

Directed assembly of cathode interlayers enables efficient binary organic solar cells

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Supplementary information

Directed Assembly of Cathode Interlayers Enables Efficient Binary Organic Solar Cells

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Supplementary Method:

Synthesis of Compound 2: Following a procedure described in Supplementary Figure 1, 1, 3,4,9,10-perylenetetracarboxylic dianhydride (1.0 g, 2.55 mmol), 1-bromobutane (2.81 g, 20.4 mmol), 1-butanol (1.51 g, 20.4 mmol), and 1,8-diazabicyclo[5.4.0]undec-7-ene (1.55 g, 10.2 mmol) were mixed in acetonitrile (50 mL). The mixture was refluxed overnight, cooled to room temperature, and then poured into methanol. The resulting precipitate was collected by filtration, washed thoroughly with methanol, and dried under vacuum to afford the title compound as a solid (1.63 g, 98% yield). ¹H NMR (400 MHz, CDCl₃) δ 8.12 (dd, 4H), 7.95 (dd, 4H), 4.40 – 4.33 (m, 8H), 1.84 – 1.76 (m, 8H), 1.54 – 1.47 (m, 8H), 1.01 – 0.99 (m, 12H).

Synthesis of Compound 3: To a stirred solution of compound **2** (1.0 g, 1.53 mmol) in dichloromethane (50 mL) was added sodium nitrite (0.10 g, 1.45 mmol) and concentrated HNO₃ (0.35 g, 3.6 mmol). The reaction mixture was stirred at room temperature for 5 h. Upon completion, a saturated aqueous solution of NaHCO₃ was added dropwise with vigorous stirring. The mixture was extracted with dichloromethane (2 × 100 mL). The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure. The crude residue was purified by column chromatography on silica gel, using a mixture of ethyl acetate and petroleum ether (1:15, v/v) as the eluent, to afford compound **3** as a solid (0.98 g, 88% yield). ¹H NMR (400 MHz, CDCl₃) δ 8.32 (t, 2H), 8.24 (s, 1H), 8.18 (d, 1H), 8.10 (d, 1H), 7.95 (d, 1H), 7.86 (d, 1H), 4.40 – 4.34 (m, 8H), 1.84 – 1.77 (m, 8H), 1.55 – 1.47 (m, 8H), 1.01 – 0.98 (m, 12H).

Synthesis of Compound 4: Compound **2** (1.0 g, 1.53 mmol), sodium nitrite (0.2 g, 2.90 mmol) and concentrated HNO₃ (1.4 g, 14.5 mmol) were added in 60 mL dichloromethane, and the reaction mixture was stirred for 8 h at room temperature. A saturated aqueous solution of NaHCO₃ was added dropwise to the reaction mixture with stirring. The mixture was extracted with dichloromethane (2 × 100 mL) and water (2 × 100 mL). The crude residue was purified by column chromatography on silica gel, using a mixture of ethyl acetate and petroleum ether (1:15, v/v) as the eluent, to afford compound **4** as a solid (0.80 g, 70%). ¹H NMR (400 MHz, CDCl₃) δ 8.39 (s, 1H), 8.33 (s, 1H), 8.13 (d, 1H), 8.06 (d, 2H), 8.01 (d, 1H), 4.39 – 4.33 (m, 8H), 1.84 – 1.75 (m, 8H), 1.54 – 1.47 (m, 8H), 1.03 – 0.99 (m, 12H).

Synthesis of Compound 5: Compound **3** (0.5 g, 0.71 mmol) and sulfur (0.2 g, 6.2 mmol) were added

in 20 mL DMF, and the reaction mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the mixture was extracted with dichloromethane (2 × 100 mL) and water (2 × 100 mL). The crude residue was purified by column chromatography on silica gel, using a mixture of ethyl acetate and petroleum ether (1:15, v/v) as the eluent, to afford compound **5** as a solid (0.41 g). ¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 2H), 8.35 (d, 2H), 8.16 (d, 2H), 4.41 – 4.33 (m, 8H), 1.94 – 1.73 (m, 8H), 1.61 – 1.43 (m, 8H), 1.03 – 0.98 (m, 12H).

Synthesis of Compound 6: In a 50 mL flask, compound **4** (0.5 g, 0.67 mmol) and sulfur (0.4 g, 12.5 mmol) were added in 20 mL DMF, and the reaction mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the mixture was extracted with dichloromethane (2 × 100 mL) and water (2 × 100 mL). The crude product was purified by column chromatography using a mixture of ethyl acetate and petroleum ether (1:15, v/v) as the eluent, to give the pure compound **6** (0.12 g). ¹H NMR (400 MHz, CDCl₃) δ 8.66 (s, 2H), 8.15 (s, 2H), 4.40 – 4.32 (m, 8H), 1.94 – 1.74 (m, 8H), 1.60 – 1.42 (m, 8H), 1.02 – 0.98 (m, 12H).

Synthesis of Compound 7: In a 50 mL flask, compound **5** (0.3 g, 0.44 mmol) and *p*-toluenesulfonic acid monohydrate (0.835 g, 4.40 mmol) were dissolved in toluene (20 mL). The mixture was heated at 120 °C for 24 h, during which a red precipitate initially formed and gradually turned orange. After cooling, the reaction mixture was transferred to a centrifuge tube and washed with water (3 × 30 mL) by high-speed centrifugation (8000 rpm, 3 min each), decanting the supernatant after each cycle. The solid was subsequently washed with petroleum ether (3 × 20 mL) and dichloromethane (3 × 20 mL) using the same centrifugation procedure. The resulting orange-red solid was dried under vacuum for 12 h to afford compound **7** (142 mg).

Synthesis of Compound 8: This dianhydride was prepared following a procedure analogous to that for compound **7**, using compound **6** (0.12 g, 0.17 mmol) as the starting material. Purification afforded compound **8** as an orange-red solid (69.2 mg).

Supplementary Discussions:

In simulation, for simplification of the calculation, an initial step involves the immobilization of 40 BTP-eC9 acceptor molecules along with 500 methanol molecules within a cubic box possessing an edge length of 5 nm. This immobilization is accomplished through the utilization of the Packmol software.¹ Subsequently, 10 PDISNN molecules are introduced onto the upper layer of this configuration. Following this setup, a molecular dynamics simulation under the constant volume and temperature (NVT-MD) conditions is executed for a duration of 5 ns at 300 K, with the objective of equilibrating the structures to derive the final configurations. The molecular dynamics simulations throughout this study employ the Verlet integrator, with a time step set to 1.0 fs.

The molecular dynamics (MD) simulations were carried out with the Forcite package and the pcff force field.² To accurately describe the intramolecular and intermolecular interactions for the L8-BO, PDISNN, methanol, and trifluoroethanol components, their atomic partial charges were derived by fitting the electrostatic potential (ESP) evaluated at the ω B97XD/cc-PVTZ level of theory (the relevant DFT calculations were performed with the Gaussian 16 C.01 package³). The Verlet integrator was used with a time step of 1 fs and the Berendsen thermostat was employed for temperature control. A cutoff of 12.5 Å was considered for the summation of the van der Waals interactions and the Ewald solver for the long-range Coulomb interactions. Here, all the MD simulations were run with the NVT (constant number of molecules, volume, and temperature) ensemble and at room temperature (i.e., 298.15 K). To examine the dynamic behaviors of PDISNN in the trifluoroethanol solution on the L8-BO substrate (without and with methanol layer in between the solution and the L8-BO substrate), three sets of MD simulations were considered: (i) a single PDISNN molecule in the trifluoroethanol solution on the L8-BO substrate without and with the methanol layer; (ii) a PDISNN molecular cluster in the trifluoroethanol solution on the L8-BO substrate without and with the methanol layer; and (iii) multiple PDISNN molecules in the trifluoroethanol solution on the L8-BO substrate without and with the methanol layer. For single molecular and molecular cluster states, the simulations were both implemented for 10 ns; for multiple molecular states, the simulation was first performed for 22 ns and then continued by evaporating the trifluoroethanols for 20 ns. To save computational costs, the substrate was fixed during the MD simulations.

The PDISNN molecule was initially placed with an edge-on orientation on the substrate. For the case without the methanol layer, the PDISNN molecule quickly detached the L8-BO substrate and diffused with a random orientation in the trifluoroethanol solution. For the case with the methanol layer, the PDISNN molecule interacted with the methanol layer for most of the time and occasionally detached the substrate. Here as well, the PDISNN molecular cluster was initially placed with an edge-on orientation on the substrate. For the case without the methanol layer, most PDISNN molecules in the cluster detached the substrate and cannot keep the edge-on orientation with respect to the substrate. In contrast, for the case with the methanol layer, the PDISNN cluster always maintains the edge-on orientation with respect to the substrate. Initially, the PDISNN molecules were randomly placed in the trifluoroethanol solution. For both cases, the PDISNN molecules can aggregate within the trifluoroethanol solution, due to the high concentration we adopted. In fact, during the solvent evaporation process, the concentration gradually becomes larger. During the following evaporation process, the PDISNN aggregate gradually approached the substrate. However, in the case without the methanol layer, the PDISNN aggregate and other PDISNN molecule cannot adopt the edge-on orientation with respect to the substrate; while in the case with the methanol layer, the PDISNN aggregate can adopt the edge-on orientation through the interaction between the PDISNN side chain and the methanol layer.

