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2025/44

东图·学术快报

材料科学 Nature & Science 发文（11 月）

（本期编辑：张亚浠　审校：刘丽娟）

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前言

/Foreword

前沿经典　学科热点

学术动态　工具助手

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 2025 年 11 月 Nature、Science 期刊上材料科学领域的最新论文。

材料科学 Science 论文

[1] Strengthening Ni alloys with nanoscale interfaces of negative excess energy

利用负过剩能的纳米尺度界面强化镍合金

出版信息：Science, 6 Nov 2025, VOL 390, ISSUE 6773

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全文链接: https://www.science.org/doi/10.1126/science.aea4299

国内报道： https://lam.ln.cn/lnsclsys/zyjz/2025110511580684719/index.shtml

Abstract: The strength of nanograined and nanotwinned metals is limited by the inherent instability of grain or twin boundaries below a length scale of typically about 10 nanometers. From experimental and density functional theory calculations, we found that the coherent interfaces between face-centered-cubic and hexagonal-close-packing lattices with a negative excess energy were more stable than twin boundaries in supersaturated Ni(Mo) solution. The negative excess-energy interface can be produced at extremely high density in Ni(Mo) solution with average spacing as small as about 1 nanometer, which inhibits plastic deformation and elevates the strength close to the theoretical value of the alloys. The measured Young's modulus of the Ni(Mo) alloys increases obviously with the interface density, reaching 254.5 gigapascals, well above that of the same compositional metallic glass and intermetallic compound (Ni_3Mo).

摘要翻译：纳米晶与纳米孪晶金属的强度受限于其晶界或孪晶界在特征尺度（通常约 10 纳米）以下的内在不稳定性。通过实验与密度泛函理论计算，研究者发现在过饱和 Ni(Mo)固溶体中，具有负过剩能的面心立方—六方最密堆积相干界面比孪晶界更具稳定性。这种负过剩能界面可在 Ni(Mo)固溶体中实现极高密度分布（平均间距约 1 纳米），从而有效抑制塑性变形，使材料强度逼近理论极限。实测结果表明，Ni(Mo)合金的杨氏模量随界面密度显著提升，最高达 254.5 吉帕，明显高于同成分金属玻璃与金属间化合物（Ni_3Mo）的模量值。

文中插图：

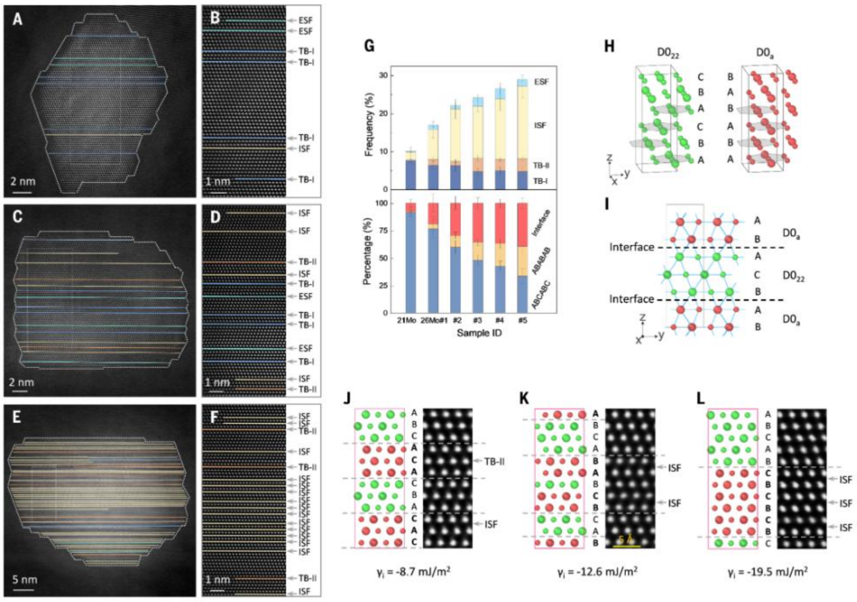

Fig. 2. Planar faults and the ABCABC/ABAB interfaces in Ni(Mo) samples.

