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本期推荐报道 2022 年 4 月 Nature、Science 期刊上材料科学领域的部分最新论文。





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# 材料科学

# 4月 Science 论文

# [1]Ferroelectric crystals with giant electro-optic property enabling ultracompact Q-switches 具有超高渗透选择性的工业气体聚合物分离膜

出版信息: Science, 22 APR 2022, VOL 376, ISSUE 6591

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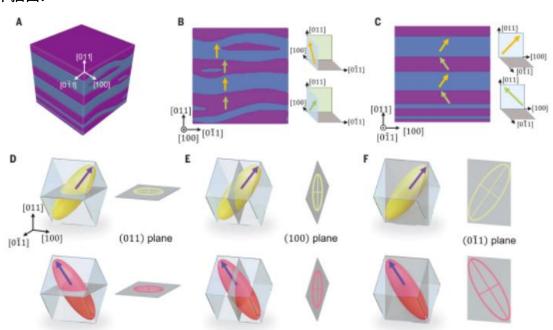
全文链接: https://www.science.org/doi/10.1126/science.abn7711

**Abstract:** Relaxor-lead titanate (PbTiO3) crystals, which exhibit extremely high piezoelectricity, are believed to possess high electro-optic (EO) coefficients. However, the optical transparency of relaxor-PbTiO3 crystals is severely reduced as a result of light scattering and reflection by domain walls, limiting electro-optic applications. Through synergistic design of a ferroelectric phase, crystal orientation, and poling technique, we successfully removed all light-scattering domain walls and achieved an extremely high transmittance of 99.6% in antireflection film – coated crystals, with an ultrahigh EO coefficient r33 of 900 picometers per volt (pm V-1), >30 times as high as that of conventionally used EO crystals. Using these crystals, we fabricated ultracompact EO Q-switches that require very low driving voltages, with superior performance to that of commercial Q-switches. Development of these materials is important for the portability and low driving voltage of EO devices.

**摘要翻译:** 弛豫钛酸铅(PbTiO3)晶体具有极高的压电性,被认为具有较高的电光(EO)系数。然而,由于畴壁的光散射和反射,弛豫 PbTiO3晶体的光学透明度严重降低,限制了其电光应用。

通过铁电相、晶体取向和极化技术的协同设计,研究组成功地消除了所有光散射畴壁,并在抗反射膜涂层晶体中实现了 99.6%的极高透射率,EO 系数 r33 高达 900 pm V-1,是常规 EO 晶体的 30 倍以上。

使用这些晶体,研究组制造了仅需极低驱动电压的超紧凑型 EOQ 开关,其性能优于商用 Q 开关。这些材料的开发对于光电器件的便携性和低驱动电压具有重要意义。



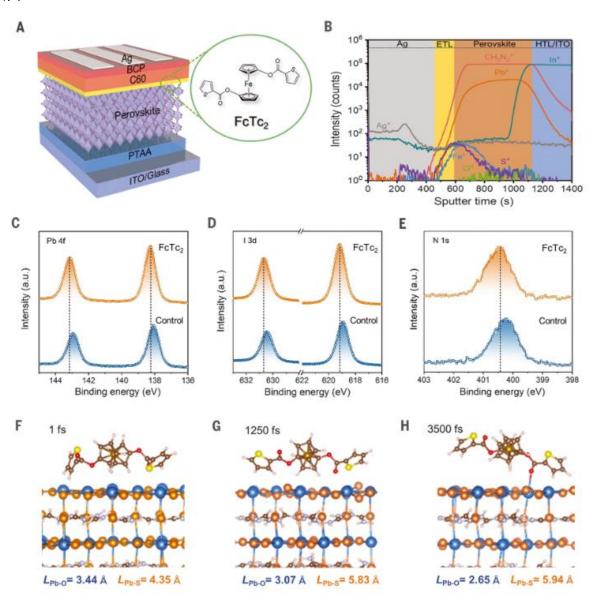
# [2]Organometallic-functionalized interfaces for highly efficient inverted perovskite solar cells 高效倒置钙钛矿太阳能电池的有机金属功能化界面

出版信息: Science, 22 APR 2022, VOL 376, ISSUE 6591

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**Abstract:** Further enhancing the performance and stability of inverted perovskite solar cells (PSCs) is crucial for their commercialization. We report that the functionalization of multication and halide perovskite interfaces with an organometallic compound, ferrocenyl-bis-thiophene-2-carboxylate (FcTc2), simultaneously enhanced the efficiency and stability of inverted PSCs. The resultant devices achieved a power conversion efficiency of 25.0% and maintained >98% of their initial efficiency after continuously operating at the maximum power point for 1500 hours under simulated AM1.5 illumination. Moreover, the FcTc2-functionalized devices passed the international standards for mature photovoltaics (IEC61215:2016) and have exhibited high stability under the damp heat test (85°C and 85% relative humidity).