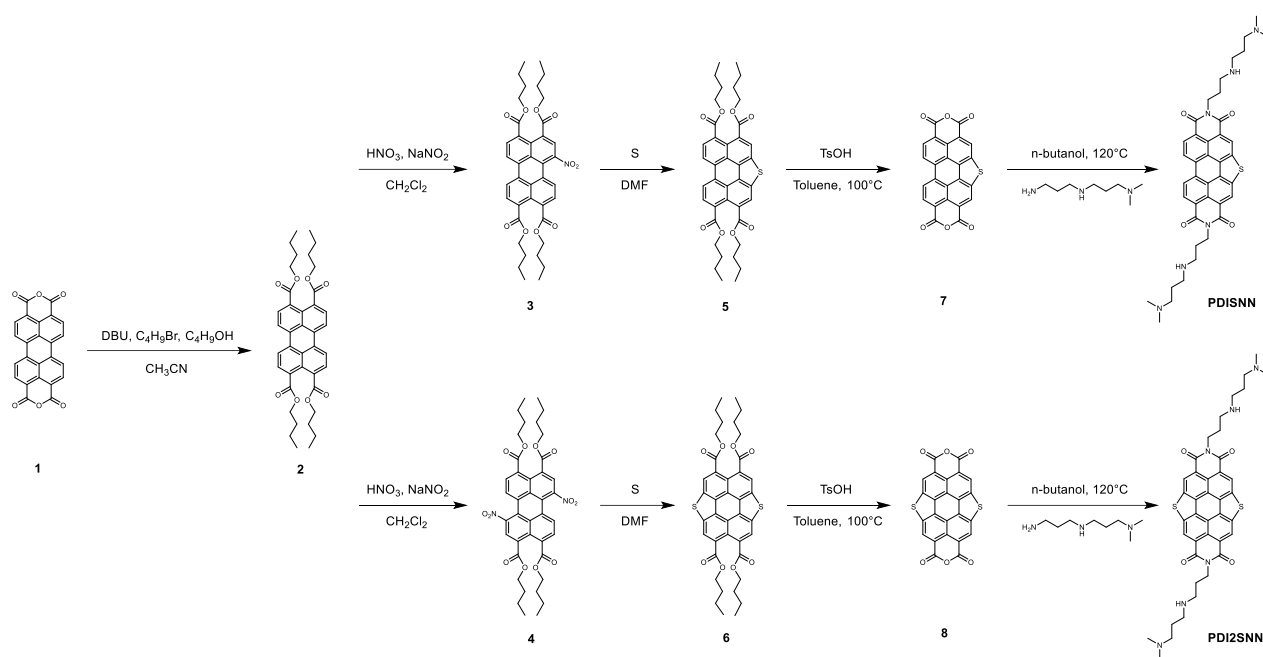
To corroborate the beneficial role of methanol pretreatment, we quantified the work function of the active layers by ultraviolet photoelectron spectroscopy (UPS). As shown in Supplementary Figure 22, the work function decreases from 4.26 eV for the pristine active layer to 4.21 eV after Method I treatment and further to 4.17 eV following Method III pretreatment. This trend aligns with the enhanced surface potential in SKPM, confirming that methanol pretreatment optimizes interfacial dipole alignment via PDISNN reorganization. The polar groups in the interlayers significantly reduce the cathode work function by forming an interfacial dipole. Moreover, when the dipole moment is oriented perpendicular to the cathode, its electrostatic effect more efficiently shifts the vacuum level, whereas parallel or disordered orientations lead to partial cancellation of the dipole. As evidenced by our UPS measurements, the variation trend indicates enhanced dipole effectiveness in Method III, which corresponds to a more perpendicular orientation of the interlayer relative to the active layer. The resulting reduction in work function improves the energy-level alignment between the cathode

and the electron quasi-Fermi level of the acceptor, thereby lowering the Schottky barrier at the interface.

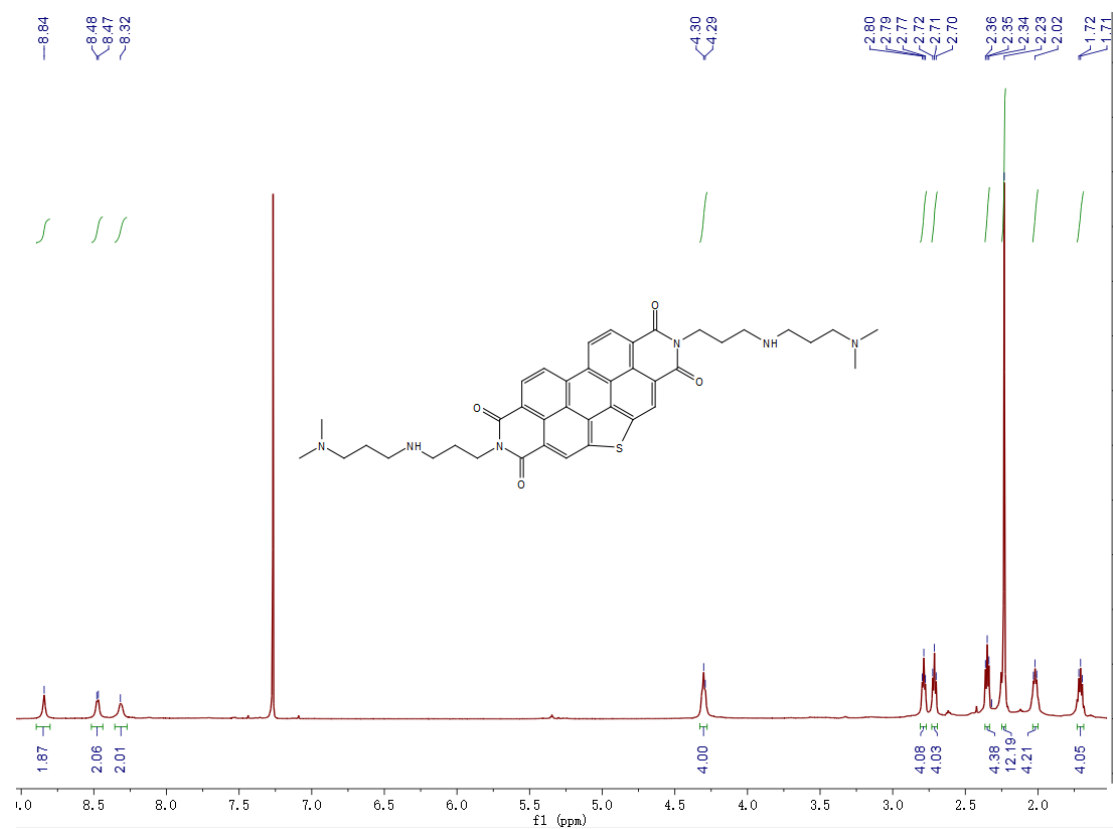
Supplementary Notes

Supplementary Note 1: The angle derived from SFG corresponds to the tilt angle of the transition dipole moment associated with the C=C stretching mode of the perylene core relative to the surface normal. A smaller tilt angle therefore indicates a more perpendicular orientation of the PDI core with respect to the substrate. In contrast, the angle obtained from NEXAFS reflects the angle between the molecular plane normal (i.e., the π^* orbital vector) and the substrate surface normal. In this convention, an angle of 90° corresponds to a molecular plane that is perfectly perpendicular to the substrate (edge-on configuration), whereas 0° indicates a face-on orientation. Although the absolute values differ due to the distinct physical quantities probed by these two techniques, they consistently reveal the same orientational trend.