[2] Atomic layer bonding contacts in two-dimensional semiconductors

二维半导体中的原子层键合接触

出版信息：Science, 20 NOV 2025, VOL 390, ISSUE 6775

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全文链接：https://www.science.org/doi/10.1126/science.adz2405

国内报道：

https://skl.ustb.edu.cn/xwzx/sysxw/0bbb539110404234b94a46daf6823705.htm

Abstract： Van der Waals contact between two-dimensional semiconductors and metals has always been inferior to covalent bond contacts used in semiconductor industry because of weak band coupling and low bond strength. Here, we report an atomic layer bonding (ALB) contact with strong band coupling and high interfacial cohesion by establishing a metallic coherent bonding interface between the transition-metal atomic layer of transition-metal dichalcogenides and metals. This contact exhibits ultralow contact resistance and superb thermomechanical stability, comparable to those of covalent bond contacts and surpassing all reported contact configurations. ALB contact formed in monolayer molybdenum disulfide and gold demonstrates a contact resistance of 70 ohm-micrometers and thermomechanical stability up to 400°C and delivers a maximum on-current of 1.1 milliamperes per micrometer after high-temperature annealing, all of which meet industrial integration.

摘要翻译：二维半导体与金属之间的范德华接触由于带耦合弱、键强度低，始终逊于半导体工业中使用的共价键接触。研究组通过在过渡金属二硫化物的过渡金属原子层与金属间构建金属相干键合界面，报道了具有强带耦合和高界面内聚力的原子层键合（ALB）接触。这种接触构型表现出超低的接触电阻和杰出的热机械稳定性，可与共价键接触相媲美，并超越了所有已报道的接触构型。在单层二硫化钼和金体系中形成的ALB接触显示出70欧姆-微米的接触电阻和高达400°C的热机械稳定性，高温退火后的最大导通电流为1.1毫安/微米，所有这些都符合工业集成的需求。

文中插图：

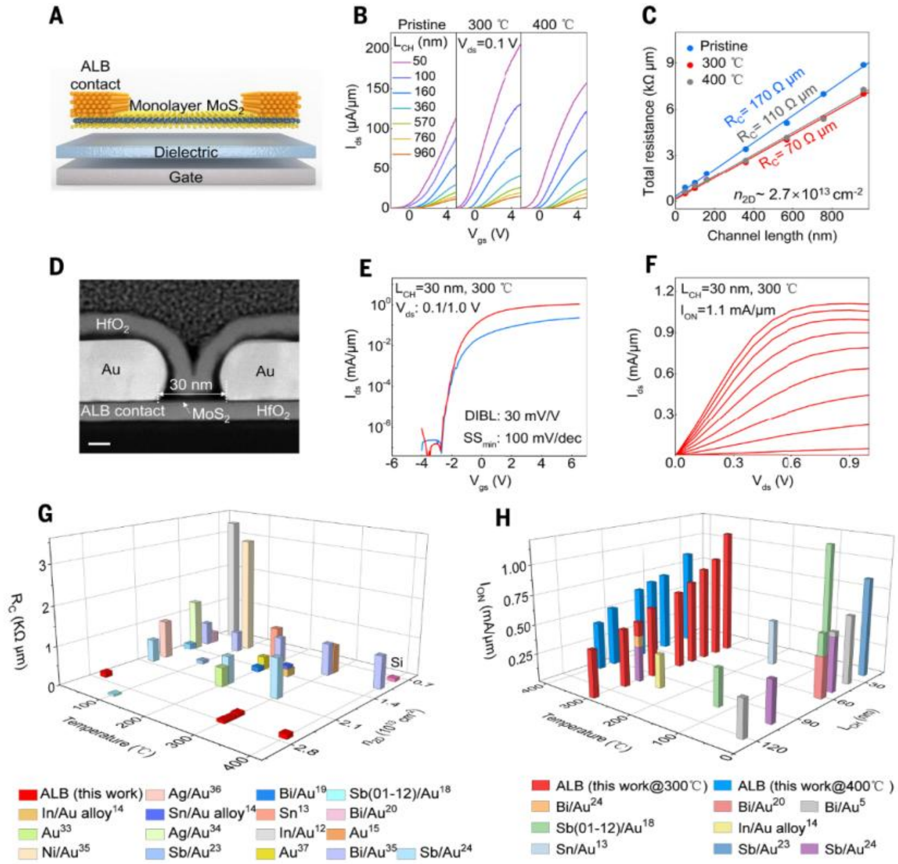

Fig. 3. Electronic properties of ALB contacts.

