Supporting Information

Conjugated Molecules Based 2D Perovskites for High-Performance Perovskite Solar Cells

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SI 1. Synthesis and characterization of PPA

SI 2. The PL characterization

SI 3. The C-V characteristics of perovskite thin film

KEYWORDS: 2D perovskites, conjugated organic molecule, organic spacer, perovskite solar cells, efficiency, and stability

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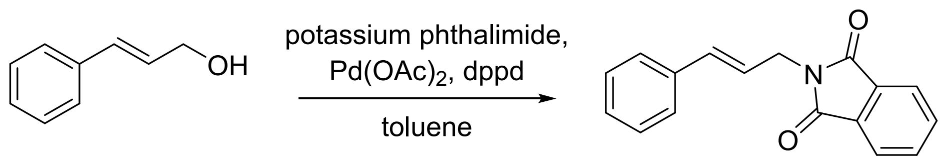
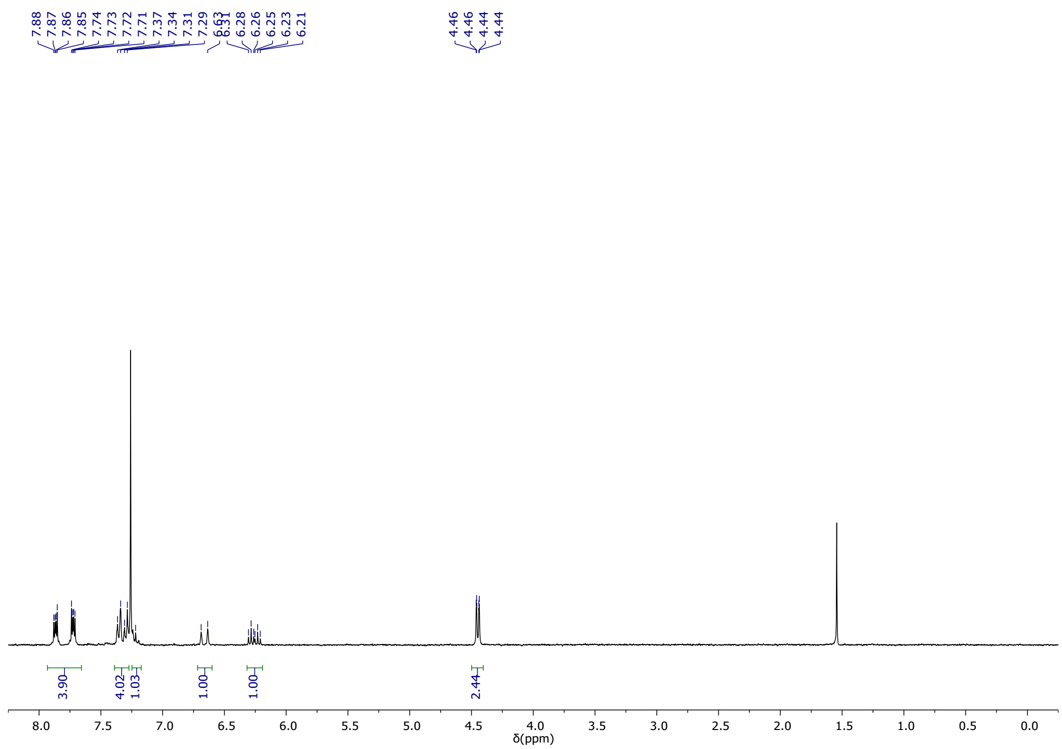
SI 1. Synthesis and characterization of PPA



Scheme 1. Synthetic steps of 2-cinnamylisoindoline-1,3-dione

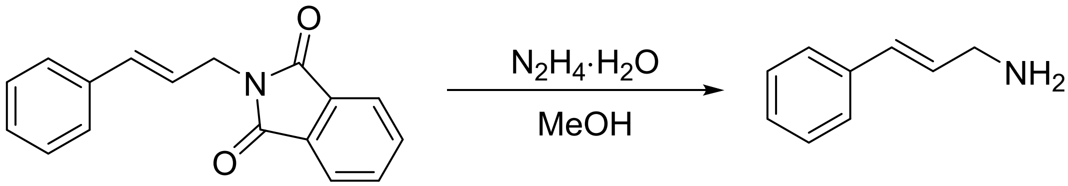
Scheme 1 describes the synthetic steps of 2-cinnamylisoindoline-1,3-dione. In an oven dried Schlenk flask was charged cinnamyl alcohol (1.0 equiv., 10 mmol, 1.34 g), potassium phthalimide (1.0 equiv., 10 mmol, 1.47 g), palladium acetate (0.025 equiv., 0.25 mmol, 94.8 g), dppd (0.05 equiv., 0.5 mmol, 213.2 mg) and 20 mL toluene. After three cycles of freeze-pump-thaw, the mixture was heated under 100 ˚C for 24 h. Toluene was removed by rotary evaporation and the residual was subjected to column chromatography, affording 2-cinnamylisoindoline-1,3-dione.

