科学通报 2026 年 第 71 卷 第 13 期: 2794 ~ 2796
悦读科学
《中国科学》杂志社
SCIENCE CHINA PRESS

离子液体调控结晶助力硒硫化锑太阳能电池效率创新高

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Ionic liquids-modulated crystallization boosts antimony sulfoselenide solar cell efficiency

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doi: 10.1360/CSB-2026-0194

在“双碳”目标引领的绿色能源浪潮中, 电力作为国家发展的“血液”, 其清洁化生产是破解能源危机、守护生态环境的关键. 自从光伏效应被发现以来, 人类就从未停止过探索高效发电技术的脚步.

在“高效低成本”的新兴光伏赛道上, 硒硫化锑($Sb_2(S,Se)_3$)太阳能电池凭借低毒、易制备、原料丰富、结构稳定、高可见光吸收系数($>10^5$ cm^{-1})和可调光学带隙(1.1~1.7 eV)的优势[1,2], 成为近年来研究热点之一. 但这款“潜力新秀”尚处发展阶段, 存在明显的“先天短板”: 晶体结构类似“一维链条”, 载流子在其中传输易受阻碍, 就像在迷宫中迂回运动, 导致传输效率较低, 仅特定[*hk1*]晶向可实现载流子的高速传输; 结晶时硫、硒元素容易“流失”, 形成大量“电荷陷阱”, 导致电子和空穴刚产生就“抱团消失”, 实验光电转换效率远低于32%的理论上限[3,4], 始终难以跟上硅基、钙钛矿等强者的步伐[5,6]. 科学家一直对症下药, 尝试过后处理、掺杂、界面工程等多种优化方案[7~11], 最终发现“后处理”是提升其性能的关键路径.

为了解决这些问题, 我们团队为它配备了一位“金牌结晶调控师”——溴化1-丁基-3-甲基咪唑离子液体([BMIM]Br), 通过简单的后处理工艺, 这位调控师化身“精准优化助手”, 给$Sb_2(S,Se)_3$薄膜带来“三重优化效应”, 同时攻克结构和缺陷两大难题[12]. 第一重效应是“防护+助长”: [BMIM]Br熔点低于100°C, 加热时先熔化成液态“防护盾”, 紧紧包裹薄膜表面, 阻止硫、硒元素挥发, 让薄膜成分接近理想的化学计量比, 从源头减少缺陷; 同时它又像“润滑剂”, 加快原子移动, 形成更大的晶粒, 减少电荷传输阻碍, 如图1(a)所示. 第二重效应是“定向引导”: 它对$Sb_2(S,Se)_3$的(211)晶面有着天然的“高亲和力”, 远强于其他晶面, 像指南针一样引导晶体沿[211]方向生长. 这个方向正是电荷传输的“快车道”, 能让电子和空穴快速抵达电极, 彻底解决准一维结构的传输难题. 第三重效应是“缺陷修正”: 它能重塑薄膜的缺陷类型, 把原本会严重“耗电”的阳离子反位缺陷(Sb_S)转化为影响极小的硒空位缺陷(V_{Se2}), 缺陷密度显著减少, 电荷未被有效利用而凭空流失的情况得到了明显遏制, 如图1(b)所示. 更难得的是, 这位“调控师”堪称“无痕优化助手”——高温处理到350°C后会完全分解成气态产物, 没有任何残留, 不会引入新杂质,

引用格式: 任栋楼, 陈烁, 章向华, 等. 离子液体调控结晶助力硒硫化锑太阳能电池效率创新高. 科学通报, 2026, 71: 2794–2796
Ren D, Chen S, Zhang X, et al. Ionic liquids-modulated crystallization boosts antimony sulfoselenide solar cell efficiency (in Chinese). Chin Sci Bull, 2026, 71: 2794–2796, doi: 10.1360/CSB-2026-0194