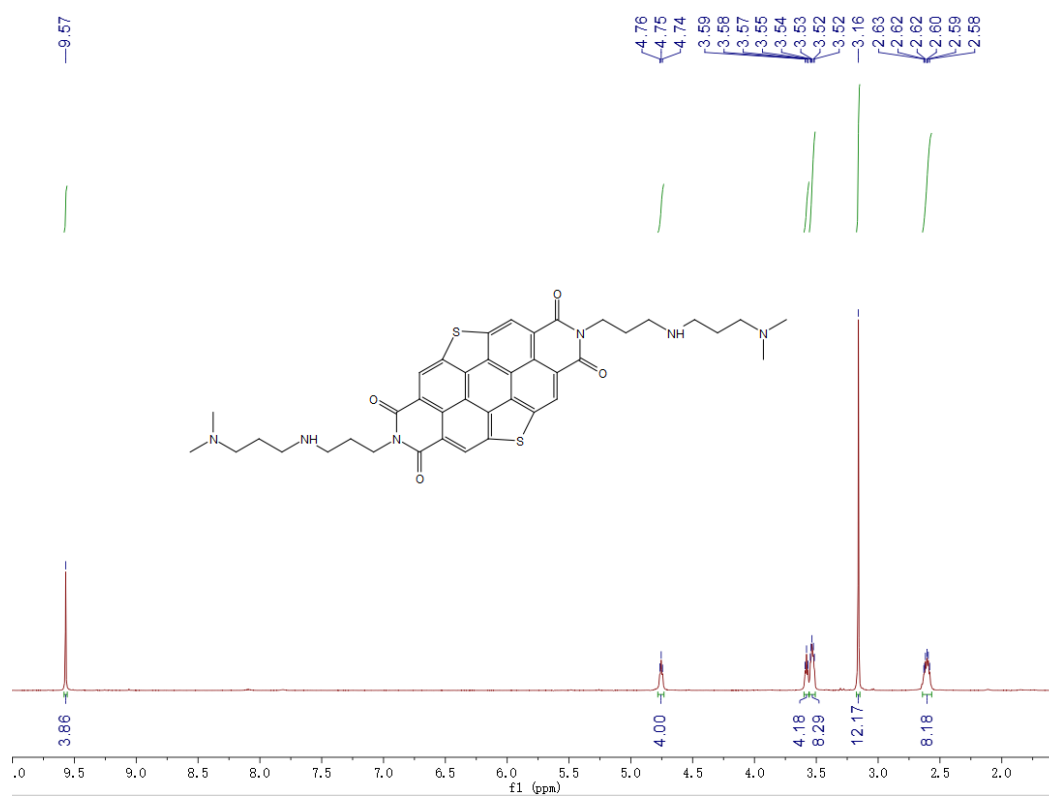
Supplementary Figures



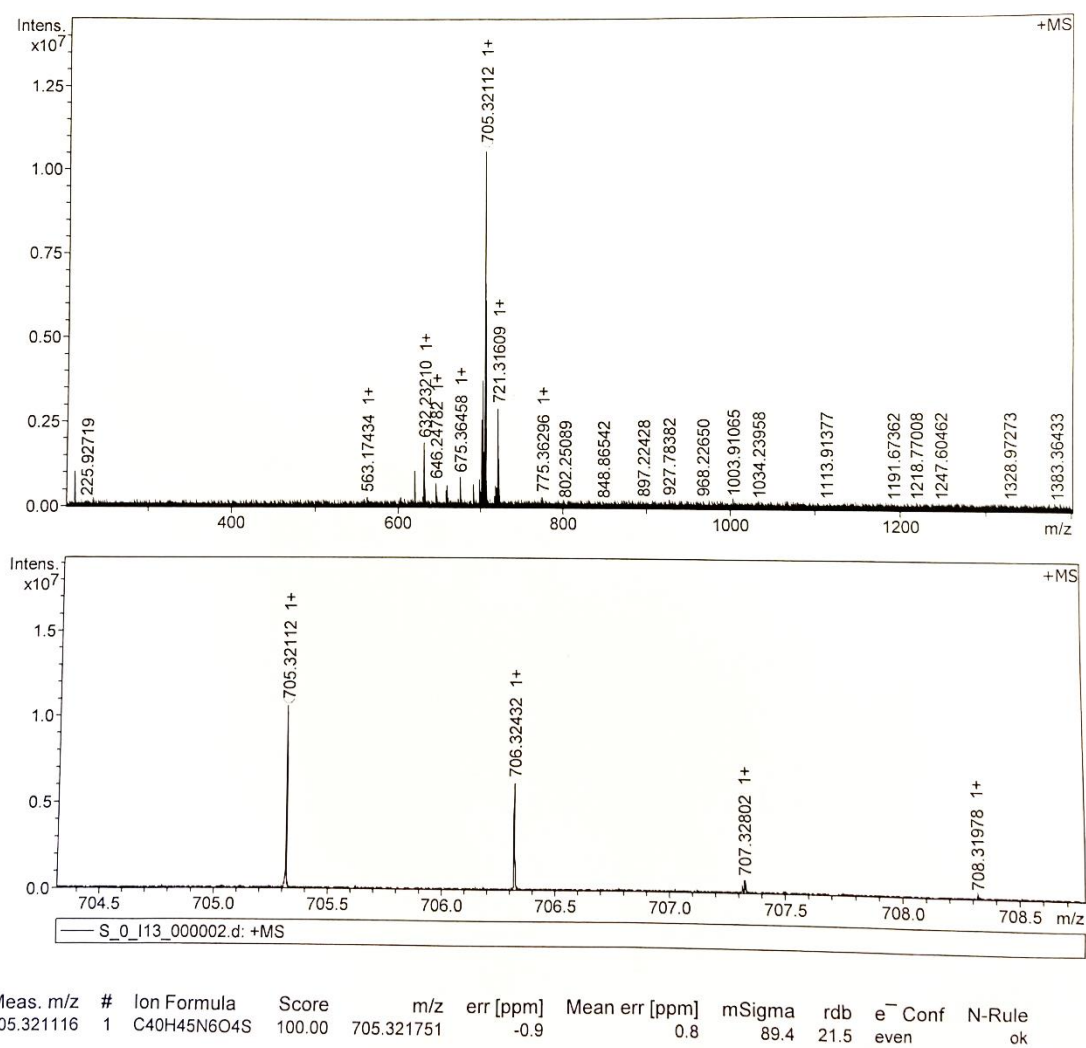
Supplementary Figure 1. Detailed synthesis route of PDISNN and PDI2SNN.



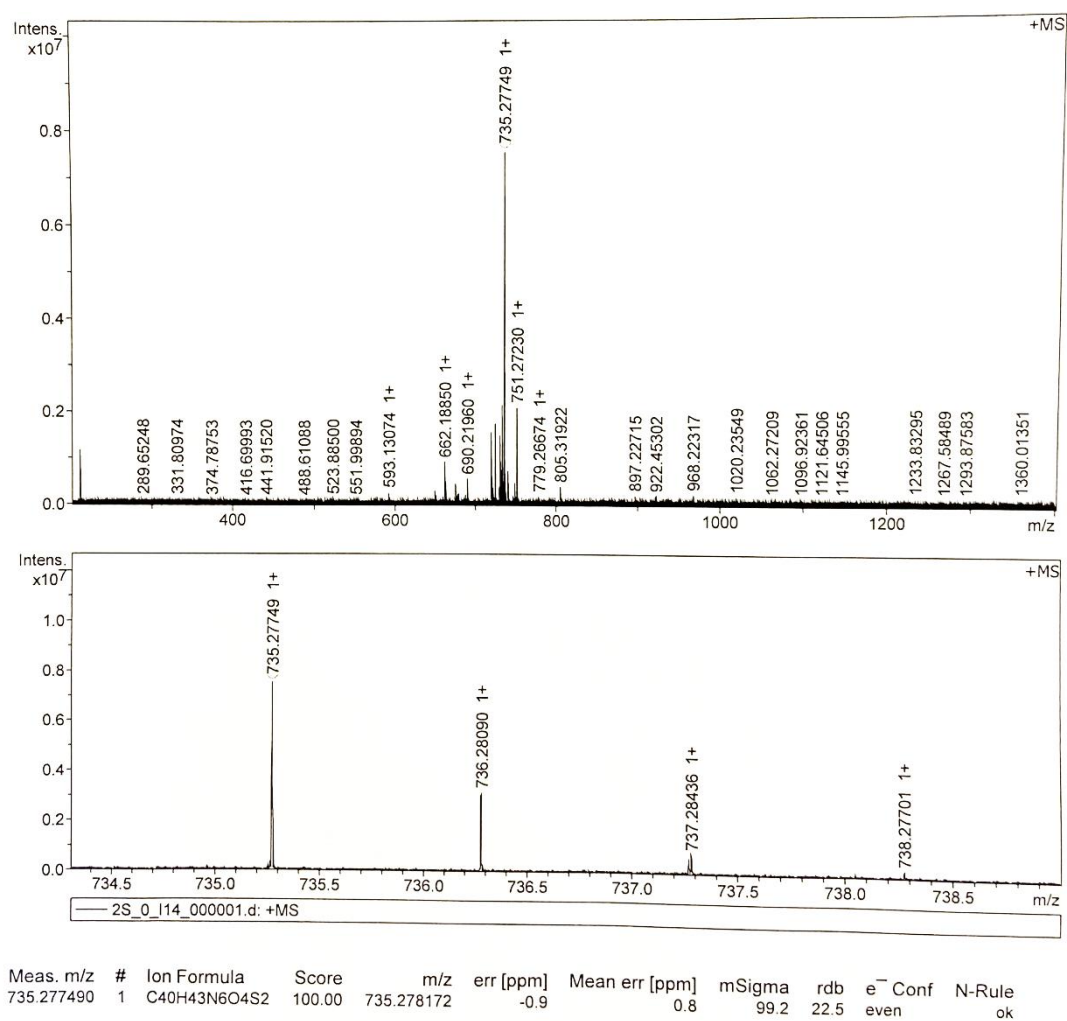
Supplementary Figure 2. ^1H -NMR spectrum (400 MHz) of PDISNN.