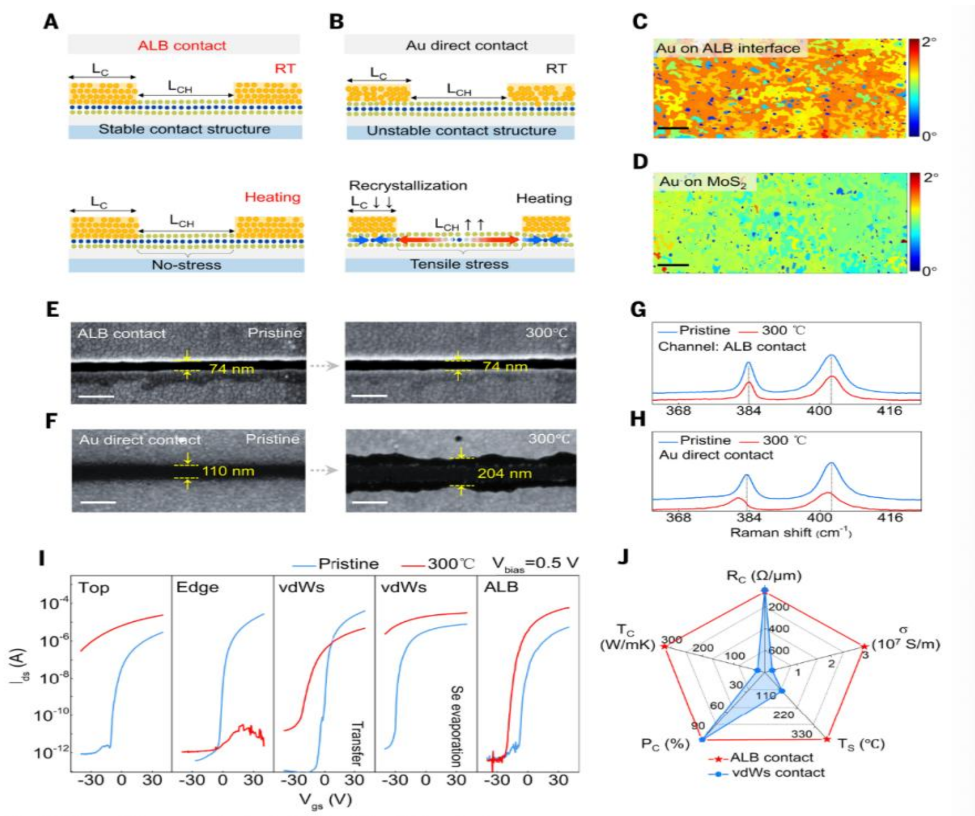

Fig. 4. Enhanced thermomechanical stability of the ALB contact.

[3] Increasing the dimensionality of transistors with hydrogels

用水凝胶拓展晶体管的维度

出版信息： Science, 20 NOV 2025, VOL 390, ISSUE 6775

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全文链接： https://www.science.org/doi/10.1126/science.adx4514

国内报道： https://www.eee.hku.hk/20251124-2/

Abstract： Transistors, fundamental to modern electronics, are traditionally rigid, planar, and two-dimensional (2D), limiting their integration with the soft, irregular, and three-dimensional (3D) nature of biological systems. Here, we report 3D semiconductors, integrating organic electronics, soft matter, and electrochemistry. These 3D semiconductors, in the form of hydrogels, realize millimeter-scale modulation thickness while achieving tissue-like softness and biocompatibility. This breakthrough in modulation thickness is enabled by a templated double-network hydrogel system, where a secondary porous hydrogel guides the 3D assembly of a primary redox-active conducting hydrogel. We demonstrate that these 3D semiconductors enable the exclusive fabrication of 3D spatially interpenetrated transistors that mimic real neuronal connections. This work bridges the gap between 2D electronics and 3D living systems, paving the way for advanced bioelectronics systems such as biohybrid sensing and neuromorphic computing.