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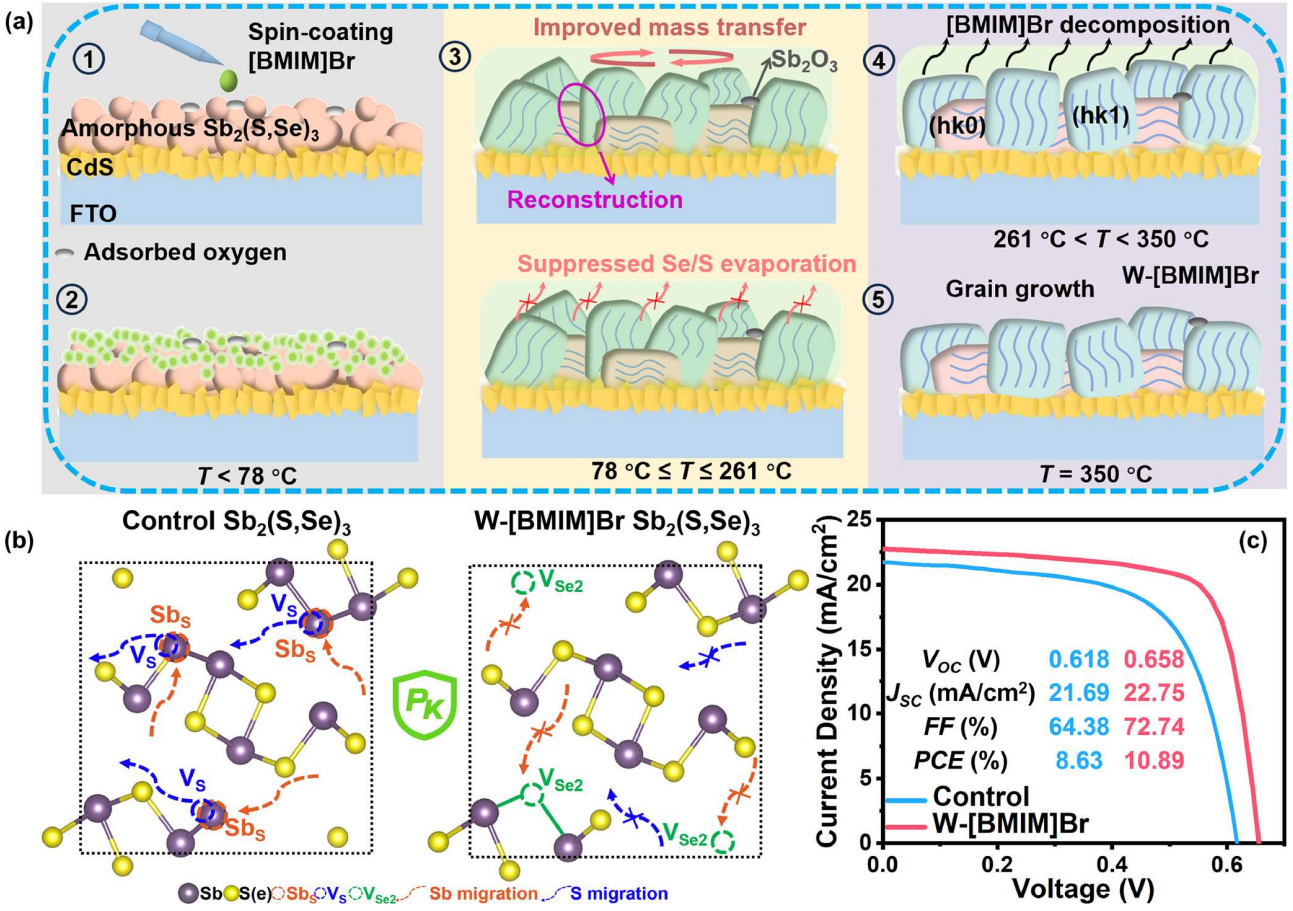


图 1 (网络版彩色)(a) [BMIM]Br辅助$Sb_2(S,Se)_3$薄膜晶化示意图(W-[BMIM]Br). (b) 参比薄膜(Control)和[BMIM]Br处理薄膜的缺陷演化示意图. (c) 参比器件和W-[BMIM]Br器件的电流密度与电压特性曲线[12]. Copyright © 2026, John Wiley and Sons

Figure 1 (Color online) (a) Schematic of $Sb_2(S,Se)_3$ film crystallization assisted by [BMIM]Br (W-[BMIM]Br). (b) Schematic of defect evolution in the reference film (Control) and the [BMIM]Br-treated film. (c) Current density versus voltage characteristics of the control and W-[BMIM]Br cells[12]. Copyright © 2026, John Wiley and Sons

既保证了薄膜高纯度，又实现了高效优化的“润物无声”. 性能测试中，这款“潜力新秀”的表现令人振奋：光电转换效率从8.63%跃升至10.89%，填充因子从64.38%提升至72.74%，两项关键指标均跻身$Sb_2(S,Se)_3$太阳能电池的顶尖水平，如图1(c)所示.

这项工作用简单的离子液体后处理策略，不仅精准调节了$Sb_2(S,Se)_3$薄膜的微观结构，还修复了其中的缺陷，为低成本、高效率太阳能电池研发提供了新范式. 然而，离子液体与$Sb_2(S,Se)_3$薄膜之间的原子级实时作用机制仍不明确. 未来可结合原位X射线光电子能谱和原位X射线衍射等先进表征技术，深入揭示二者的动态相互作用机制，这将有助于设计更高效的晶化调控体系，从而最大限度地抑制载流子复合损耗, 进一步提升器件性能. 此外, 本研究提出的后处理策略具有良好的普适性，有望拓展至其他锑基硫属化物半导体器件(如光电探测器和光解水制氢)，为推动该类材料在光电器件领域的研发提供新思路.

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