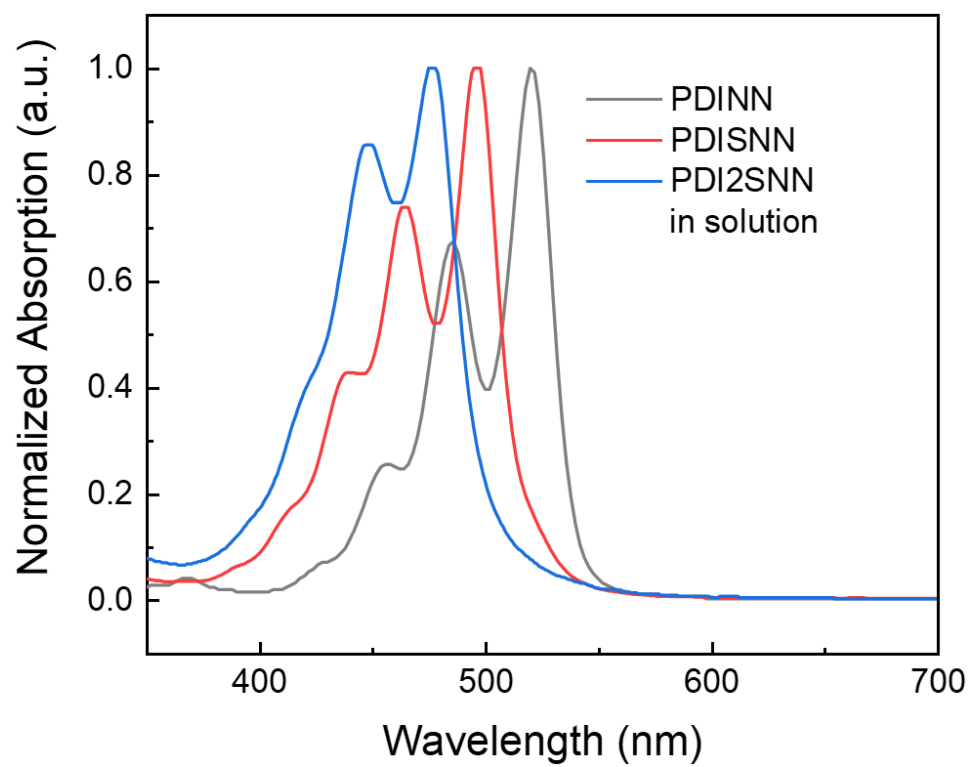
Supplementary Figure 3. ¹H-NMR spectrum (400 MHz) of PDI2SNN.



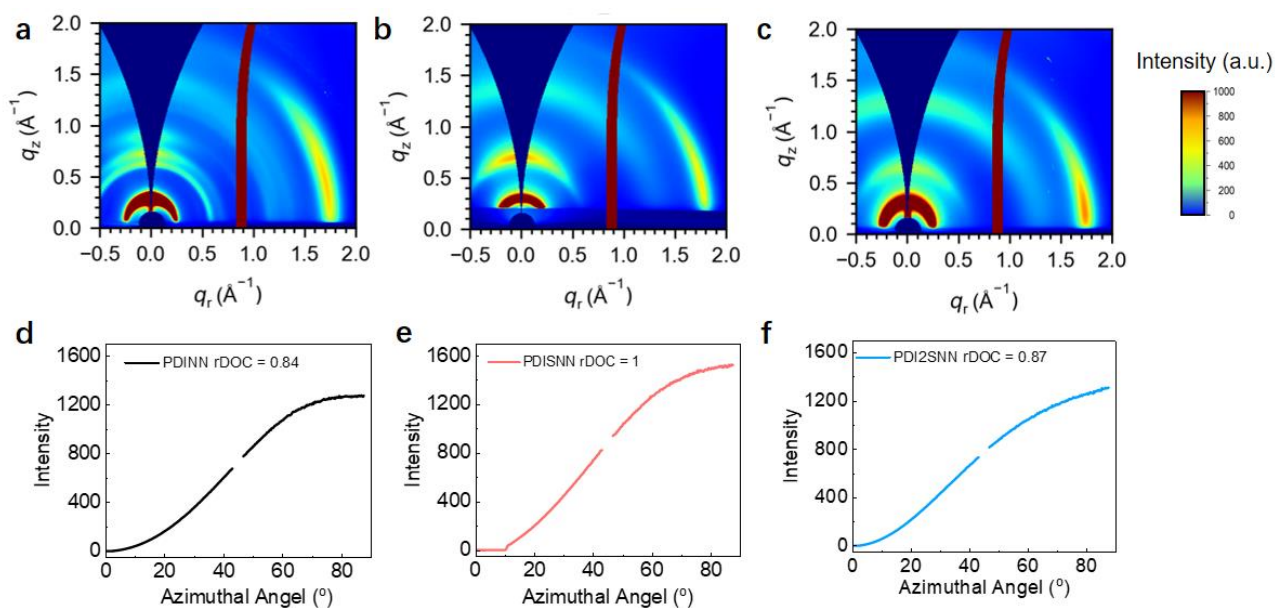
Supplementary Figure 4. The MALDI-TOF spectrum of PDISNN.



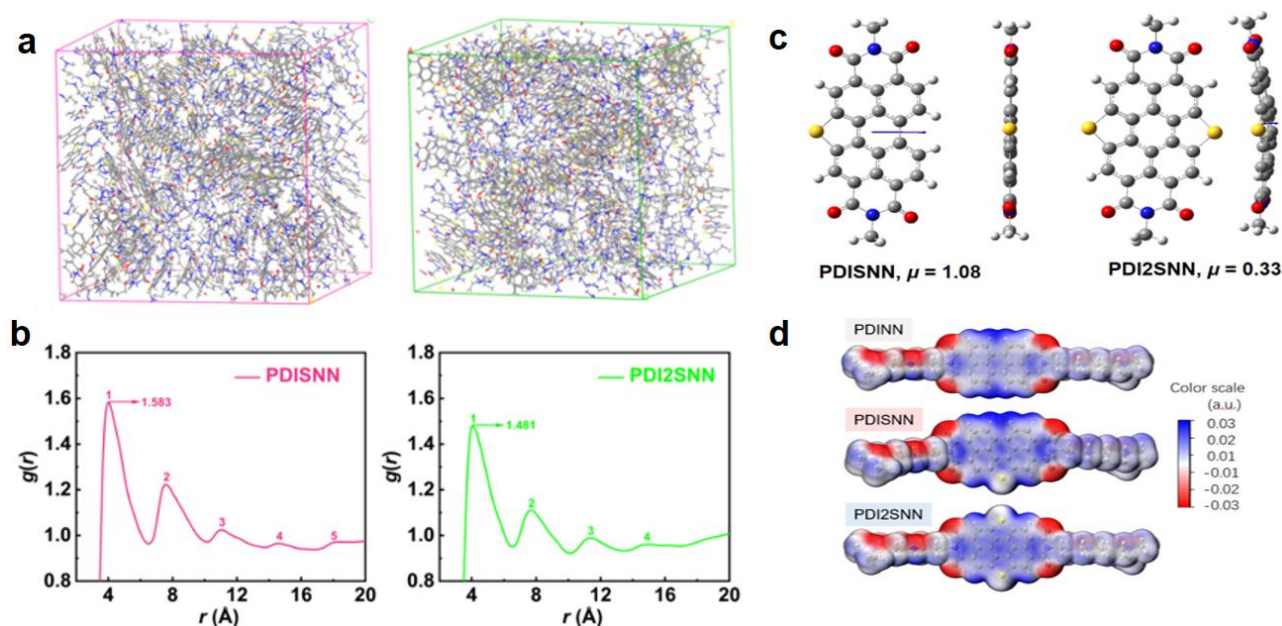
Supplementary Figure 5. The MALDI-TOF spectrum of PDI2SNN.