摘要翻译： 晶体管是现代电子学的基础，传统上为刚性、平面和二维（2D）结构，这限制了其与生物系统的柔软、不规则的和三维（3D）性质的集成。研究组报道了一种 3D 半导体，集成了有机电子学、软物质和电化学技术。这些 3D 半导体以水凝胶的形式实现了毫米级的调控厚度，同时实现了组织般的柔软性和生物相容性。调控厚度的这一突破通过模板化的双网络水凝胶系统实现，其中次级多孔水凝胶引导初级氧化还原活性导电水凝胶的 3D 组装。研究组证明了这些 3D 半导体能够独家制造模拟真实神经元连接的 3D 空间互穿晶体管。这项工作弥合了 2D 电子学和 3D 生命系统之间的差距，为生物混合传感和神经形态计算等高级生物电子系统开辟了途径。

文中插图：

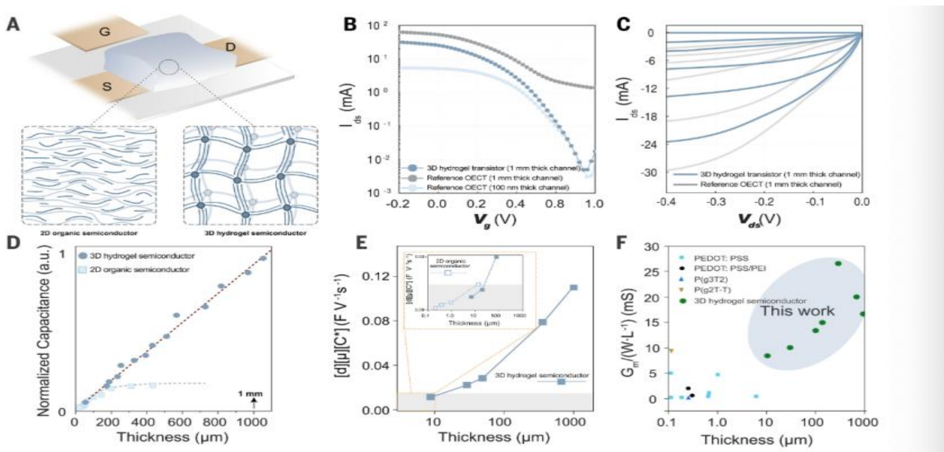

Fig. 4. Electrical performance of 3D hydrogel transistors.

[4] A cross-linked molecular contact for stable operation of perovskite/silicon tandem solar cells

钙钛矿/硅叠层太阳能电池稳定运行的交联分子接触

出版信息：Science, 20 NOV 2025, VOL 390, ISSUE 6775

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全文链接：https://www.science.org/doi/10.1126/science.ady6874

国内报道：

https://news.uestc.edu.cn/?n=UestcNews.Front.DocumentV2.ArticlePage&Id=98004

Abstract： Monolithic perovskite/silicon tandem solar cells surpass the power-conversion efficiency limits of single-junction solar cells but face challenges in operational stability. We identified fill factor diminution as a key performance-loss mode in the state-of-the-art tandem architecture. We reveal that widely used hole-selective molecular contacts, which enhance tandem cell performance, undergo thermal degradation that undermines charge transport. At elevated temperatures, the resistance of conventional monomeric contacts increases by about sixfold because of thermal-induced disorder. To stabilize interfacial structures, we introduce in situ synthesized cross-linked molecular contacts based on Schiff base linkages. One-square-centimeter perovskite/silicon tandem solar cells achieved power-conversion efficiencies exceeding 34% (33.61% certified), and three independent devices retained 96.2 ± 1.7% of their initial performance after about 1200-hour maximum power point operation under AM1.5G illumination at 65°C.

摘要翻译：单片钙钛矿/硅叠层太阳能电池超越了单结太阳能电池的功率转换效率极限，但在运行稳定性方面仍存在挑战。研究组确定在最先进叠层电池结构中，填充因子减少是一种关键的性能损失模式。他们发现，广泛使用的空穴选择性分子接触可提高串联电池的性能，但会经历热降解，从而破坏电荷传输。在高温下，由于热致失序，传统单体接触的电阻将增加约六倍。为了稳定界面结构，研究组引入了基于席夫碱键的原位合成交联分子接触。使用该技术的一平方厘米钙钛矿/硅叠层太阳能电池的功率转换效率超过 34%（经认证为 33.61%），三组独立器件在 65℃、AM1.5G 光照、最大功率点运行约 1200 小时后，仍可保持初始性能的 96.2±1.7%。

