小模型系统, 具有可编程的 DNA 相互作用, 引导它们向下折叠成特定的几何形状。液滴在真实时空中观测, 揭示了折叠规则。结合实验、模拟和理论, 研究组表明, 控制相互作用的开启顺序可直接将胶体液滴折叠成独特的结构, 并将其称之为胶体折叠体。最多 13 个液滴的最简单交替序列 (ABAB...) 产生了 11 个二维折叠体和 1 个三维折叠体。通过优化液滴序列和添加额外种类, 可对 619 个可能的二维几何图形中的多半进行独特编程。由至少 13 个液滴组成的折叠体显示有孔的开放结构, 可提供多孔设计。数值模拟表明, 这些折叠体可进一步相互作用, 形成复杂的超胶体结构, 如二聚体、带状体和镶嵌体。该研究结果与动力学无关, 因此适用于所有长度尺度上具有层级相互作用的聚合物材料, 从有机分子一直到“魔尺”。该工具箱使大规模设计编码短聚合物序列成为可能, 将折叠设计置于材料自组装的前沿。

文中插图:



[2]

Low-hysteresis shape-memory ceramics designed by multimode modelling

多模态建模设计低滞回形状记忆陶瓷

出版信息: Nature, 20 October 2022, VOL 610, ISSUE 7932

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全文链接: <https://www.nature.com/articles/s41586-022-05210-1>

Abstract: Zirconia ceramics exhibit a martensitic phase transformation that enables large strains of order 10%, making them prospects for shape-memory and superelastic applications at high temperature. Similarly to other martensitic materials, this transformation strain can be engineered by carefully alloying to produce a more commensurate transformation with reduced hysteresis (difference in transformation temperature on heating and cooling). However, such ‘lattice engineering’ in zirconia is complicated by additional physical constraints: there is a secondary need to manage a large transformation volume change, and to achieve transformation temperatures high enough to avoid kinetic barriers. Here we present a method of augmenting the lattice engineering approach to martensite design to address these additional constraints, incorporating modern computational thermodynamics and data science tools to span complex multicomponent spaces for which no data yet exist. The result is a new zirconia composition with record low hysteresis of 15 K, which is about ten times less transformation hysteresis compared to typical values (and approximately five times less than the best values reported so far). This finding demonstrates that zirconia ceramics can exhibit hysteresis values of the order of those of widely deployed shape-memory alloys, paving the way for their use as viable high-temperature shape-memory materials.

摘要翻译: 氧化锆陶瓷表现出马氏体相变, 能产生高达 10% 的大应变, 使其在高温下具有形状记忆和超弹性的应用前景。与其他马氏体材料类似, 这种相变应变可通过精确合金化来设计, 以产生减少滞回 (加热和冷却时的相变温度差异) 的更相称相变。然而, 氧化锆中的这种“晶格工程”由于附加的物理约束而变得复杂: 其次需要管理较大的相变体积变化, 并实现足够高的相变温度以避免动力学障碍。研究组提出了一种将晶格工程方法扩展到马氏体设计的方法, 以解决这些额外的约束, 结合现代计算热力学和数据科学工具, 跨越数据空白的复杂多组分空间。结果得到一种新的氧化锆组分, 具有 15K 的低滞回记录, 相变滞回比典型值低约 10 倍 (比目前报道的最佳值低约 5 倍)。这一发现表明, 氧化锆陶瓷表现出可与广泛应用的形状记忆合金相媲美的滞回值, 有望应用于可行的高温形状记忆材料。

文中插图:

