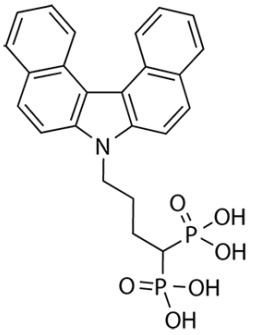
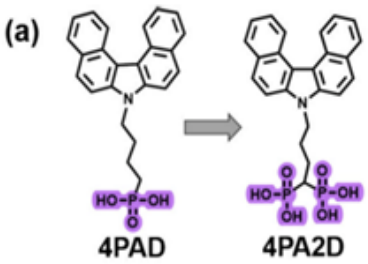
Perovskite Solar Cells

Self-Assembled Monolayers Materials



LT-S8100 4PA2D >98%

Bisphosphonic acid-based self-assembled monolayer, 4PA2D. By incorporating dual phosphonic acid groups linked through a stable alkyl chain to a dibenzocarbazole core, 4PA2D enables robust tridentate anchoring on ITO substrates, leading to stronger interfacial binding, improved energy-level alignment, and effective defect passivation. As a result, the optimized PSCs achieve a champion PCE of 25.31% , with a high *Voc* of 1.177 V and a FF of 86.74%, while large-area devices (1.055 cm^2) reach 23.99% efficiency. Moreover, the devices demonstrate excellent thermal and operational stability, retaining 95.6% of their initial PCE after 1500 h at 65 °C.



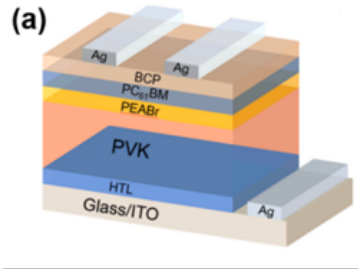
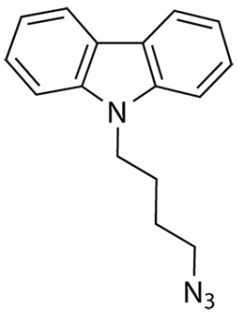


Table S5 Forward and reverse scanning parameters of the device.

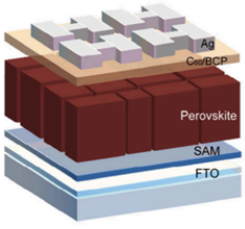
Sample	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	Average PCE (%)
4PAD-R	1.144	24.64	85.25	24.03	23.71
4PAD-F	1.136	24.53	81.01	23.41	
4PA2D-R	1.177	24.79	86.74	25.31	25.11
4PA2D-F	1.177	24.75	85.85	24.91	

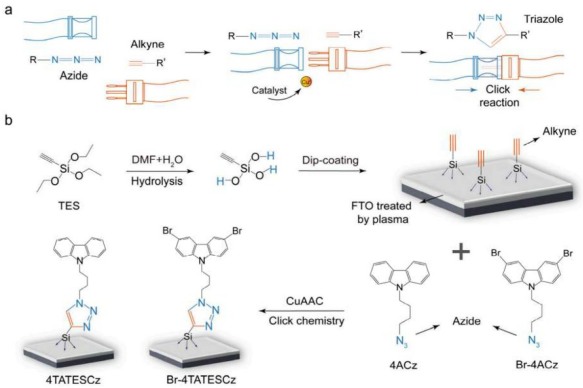
DOI:10.1016/j.cej.2026.173863



LT-S8102 4ACz >98%

An in situ click chemistry strategy to construct mixed SAMs with precisely tunable energy levels under mild conditions and high intrinsic reactivity. By adjusting the precursor ratio of 4ACz and Br-4ACz, the energy alignment of the SAMs can be finely controlled, effectively overcoming the steric-hindrance–anchoring trade-off found in conventional SAM formation and enabling high-quality hole transport layers. Theoretically and experimentally, the click-chemistry-engineered interfaces enhance charge transport and suppress nonradiative recombination. Consequently, 1.53 eV inverted perovskite solar cells achieve a champion PCE of 26.83% and maintain 93% of their initial efficiency after 2,000 hours under ISOS-L-2 conditions.





	Voc (V)	*FF (%)*	*Jsc (mA cm^{-2})*	*PCE (%)*
4PACz-based	1.164	80.51	26.45	24.78
4PACz (after treated)	1.130	78.29	26.08	23.07
3-2 SAM-based	1.192	84.33	26.48	26.62
3-2 SAM-based (after treated)	1.189	84.07	26.48	26.47

DOI:10.1021/acs.nanolett.5c06186

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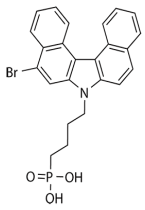
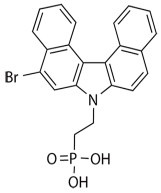
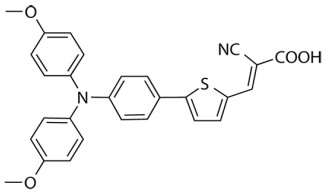
LT-S8096 1Br4PADCB
>98%



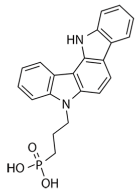
LT-S8097 1Br2PADCB
>98%



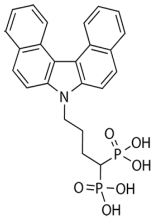
LT-S8098 MPA-Th-CA
>98%



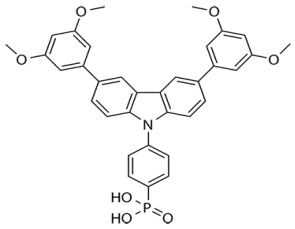
LT-S8099 M3PAICz-1
>98%



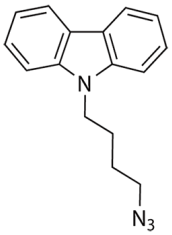
LT-S8100 4PA2D
>98%



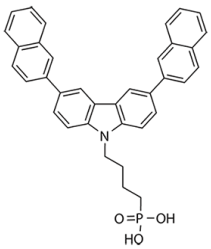
LT-S8101 DMPP
>98%



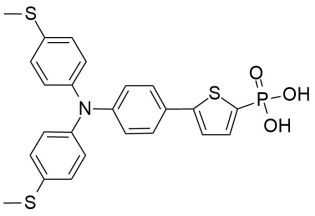
LT-S8102 4ACz
>98%



LT-S8103 NaPh-4PACz
>98%



LT-S8105 SMe-TPA-THPA
>98%



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