文中插图：

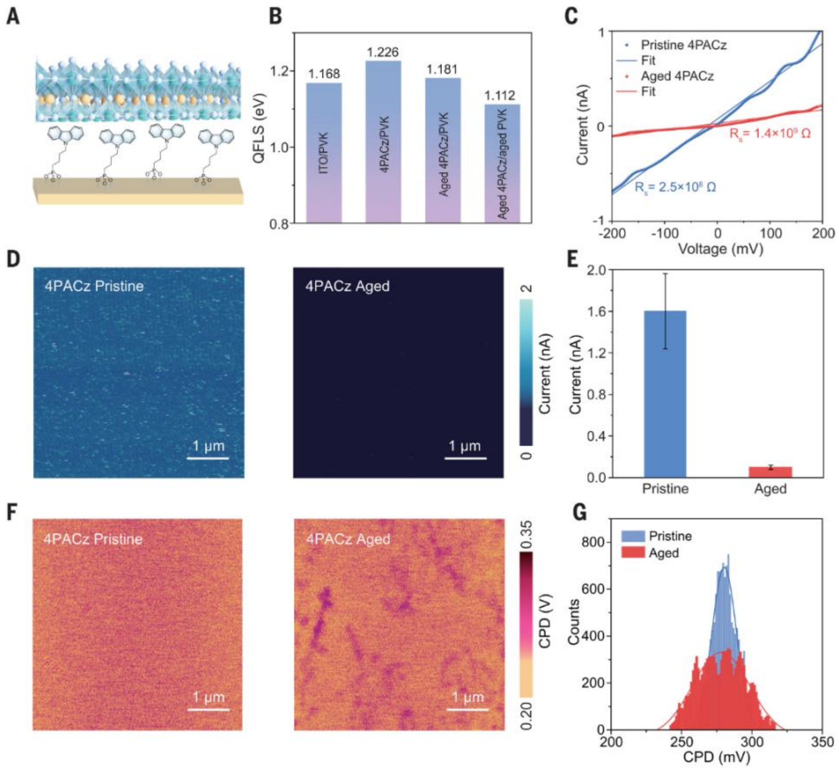

Fig. 2. Thermal aging degrades charge transport in monomeric 4PACz SAMs.

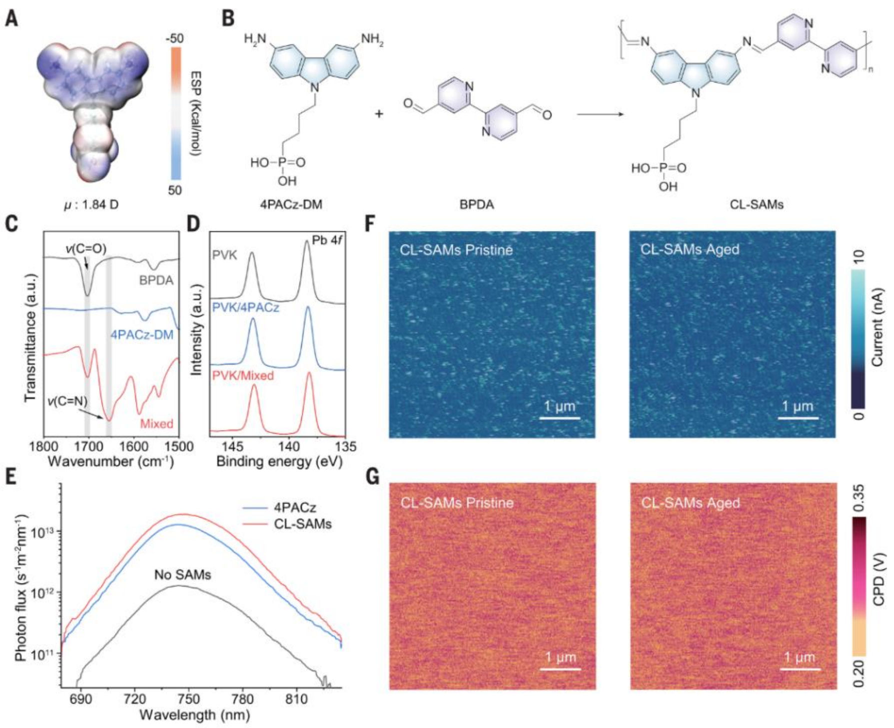

Fig. 3. Design and thermal robustness of polymeric CL-SAMs.

