

GLASS-FORMING HOLE-TRANSPORT MATERIALS WITH TAILORED SURFACE ROUGHNESS FOR ENHANCED PERFORMANCE IN PEROVSKITE SOLAR CELLS

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Charge transport materials in heterojunction solar cells, particularly perovskite solar cells (PSCs), are critical for optimal charge dynamics and device stability[1][2]. Conventional hole transport materials (HTMs) such as spiro-OMeTAD and PTAA demonstrate strong photovoltaic performance due to high thin-film quality and energy alignment[3][4]. However, they often show high material cost, low carrier mobility and poor stability, which greatly limit their practical applications. In our pursuit of low-cost, accessible organic HTMs with attributes such as enhanced thermal and photochemical stability, higher glass transition temperatures, and improved hole mobility, we designed and synthesized novel dibenzothiophene and spiro[1,3-dithiolane-2,9'-fluorene]-based compounds utilizing microwave-assisted Buchwald–Hartwig reactions. Notably, surface roughness analyses of the resulting materials revealed a general average roughness of 6.129 to 8.028 nm, influencing their charge transport dynamics. The synthesized materials exhibited excellent thermal stability, with decomposition temperatures between 309 and 408 °C and glass transition temperatures ranging from 99 to 163 °C. Photoelectron emission spectroscopy indicated ionization potentials from 5.03 to 5.16 eV. Additionally, time-of-flight (TOF) and charge extraction by linearly increasing voltage (CELIV) measurements demonstrated efficient hole transport in vacuum-deposited films, achieving hole mobilities as high as $4 \times 10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at an electric field of $9 \times 10^5 \text{ V cm}^{-1}$. Among the materials evaluated, the compound 2',7'-bis[(4-methoxyphenyl)(9-ethylcarbazol-3-yl)amino]-spiro[1,3-dithiolane-2,9'-fluorene] showcased the best device performance, attaining optimized power conversion efficiencies of 7.5% (forward scan) and 13.5% (reverse scan) under 1-sun illumination, alongside 14.55% (FW) and 26.5% (RV) under 3000 K LED illumination (1000 lx).

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