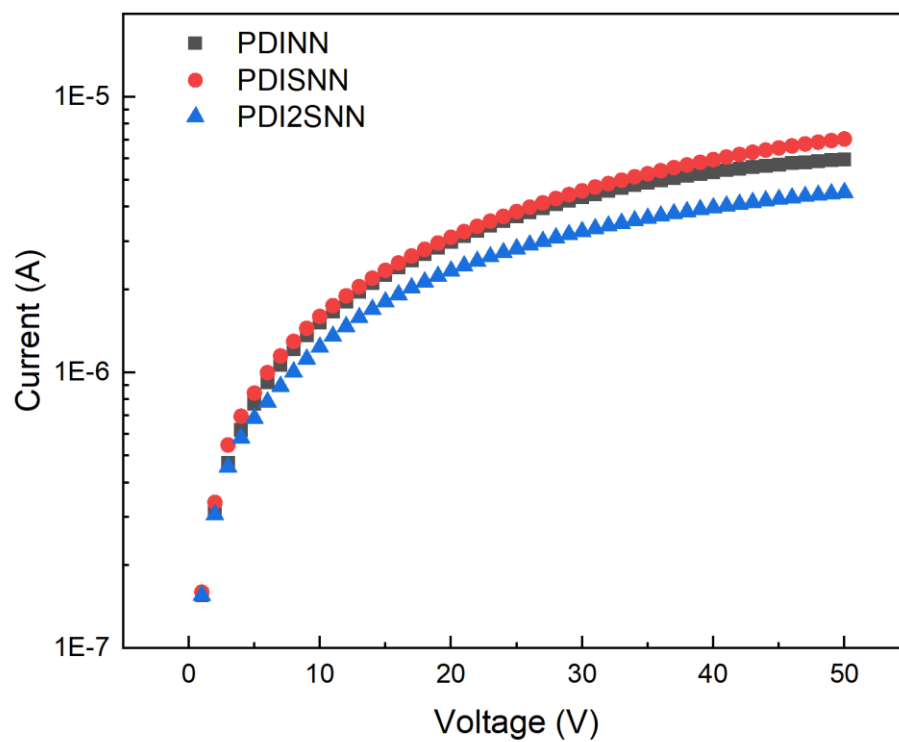
Supplementary Figure 6. Normalized absorption spectra of PDINN, PDISNN and PDI2SNN in dilute solution.



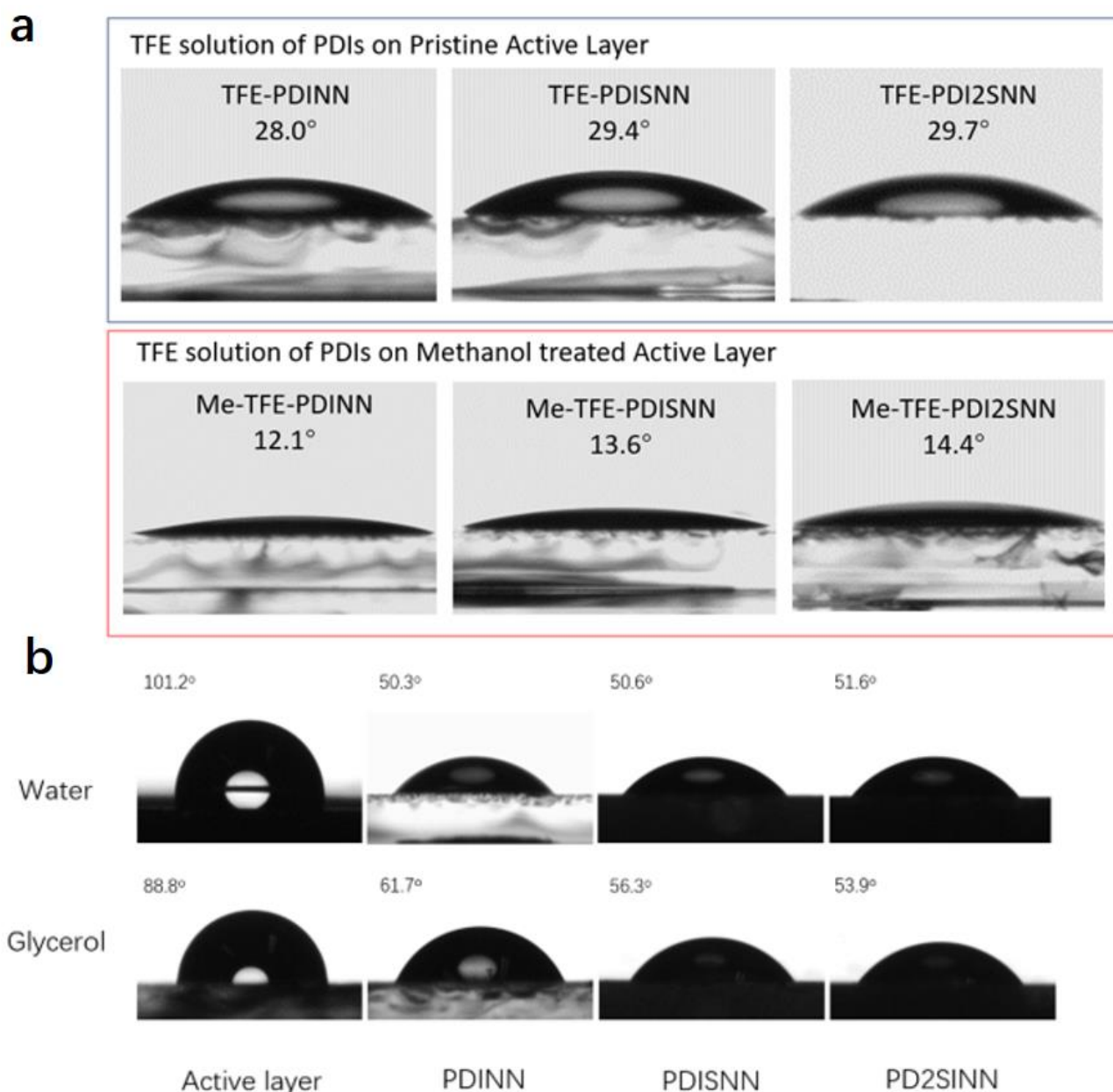
Supplementary Figure 7. 2D GIWAXS patterns of the PDIs fabricated by using different methods on silicon substrates. a, GIWAXS patterns of PDINN. **b,** GIWAXS patterns of PDISNN. **c,** GIWAXS patterns of PDI2SNN. **d,** The integrated scattering curves with different azimuthal angles for PDINN. **e,** The integrated scattering curves with different azimuthal angles for PDISNN. **f,** The integrated scattering curves with different azimuthal angles for PDI2SNN.



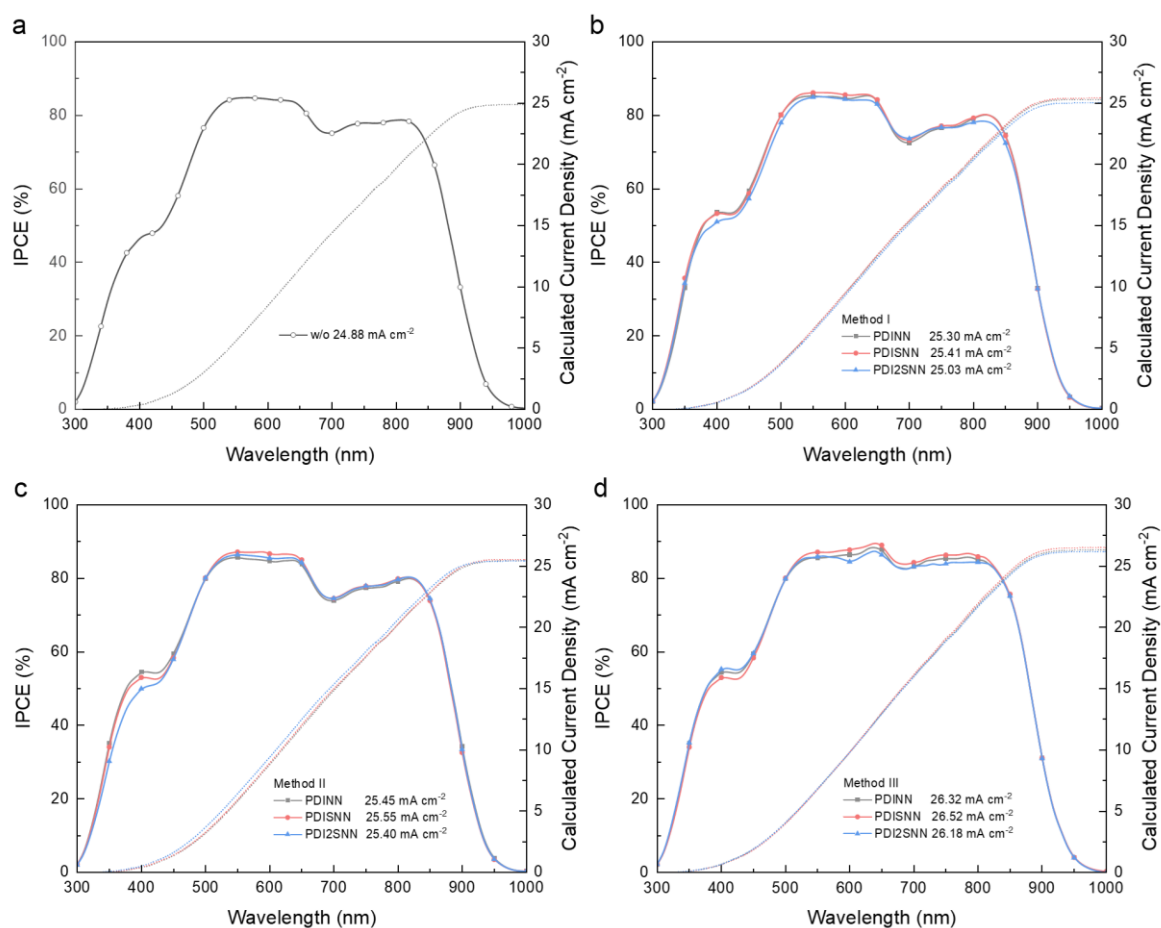
Supplementary Figure 8. MD simulation results. **a**, Snapshots of MD simulation molecular packing morphology of PDISNN and PDI2SNN. Extracted from MD-simulated PDISNN and PDI2SNN films, the intermolecular packing pairs numbered 266 and 249, respectively. The π - π stacking pairs were 92 (34.59%) for PDISNN and 75 (30.12%) for PDI2SNN, with corresponding interaction energies of -24.39 and -22.56 kcal/mol. **b**, The radial distribution function (RDF). **c**, The geometry and molecular dipole moment. **d**, ESP distribution of PDI-molecules. The RDF measures the variation in density (or probability of finding a particle) of particles as a function of distance from a reference particle. If ρ_{global} denotes the global density, the density at a local distance r is simply $\rho_{\text{global}} \cdot g(r)$. Therefore, with a similar ρ_{global} , a higher $g(r)$ peak corresponds to a larger intermolecular packing density. The first $g(r)$ peak corresponds to the nearest-neighbor packing, the second one to the next-nearest-neighbor packing, and so forth; the larger numbers of $g(r)$ peaks, the better film crystallinity.