材料科学 Nature 论文

[1] Atomically resolved edges and defects in lead halide perovskites

卤化铅钙钛矿的原子分辨边缘和缺陷分析

出版信息：Nature, 13 November 2025, Volume 647, Issue 8089

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全文链接：https://www.nature.com/articles/s41586-025-09693-6

国内报道：https://www2.scut.edu.cn/emc/2025/0530/c37838a592839/page.htm

Abstract： Although edges and defects constitute only a small fraction of crystalline materials, they exert an outsized impact on a material′s properties. Organic–inorganic halide perovskites are promising next-generation semiconductor materials with superior cost effectiveness and interesting optoelectronic properties. However, clear images of their edges have remained challenging to obtain owing to their extreme sensitivity. Using truly high-speed ultralow-dose four-dimensional scanning transmission electron microscopy with dose fractionation, we perform ptychography at, to our knowledge, the lowest-dose atomic resolution to date, revealing not only the detailed atomic structure of the edges of a halide perovskite but also their structural dynamics. A majority methylammonium (MA) and iodine (I) edge termination is observed in methylammonium lead iodide ($MAPbI_3$), and the damage rate of its edges and internal defects is found to depend on the concentration and type of vacancies present, with a preponderance of I vacancies in particular correlating with higher rates of damage.

摘要翻译：虽然边缘和缺陷只构成晶体材料的一小部分，但它们对材料的性能产生巨大的影响。有机—无机卤化物钙钛矿是颇具前景的下一代半导体材料，具有优越的成本效益和有趣的光电性能，但因其极端敏感性，获得边缘的清晰图像仍颇具挑战。研究组采用真正高速超低剂量四维扫描透射电子显微镜技术，结合剂量分割法，实现了迄今所知最低剂量的原子分辨率叠层成像，不仅揭示了卤化物钙钛矿边缘的精细原子结构，还揭示了边缘结构动力学。研究组在甲基铵铅碘（$MAPbI_3$）中观察到大多数甲基铵（MA）和碘（I）在边缘的末端结构，并发现其边缘和内部缺陷的损坏率取决于存在空位的浓度和类型，特别是碘空位的优势与更高的损坏率相关。

文中插图：

Fig. 1: Ultralow-dose 4D-STEM imaging of $MAPbI_3$.