**摘要翻译:** 进一步提高倒置钙钛矿太阳能电池(PSC)的性能和稳定性对其商业化至关重要。研究组报道了一种有机金属化合物(二茂铁-双噻吩-2-羧酸盐[FcTc2])对卤化物钙钛矿界面的多功能化,同时提高了倒置 PSC 的效率和稳定性。在模拟 AM 1.5 光照条件下,在最大功率点连续运行 1500 小时后,合成装置的功率转换效率达到 25.0%,并保持其初始效率的 98%以上。此外,FcTc2 功能化设备通过了成熟的光伏国际标准(IEC61215:2016),并在湿热试验(85℃和 85%相对湿度)中表现出高稳定性。



[3] Volumetric additive manufacturing of silica glass with microscale computed axial lithography

### 微尺度计算轴向光刻上的硅玻璃体积增材制造

出版信息: Science, 15 APR 2022, VOL 376, ISSUE 6590

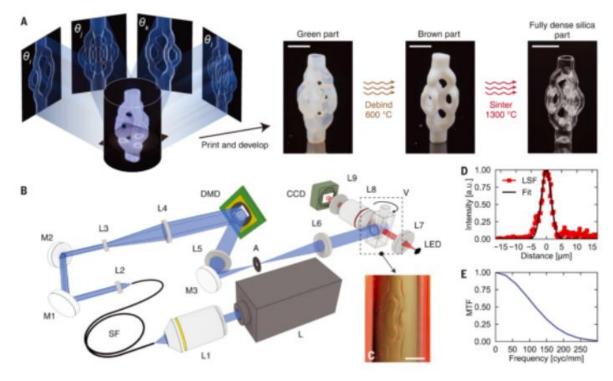
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全文链接: https://www.science.org/doi/10.1126/science.abm6459

**Abstract:** Glass is increasingly desired as a material for manufacturing complex microscopic geometries, from the micro-optics in compact consumer products to microfluidic systems for chemical synthesis and biological analyses. As the size, geometric, surface roughness, and mechanical strength requirements of glass evolve, conventional processing methods are challenged. We introduce microscale computed axial lithography (micro-CAL) of fused silica components, by tomographically illuminating a photopolymer-silica nanocomposite that is then sintered. We fabricated three-dimensional microfluidics with internal diameters of 150 micrometers, free-form micro-optical elements with a surface roughness of 6 nanometers, and complex high-strength trusses and lattice structures with minimum feature sizes of 50 micrometers. As a high-speed, layer-free digital light

**摘要翻译:** 从消费品的微光学到用于化学合成和生物分析的微流体系统,玻璃作为制造复杂的微观几何形状的材料越来越受欢迎。随着玻璃尺寸、几何形状、表面粗糙度和机械强度要求的发展,传统的加工方法受到了挑战。我们介绍了熔融二氧化硅元件的微尺度轴向计算光刻技术(micro-CAL),即对随后烧结的光致聚合物—二氧化硅纳米复合材料进行层析成像。我们制作了内径为150微米的三维微流体,表面粗糙度为6纳米的自由曲面微光学元件,以及最小特征尺寸为50微米的复杂高强度桁架和晶格结构。micro-CAL作为一种高速的数字化轻制造工艺,可以加工高固含量、高几何自由度的纳米复合材料,实现了新的器件结构和应用。



[4]Damp heat-stable perovskite solar cells with tailored-dimensionality 2D/3D heterojunctions