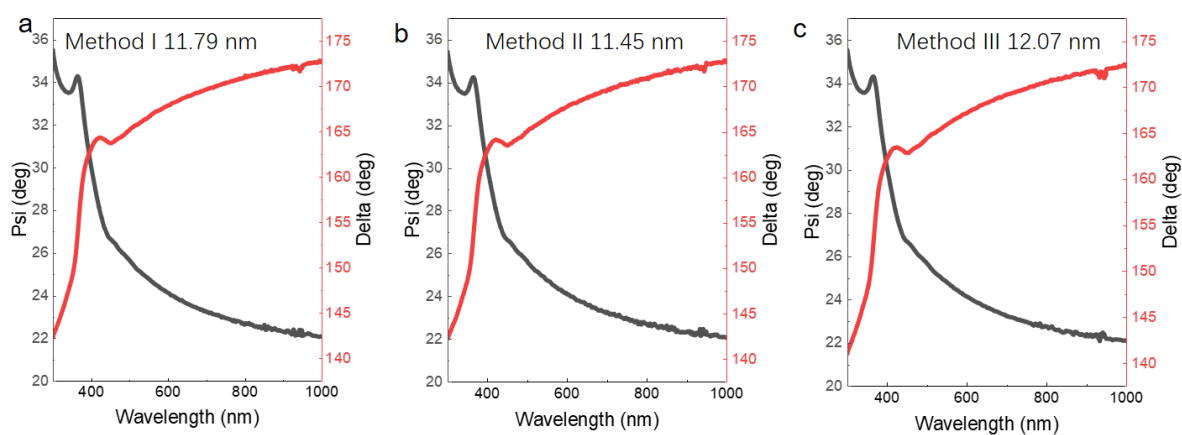
Supplementary Figure 9. Current–voltage measurements of these small-molecule thin films.



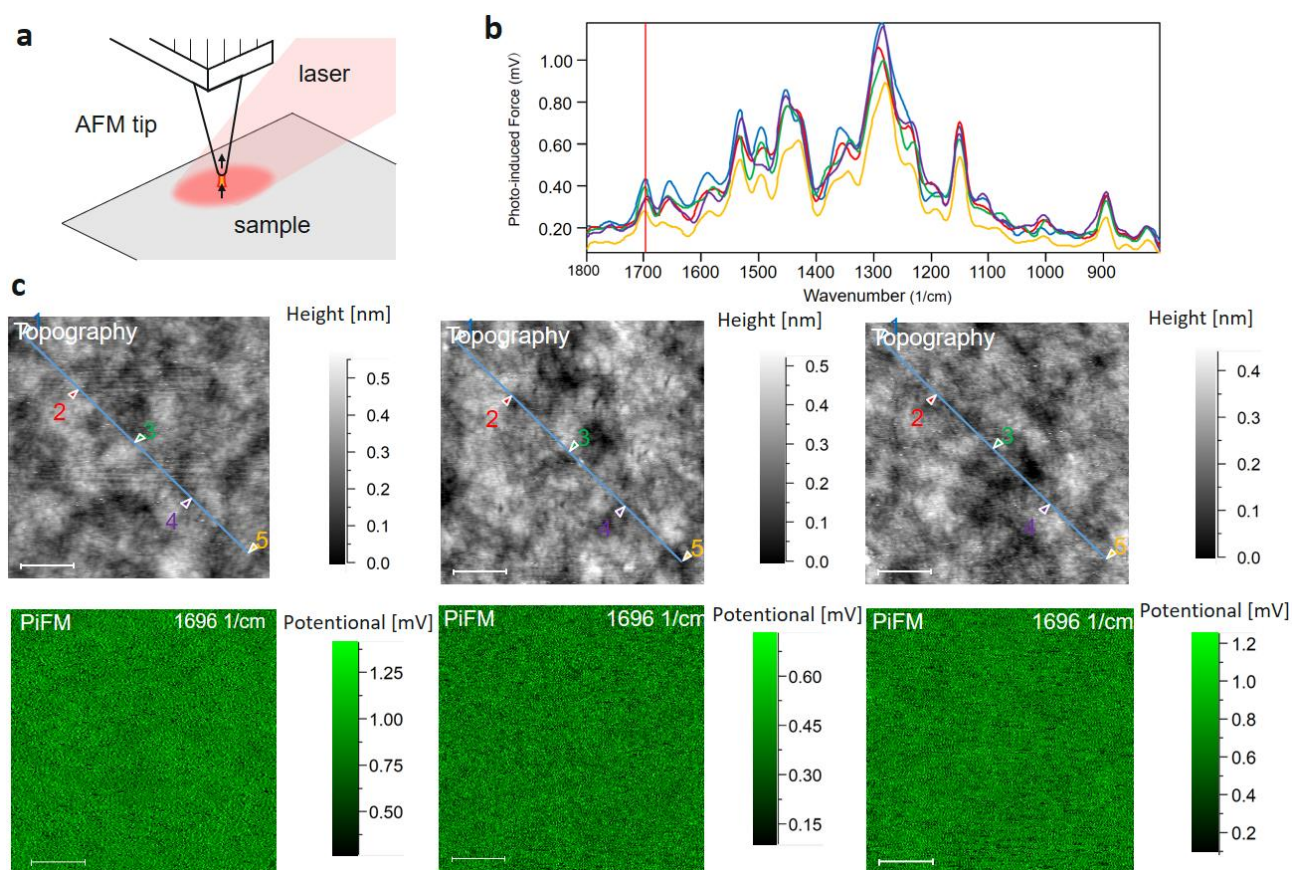
Supplementary Figure 10. Influence of methanol treatment on surface properties. a, Photographs of TFE solution droplets of PDIs on pristine active layer and on methanol treated active layer. **b,** Photographs of water (top row) and glycerol (bottom row) droplets in contact with the various surfaces. The measured surface energies of active layer, PDINN, PDISNN, PD2SINN, PM6, eC9 are 19.1, 57.3, 51.6, 48.9, 17.6, 25.0 mNm⁻¹.



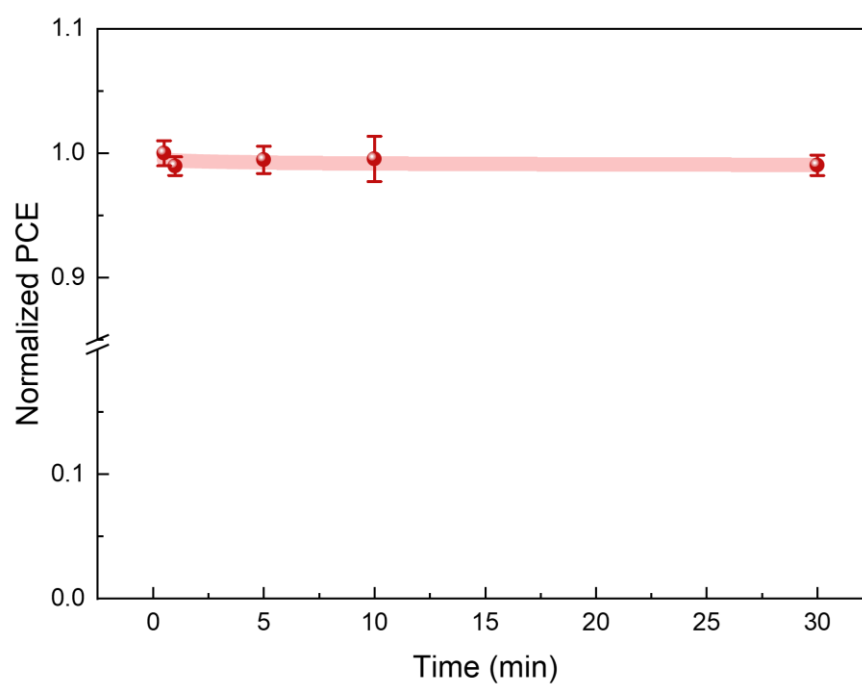
Supplementary Figure 11. IPCE spectra and integrated current densities of the devices. a, without PDI-interlayers. **b,** PDI-interlayers deposited via method I. **c,** PDI-interlayers deposited via method II. **d,** PDI-interlayers deposited via method III.