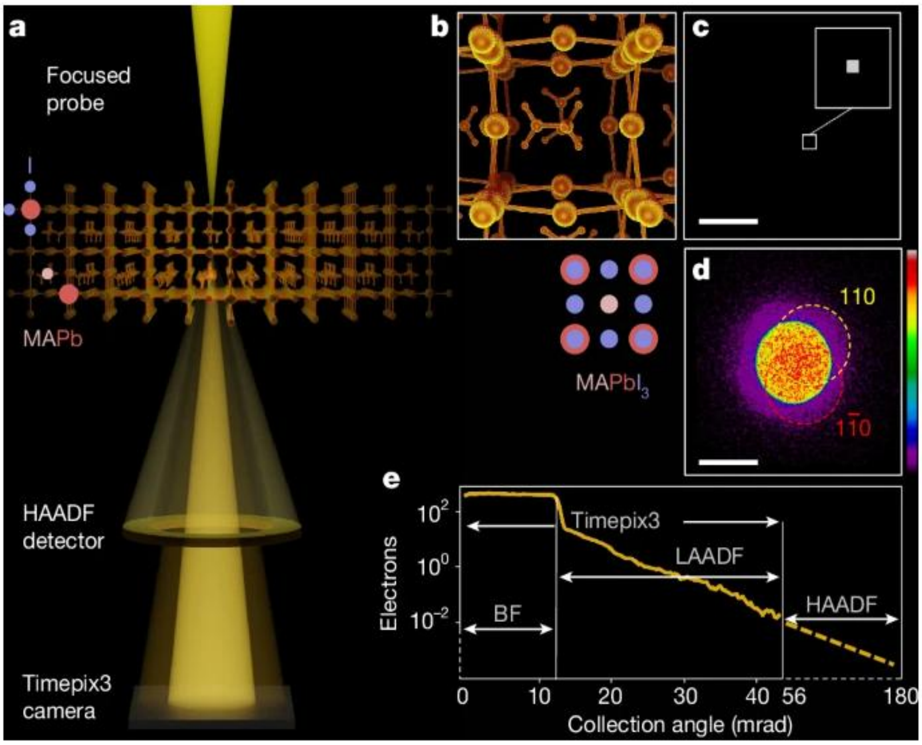
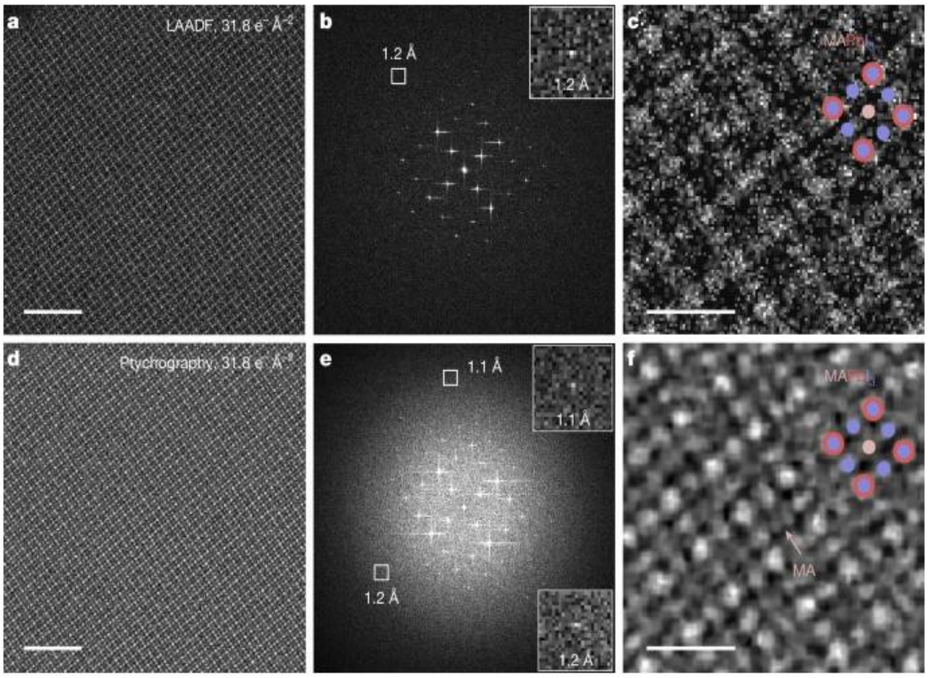


Fig. 2: Atomic-resolution imaging of $MAPbI_3$.



[2] Silicon solar cells with hybrid back contacts

杂化背接触结构硅太阳能电池

出版信息：Nature, 13 November 2025, Volume 647, Issue 8089

作者：Genshun Wang, Mingzhe Yu, Hua Wu, Yunpeng Li, Lei Xie, Junzhe Wei, et al.

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全文链接：https://www.nature.com/articles/s41586-025-09681-w

国内报道：https://materials.sysu.edu.cn/article/766

Abstract: Silicon solar cells are essential for sustainable energy but remain limited by efficiency losses, particularly in the fill factor. Here we develop a hybrid interdigitated back-contact solar cell that combines advanced all-surface passivation with laser-treated tunnelling contacts. This approach achieves a power conversion efficiency of 27.81%, approaching 95% of the theoretical limit. By integrating high- and low-temperature processes, we suppress recombination and enhance contact performance, achieving a fill factor of 87.55%—nearly 98% of the theoretical limit. A model links the ideality factor to carrier loss mechanisms, elucidating carrier recombination in both the bulk and the surface and clarifies key fill factor losses owing to recombination. These innovations provide both experimental and theoretical advances towards scalable, high-efficiency silicon photovoltaics.

摘要翻译：硅太阳能电池对可持续能源至关重要，但仍受到效率损失的限制，特别是在填充因子方面。研究组开发了一种杂化背接触结构太阳能电池，其结合了先进的全表面钝化和激光加工隧穿接触。该策略实现了 27.81%的功率转换效率，接近理论极限的 95%。通过整合高低温工艺，研究组抑制了复合，提高了接触性能，实现了 87.55%（接近理论极限 98%）的填充因子。该模型将理想因子与载流子损失机制联系起来，阐明了在体相和表面的载流子复合，以及由复合引起的关键填充因子损失。这些创新为可扩展、高效的硅光伏电池提供了实验和理论上的进展。

文中插图：

Fig. 2: Laser treatment effects on the i-a-Si/p-a-Si stack of the HIBC cell.