### 具有定制二维/三维异质结的湿热稳定钙钛矿太阳能电池

出版信息: Science, 1 APR 2022, VOL 376, ISSUE 6588

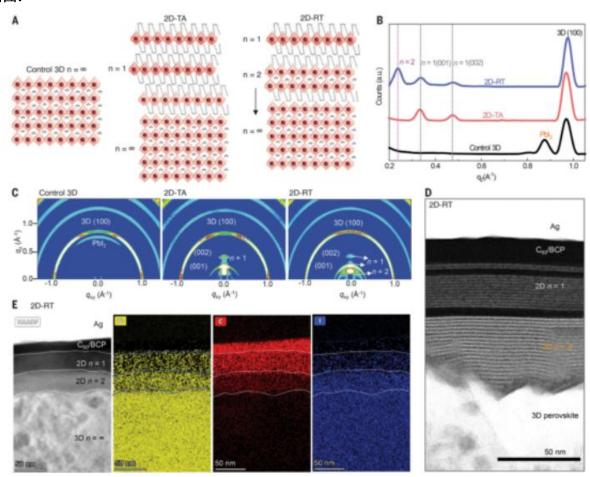
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全文链接: https://www.science.org/doi/10.1126/science.abm5784

**Abstract:** If perovskite solar cells (PSCs) with high power conversion efficiencies (PCEs) are to be commercialized, they must achieve long-term stability, which is usually assessed with accelerated degradation tests. One of the persistent obstacles for PSCs has been successfully passing the damp-heat test (85°C and 85% relative humidity), which is the standard for verifying the stability of commercial photovoltaic (PV) modules. We fabricated damp heat—stable PSCs by tailoring the dimensional fragments of two-dimensional perovskite layers formed at room temperature with oleylammonium iodide molecules; these layers passivate the perovskite surface at the electron-selective contact. The resulting inverted PSCs deliver a 24.3% PCE and retain >95% of their initial value after >1000 hours at damp-heat test conditions, thereby meeting one of the critical industrial stability standards for PV modules.

**摘要翻译:** 若要将具有高功率转换效率(PCE)的钙钛矿太阳能电池(PSC)商业化,它们必须实现长期稳定性,这通常由加速降解测试进行评估。PSC的持久障碍之一是成功通过湿热测试(85℃和85%相对湿度),这是验证商用光伏(PV)组件稳定性的标准。研究组用油胺碘分子定制室温下形成的二维钙钛矿层多维碎片,制备了湿热稳定的PSCs,在电子选择性接触时钝化钙钛矿表面。在湿热试验条件下超过1000小时后,产生的倒置PSCs的PCE为24.3%,并保留其初始值的95%以上,从而满足光伏组件稳定性的关键工业标准之一。



[5] An integrated materials approach to ultrapermeable and ultraselective CO2 polymer membranes

## 超渗透性和超选择性 CO2 聚合膜的集成材料方法

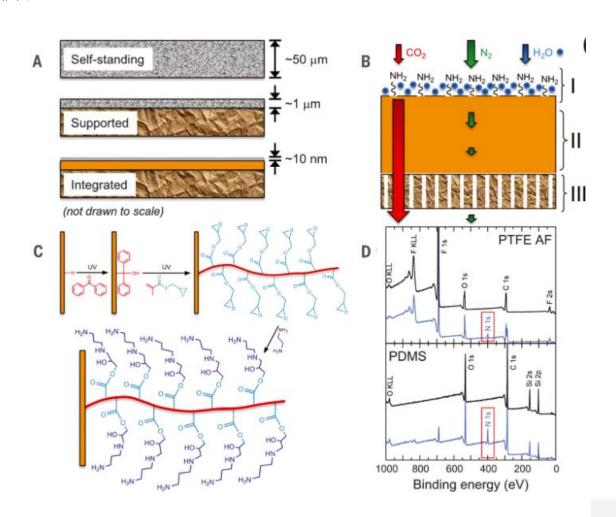
出版信息: Science, 1 APR 2022, VOL 376, ISSUE 6588

作者: MARIUS SANDRU, EUGENIA M. SANDRU, WADE F. INGRAM, JING DENG, PER M. STENSTAD, LIYUAN DENG.

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Abstract: Advances in membrane technologies that combine greatly improved carbon dioxide (CO2) separation efficacy with low costs, facile fabrication, feasible upscaling, and mechanical robustness are needed to help mitigate global climate change. We introduce a hybrid-integrated membrane strategy wherein a high-permeability thin film is chemically functionalized with a patchy CO2-philic grafted chain surface layer. A high-solubility mechanism enriches the concentration of CO2 in the surface layer hydrated by water vapor naturally present in target gas streams, followed by fast CO2 transport through a highly permeable (but low-selectivity) polymer substrate. Analytical methods confirm the existence of an amine surface layer. Integrated multilayer membranes prepared in this way are not diffusion limited and retain much of their high CO2 permeability, and their CO2 selectivity is concurrently increased in some cases by more than ~150-fold.