^{1}H NMR (300 MHz, $CDCl_3$) spectrum for 2-cinnamylisoindoline-1,3-dione is shown in **Scheme 2.** ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.80 (ddd, J = 43.0, 5.5, 3.1 Hz, 4H), 7.39-7.18 (m, 5H), 6.66 (d, *J* = 16.1 Hz, 1H), 6.26 (dt, *J* = 15.8, 6.4 Hz, 1H), 4.50-4.39 (dd, *J* = 6.5, 1.2 Hz, 2H).



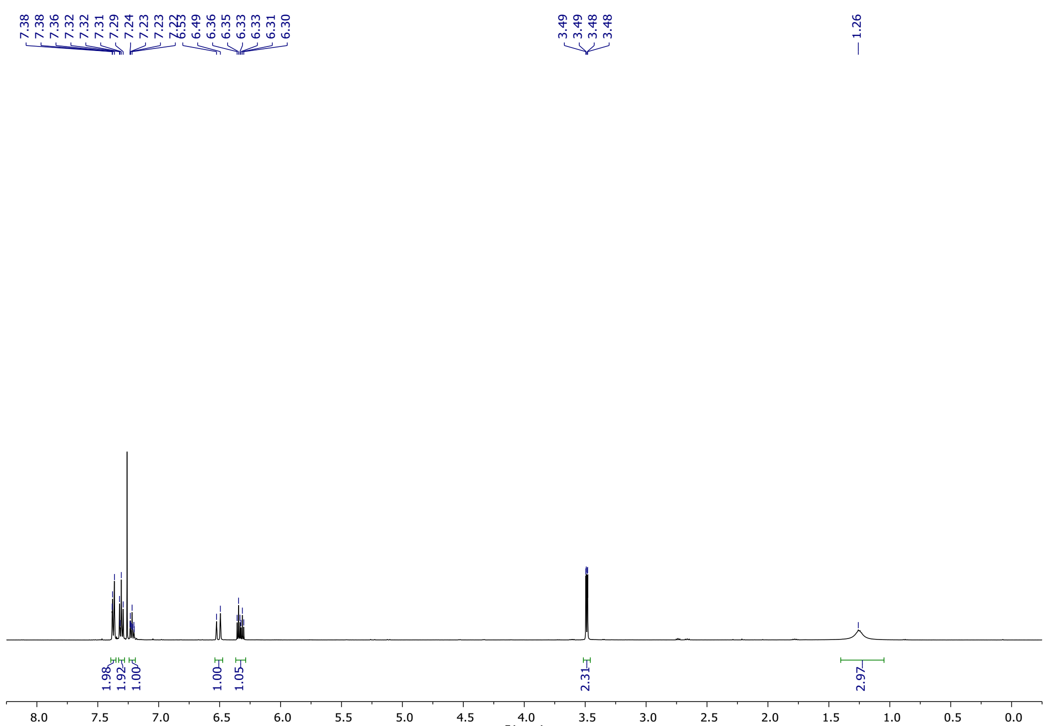
Scheme 2. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum for 2-cinnamylisoindoline-1,3-dione.

Scheme 3 displays synthetic steps of PPA. In a round bottom flask was charged 2-cinnamylisoindoline-1,3-dione (1.0 equiv., 1.0 mmol, 263.3 mg), hydrazine hydrate (50%~60% hydrazine, 3.0 equiv., 3.0 mmol, 187 μL) and MeOH (3 mL). After refluxing overnight, the mixture was cooled down, and to it were added 5 mL DCM and 5 mL 1 M NaOH(aq). The mixture was stirred for an additional 30 min. The mixture was extracted with DCM and the combined organic phase was then washed with water and brine and dried over sodium sulfate. Preparative Gel Permeation Chromatography was performed for purification to render 3-phenyl-2-propen-1-amine.