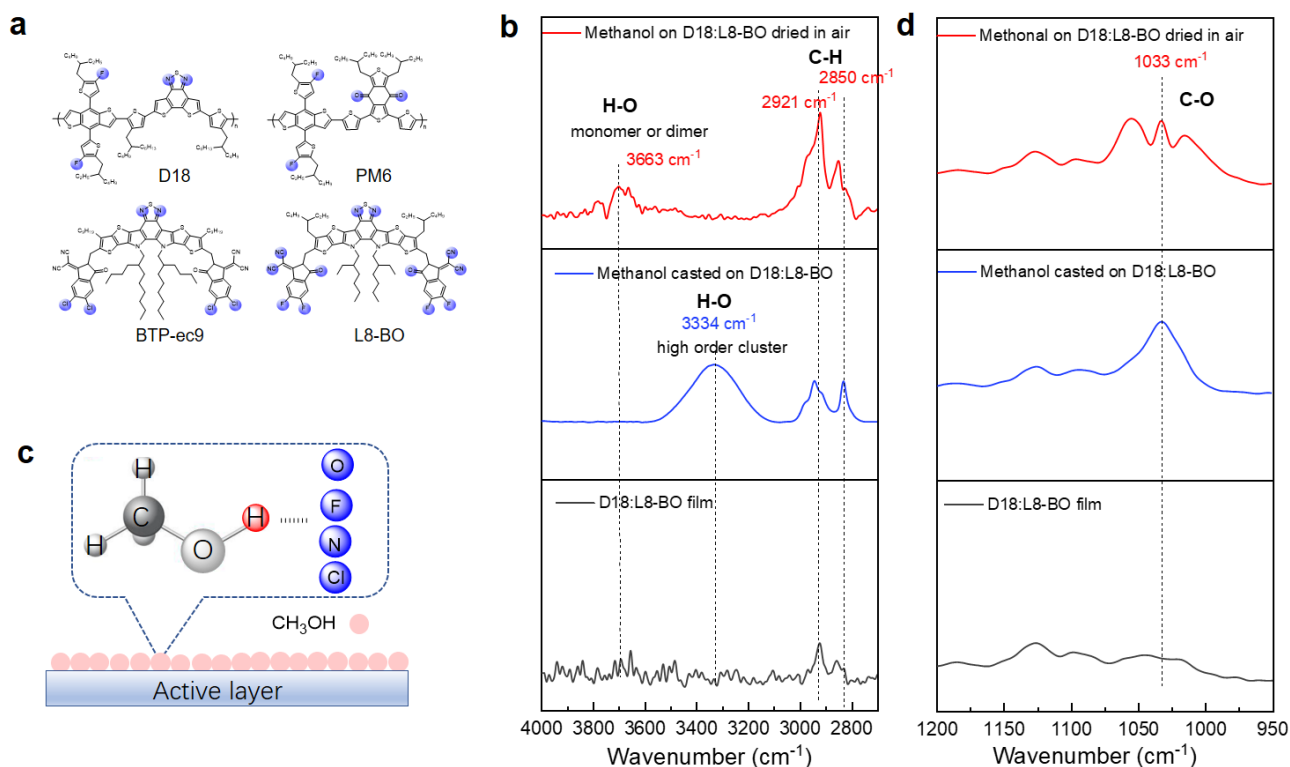
Supplementary Figure 12. Ellipsometry spectra of the samples. a, Prepared with method I. **b,** prepared with method II. **c,** Prepared with method III.



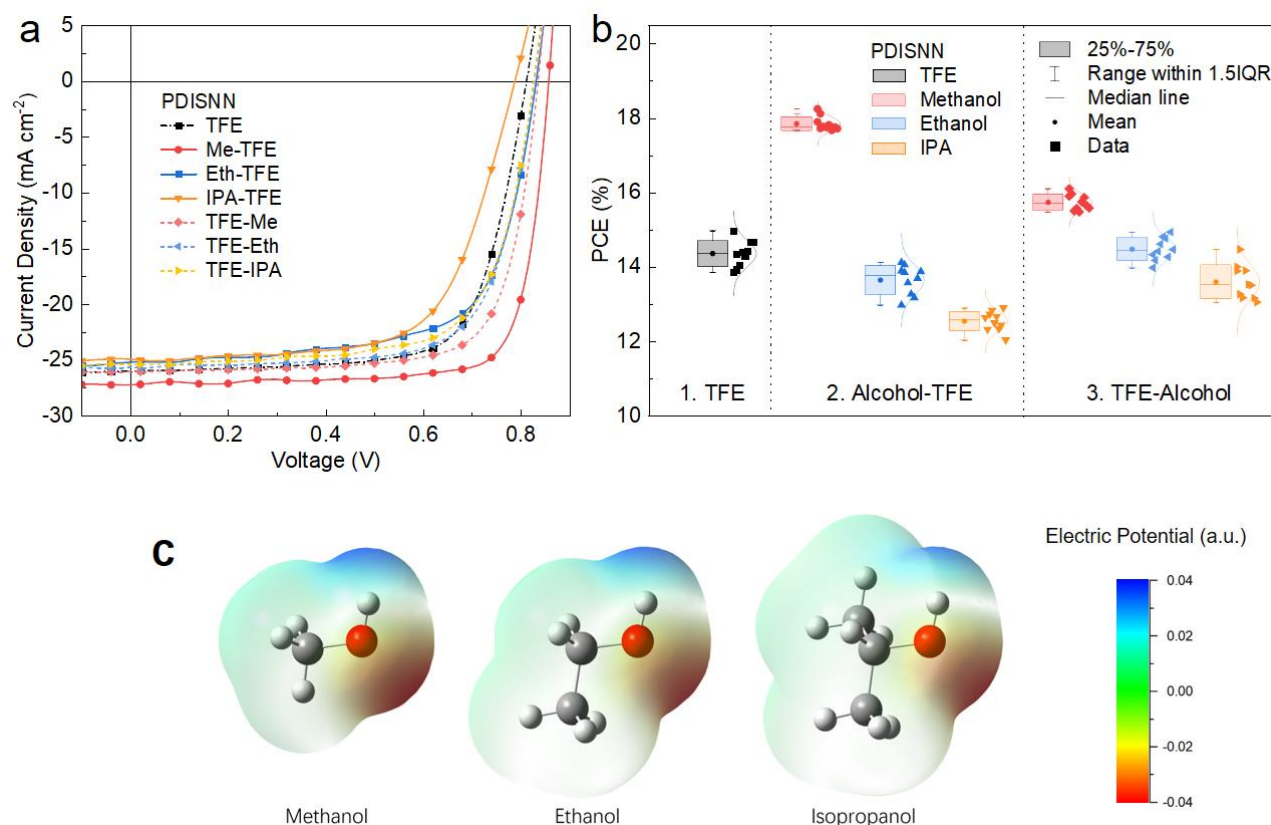
Supplementary Figure 13. Surface coverage. **a**, Illustration of the working mechanism of PIFM where an AFM tip is used to mechanically detect the force interaction between the tip and sample due to laser excitation. **b**, PiF-IR spectra of the interlayer. **c**, AFM image and PiFM images of the three samples fabricated with different method, PDI-molecules are marked with green in PiFM images. The scale bar is 200 nm.