**摘要翻译:** 膜技术的进步将大大提高二氧化碳(CO2)分离效率与低成本、易于制造、可扩大规模和机械稳定性结合起来,以帮助缓解全球气候变化。研究组介绍了一种混合集成膜策略,其中高渗透性薄膜通过零散亲 CO2接枝链表面层实现化学功能化。高溶解度机制使目标气流中天然存在的水蒸气水化表层的 CO2浓度增加,随后 CO2通过高渗透性(但低选择性)聚合物基质快速传输。分析方法证实了胺表层的存在。以这种方式制备的集成多层膜不受扩散限制,并保留了大部分高 CO2渗透性,在某些情况下,其 CO2选择性同时提升了约 150 倍以上。



# 材料科学

# 4月 Nature 论文

### [1]Uniting tensile ductility with ultrahigh strength via composition undulation

### 通过成分起伏同时实现拉伸塑性与超高强度

出版信息: Nature, 13 April 2022, VOL 604, ISSUE 7905

作者: Heng Li, Hongxiang Zong, Suzhi Li, Shenbao Jin, Yan Chen, Matthew J. Cabral, et al.

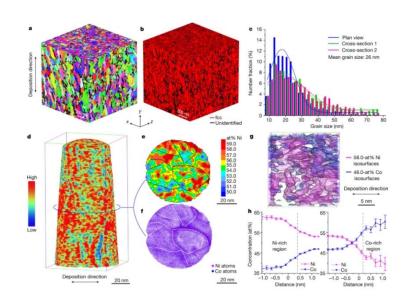
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国内相关报道: https://news.jlu.edu.cn/info/1306/55583.htm

全文链接: https://www.nature.com/articles/s41586-022-04459-w

Abstract: Metals with nanocrystalline grains have ultrahigh strengths approaching two gigapascals. However, such extreme grain-boundary strengthening results in the loss of almost all tensile ductility, even when the metal has a face-centred-cubic structure—the most ductile of all crystal structures. Here we demonstrate that nanocrystalline nickel—cobalt solid solutions, although still a face-centred-cubic single phase, show tensile strengths of about 2.3 gigapascals with a respectable ductility of about 16 per cent elongation to failure. This unusual combination of tensile strength and ductility is achieved by compositional undulation in a highly concentrated solid solution. The undulation renders the stacking fault energy and the lattice strains spatially varying over length scales in the range of one to ten nanometres, such that the motion of dislocations is thus significantly affected. The motion of dislocations becomes sluggish, promoting their interaction, interlocking and accumulation, despite the severely limited space inside the nanocrystalline grains. As a result, the flow stress is increased, and the dislocation storage is promoted at the same time, which increases the strain hardening and hence the ductility. Meanwhile, the segment detrapping along the dislocation line entails a small activation volume and hence an increased strain-rate sensitivity, which also stabilizes the tensile flow. As such, an undulating landscape resisting dislocation propagation provides a strengthening mechanism that preserves tensile ductility at high flow stresses.

**摘要翻译:** 具有纳米晶粒的金属有接近 2 GPa 的超高强度。然而,这种极端的晶界强化导致几乎所有拉伸塑性的丧失,即使当金属具有面心立方结构(所有晶体结构中塑性最强的结构)时亦如此。研究组证明了纳米晶镍-钴固溶体虽仍是面心立方单相,但其拉伸强度约为 2.3 GPa,塑性断裂伸长率约为 16 %。这种不寻常的拉伸强度和塑性的结合是通过高浓度固溶体中的成分起伏实现的。这种起伏使得层错能和晶格应变在 1-10 纳米的尺度范围内发生空间变化,从而显著影响了位错运动。尽管纳米晶粒内部空间非常有限,但位错运动变得缓慢,促进了它们的交互作用、联锁和增殖。因此,流动应力增加,同时位错储存增加,从而提升了应变硬化能力,提高了塑性。同时,沿位错线的分段脱捕需要较小的激活体积,因此应变速率敏感性增加,这也稳定了拉伸流动。因此,抗位错传播的起伏结构提供了一种强化机制,可在高流动应力下保持拉伸塑性。



### [2]Perovskite - organic tandem solar cells with indium oxide interconnect

#### 钙钛矿-氧化铟互连有机串联太阳能电池

出版信息: Nature, 14 April 2022, VOL 604, ISSUE 7905

作者: Zhitao Zhang, Weichen Wang, Yuanwen Jiang, Yi-Xuan Wang, Yilei Wu, Jian-Cheng Lai, et al.