Scheme 3. Synthetic steps of PPA

Scheme 4 shows the ^{1}H NMR results of PPA. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.39-7.35 (m, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.24-7.19 (m, 1H), 6.51 (d, *J* = 15.9 Hz, 1H), 6.33 (dt, *J* = 15.9, 5.9 Hz, 1H), 3.51-3.46 (dd, *J* = 5.9, 1.5 Hz, 2H), 1.40-1.05 (br, 2H).



Scheme 4 . ^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 3-phenyl-2-propen-1-amine.

SI 2. The PL characterization

Fig. S1 displays the photoluminescence (PL) spectra of $MAPbI_3$ thin film and the $(PPA)_x(MAPbI_3)_{1-x}/MAPbI_3$ bilayer thin film coated on the top of quartz. The PL intensity increased obviously in the $(PPA)_x(MAPbI_3)_{1-x}/MAPbI_3$ bilayer thin film, implying that non-radiative recombination within the $(PPA)_x(MAPbI_3)_{1-x}/MAPbI_3$ bilayer thin film was significantly suppressed.

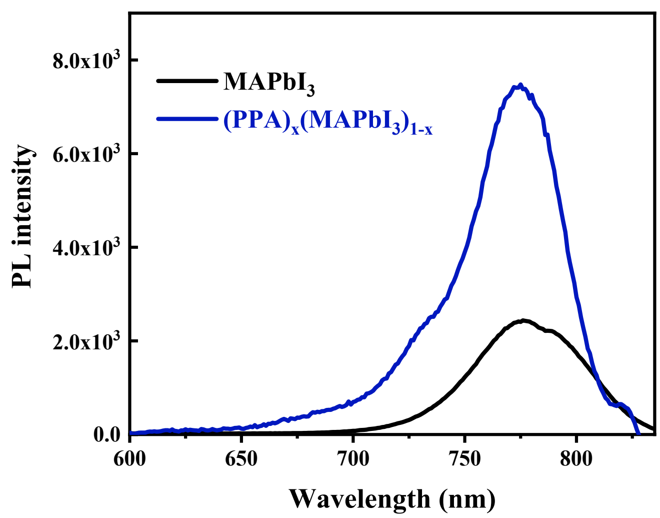


Fig. S1. The PL spectra of $MAPbI_3$ and the $(PPA)_x(MAPbI_3)_{1-x}/MAPbI_3$ thin films from front side.

SI 3. The capacitance versus frequency characteristics of perovskite thin film

The capacitance versus frequency characteristics of photodiodes with a device structure of ITO/perovskite active layer/Al, where the active layer is either the $(PPA)_x(MAPbI_3)_{1-x}/MAPbI_3$ bilayer thin film or $MAPbI_3$ thin film are **Fig. S2**). The ε is the dielectric constant for perovskite thin film is described by: $C = \varepsilon\varepsilon_0\frac{A}{d}$ (where A is the device area and d is the film thickness of perovskite thin film) [41-44]). Thus**,** the ε values are calculated to be 26.6 and 25.4 for the $(PPA)_x(MAPbI_3)_{1-x}/MAPbI_3$ bilayer thin film and $MAPbI_3$ thin film, respectively.

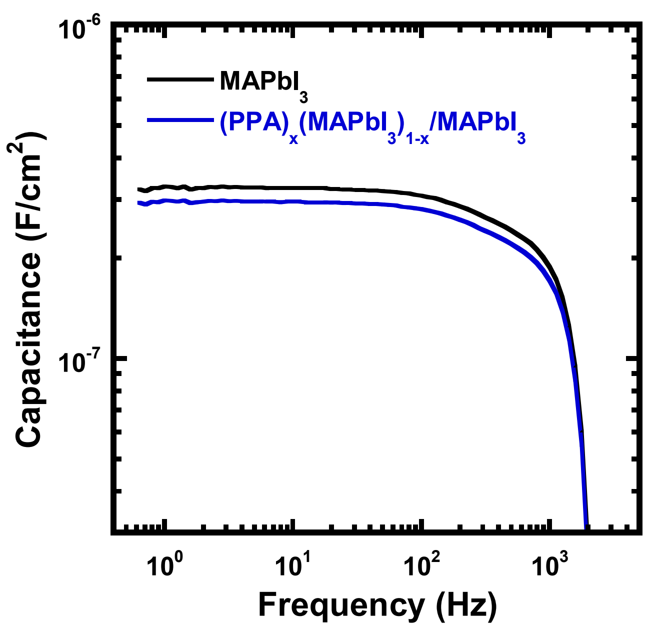


Fig. S2. The C-V characteristics of perovskite thin films