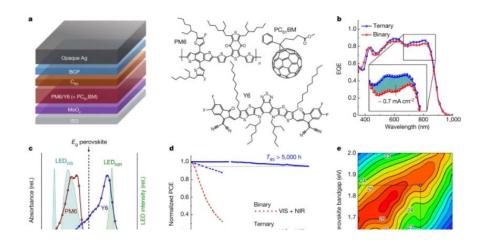
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### 全文链接: https://www.nature.com/articles/s41586-022-04400-1

**Abstract:** Multijunction solar cells can overcome the fundamental efficiency limits of single-junction devices. The bandgap tunability of metal halide perovskite solar cells renders them attractive for multijunction architectures. Combinations with silicon and copper indium gallium selenide (CIGS), as well as all-perovskite tandem cells, have been reported. Meanwhile, narrow-gap non-fullerene acceptors have unlocked skyrocketing efficiencies for organic solar cells. Organic and perovskite semiconductors are an attractive combination, sharing similar processing technologies. Currently, perovskite - organic tandems show subpar efficiencies and are limited by the low open-circuit voltage (Voc) of wide-gap perovskite cells and losses introduced by the interconnect between the subcells. Here we demonstrate perovskite - organic tandem cells with an efficiency of 24.0 per cent (certified 23.1 per cent) and a high Voc of 2.15 volts. Optimized charge extraction layers afford perovskite subcells with an outstanding combination of high Voc and fill factor. The organic subcells provide a high external quantum efficiency in the near-infrared and, in contrast to paradigmatic concerns about limited photostability of non-fullerene cells, show an outstanding operational stability if excitons are predominantly generated on the non-fullerene acceptor, which is the case in our tandems. The subcells are connected by an ultrathin (approximately 1.5 nanometres) metal-like indium oxide layer with unprecedented low optical/electrical losses. This work sets a milestone for perovskite - organic tandems, which outperform the best p - i - n perovskite single junctions and are on a par with perovskite - CIGS and all-perovskite multijunctions.

摘要翻译:多结太阳能电池可以克服单结器件的基本效率限制。金属卤化物钙钛矿型太阳能电池的带隙可调性使其在多结结构中具有吸引力。硅和铜铟硒化镓(CIGS)以及全钙钛矿串联电池的组合已有报道。与此同时,窄间隙非富勒烯受体为有机太阳能电池带来了快速提升的效率。有机和钙钛矿半导体是一种很有吸引力的组合,具有相似的加工技术。目前,钙钛矿-有机串联电池的效率低于标准,并且受到宽间隙钙钛矿电池的低开路电压(Voc)和子电池之间互连引入损耗的限制。研究组展示了钙钛矿-有机串联电池的效率为 24.0%(认证为 23.1%),Voc 高达 2.15 伏特。优化的电荷提取层使钙钛矿子电池具有高 Voc 和填充因子的出色组合。该串联电池的有机子电池在近红外下提供了高外部量子效率,与对非富勒烯电池有限光稳定性的典型担忧相反,如果激子主要在非富勒烯受体上产生,则表现出出色的操作稳定性。子电池由一层超薄(约 1.5 纳米)类金属氧化铟层连接,具有前所未有的低光/电损耗。这项工作为钙钛矿-有机串联电池竖了一座里程碑,它优于最好的 p-i-n 钙钛矿单结,并与钙钛矿-CIGS 和所有钙钛矿多结相媲美。



### [3] Charge-density-wave-driven electronic nematicity in a kagome superconductor

### 笼目超导体中发现新型电子向列相

出版信息: Nature, 7 April 2022, Volume 604 Issue 7904

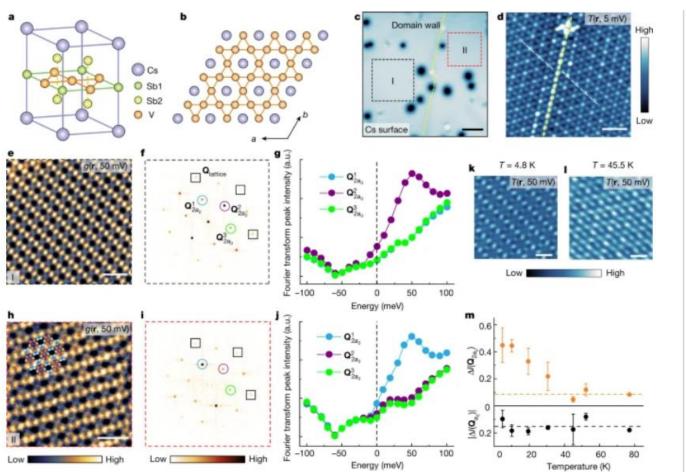
作者: Linpeng Nie, Kuanglv Sun, Wanru Ma, Dianwu Song, Lixuan Zheng et al.

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全文链接: https://www.nature.com/articles/s41586-022-04493-8

**Abstract:** Here we report evidence for the existence of electronic nematicity in CsV3Sb5, using a combination of elastoresistance measurements, nuclear magnetic resonance (NMR) and scanning tunnelling microscopy/spectroscopy (STM/S). The temperature-dependent elastoresistance coefficient (m11 minus m12) and NMR spectra demonstrate that, besides a C2 structural distortion of the 2a0 × 2a0 supercell owing to out-of-plane modulation, considerable nematic fluctuations emerge immediately below the CDW transition (approximately 94 kelvin) and finally a nematic transition occurs below about 35 kelvin. The STM experiment directly visualizes the C2-structure-pinned long-range nematic order below the nematic transition temperature, suggesting a novel nematicity described by a three-state Potts model.

**摘要翻译:** 我们通过弹性电阻、核磁共振(NMR)和扫描隧道显微镜/光谱(STM/S)三种技术的结合,发现了笼目超导体 CsV3Sb5 中存在电子向列相的证据。随温度变化的弹性电阻系数(m11 - m12 和核磁共振谱表明,2a0 × 2a0 超级单体由于面外调制而产生 C2 结构畸变,在电荷密度波跃迁(约 94 开尔文)下方会出现相当大的向列波动,最后在 35 开尔文以下会出现向列跃迁。STM 实验实现了 C2 -结构固定的长程向列向转变温度以下的向列相,提出了一种由 three state Potts 模型描述的新型向列相。



# [4]Ultrathin ferroic HfO2 - ZrO2 superlattice gate stack for advanced transistors 可用于先进晶体管的超薄铁质 HfO2 - ZrO2 超晶格栅叠层

出版信息: Nature, 7 April 2022, Volume 604 Issue 7904

作者: Suraj S. Cheema, Nirmaan Shanker, Li-Chen Wang, Cheng-Hsiang Hsu et al.

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全文链接: <a href="https://www.nature.com/articles/s41586-022-04425-6">https://www.nature.com/articles/s41586-022-04425-6</a>

**Abstract:** Here we report HfO2 - ZrO2 superlattice heterostructures as a gate stack, stabilized with mixed ferroelectric - antiferroelectric order, directly integrated onto Si transistors, and scaled down to approximately 20 ångströms, the same gate oxide thickness required for high-performance transistors. The overall equivalent oxide thickness in metal - oxide - semiconductor capacitors is equivalent to an effective SiO2 thickness of approximately 6.5 a ngstr o ms. Such a low effective oxide thickness and the resulting large capacitance cannot be achieved in conventional HfO2-based high-dielectric-constant gate stacks without scavenging the interfacial SiO2, which has adverse effects on the electron transport and gate leakage current. Accordingly, our gate stacks, which do not require such scavenging, provide substantially lower leakage current and no mobility degradation.

**摘要翻译:** 在此,我们报告 HfO2 - ZrO2 超晶格异质结构作为栅叠层,通过混合铁电性-反铁电性顺序稳定,直接集成到 Si 晶体管上,并缩小到大约 20 埃,与高性能晶体管所需的栅极氧化厚度相同。金属氧化物半导体电容器的整体等效氧化层厚度相当于 6.5 埃的二氧化硅有效厚度。

在传统的 HfO2 基高介电常数栅极堆中,如果不清除表面的二氧化硅,就无法获得如此低的有效氧化层厚度和由此产生的大电容,这对电子传输和栅极漏电流有不利影响。因此,我们的栅极堆栈不需要这样清除即可提供更低的泄漏电流和无迁移率退化。