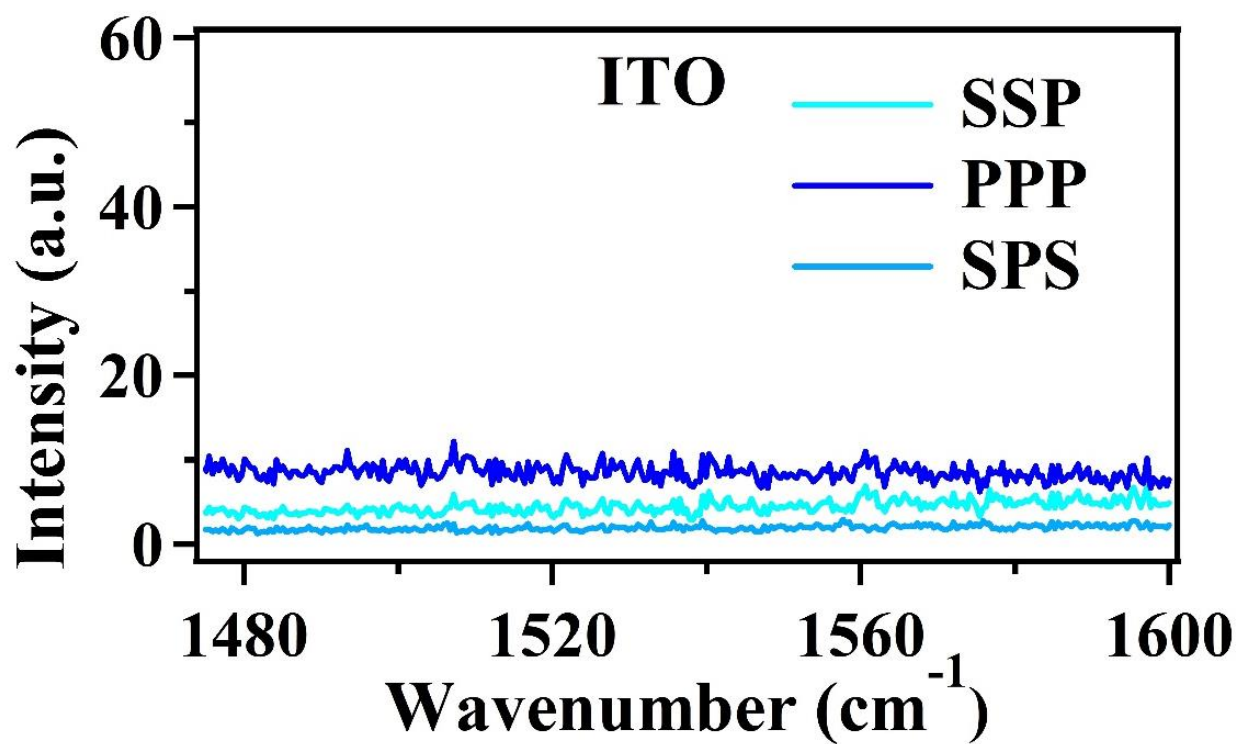
Supplementary Figure 14. The impact of the time interval between methanol pretreatment and spin-coating the TFE solution of CILs on the device performance. The error bars represent the standard error of the mean (n = 10)



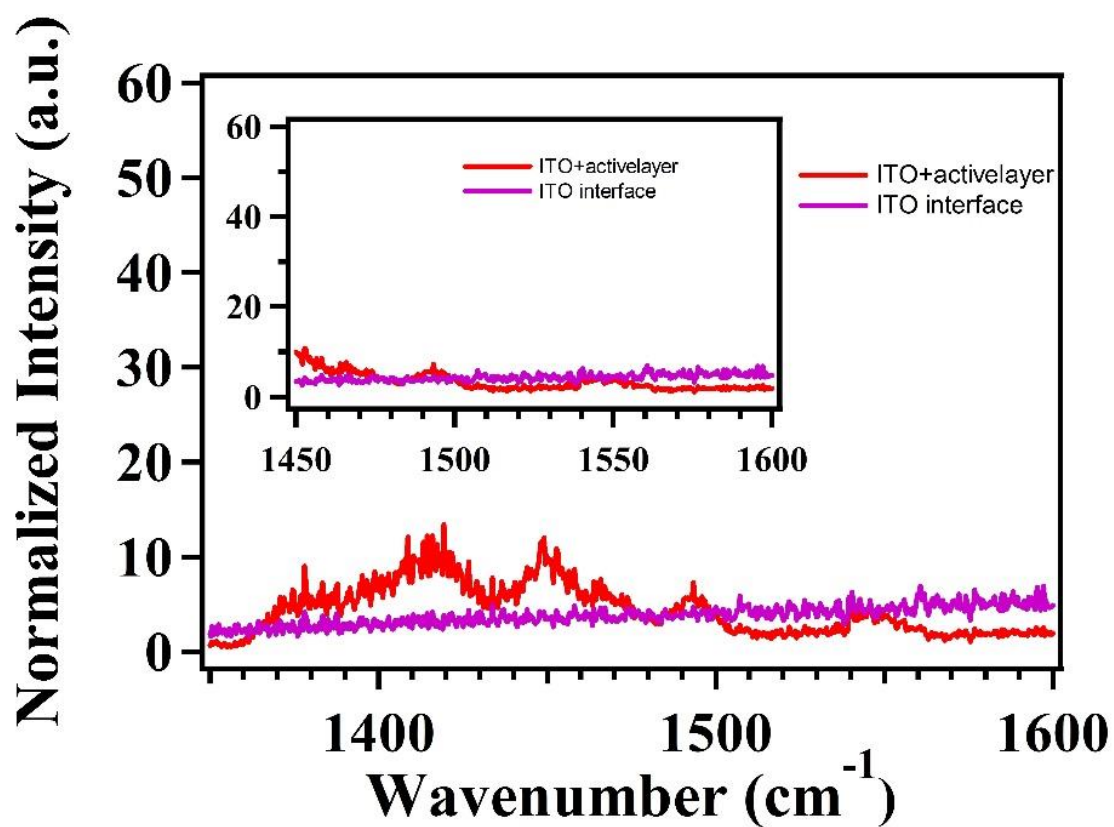
Supplementary Figure 15. Residual methanol on the active layer. **a**, Typical photovoltaic materials contain binding sites marked with blue for active hydrogen. **b**, FTIR-ATR spectroscopy of methanol modified D18:L8BO films in the range of 4000-2700 cm⁻¹. **c**, The schematic demonstrates how residual methanol, through hydrogen bonding to the active layer, serves as a template for the subsequent assembly of the PDI-interlayer. **d**, FTIR-ATR spectroscopy of methanol modified D18:L8BO films in the range of 1200-950 cm⁻¹.



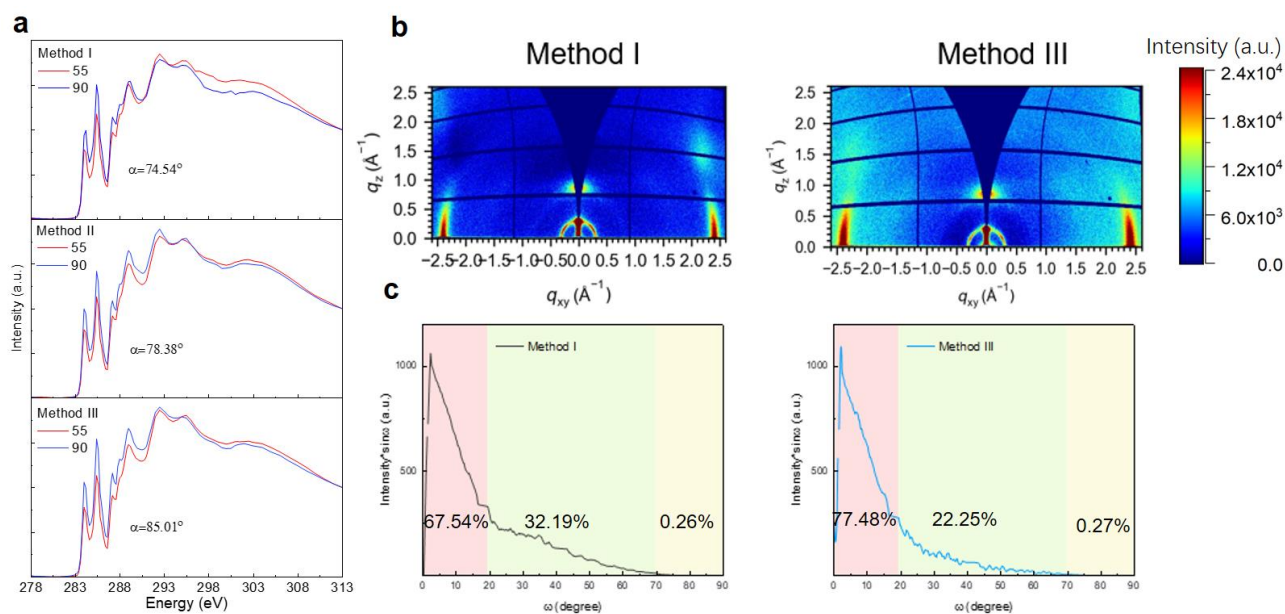
Supplementary Figure 16. Device performance of the active layer treated with different polar solvents. **a**, J - V curves of the corresponding OSCs under the illumination of AM 1.5G, 100 mW cm^{-2} . **b**, Comparison of PCE values distribution of devices based on PDISNN CILs that deposited through different methods represented as box plots. For the box plots, the central line represents the median, the bounds of the box represent the interquartile range (25th and 75th percentiles) and the whiskers extend to the minimum and maximum values within 1.5 times the interquartile range. Outliers are shown as individual points. **c**, The electric potentials of methanol, ethanol and isopropanol. Their corresponding derived rohrschneider's polarity parameters are 5.1, 4.3 and 3.9, respectively. The larger the value, the higher the polarity.



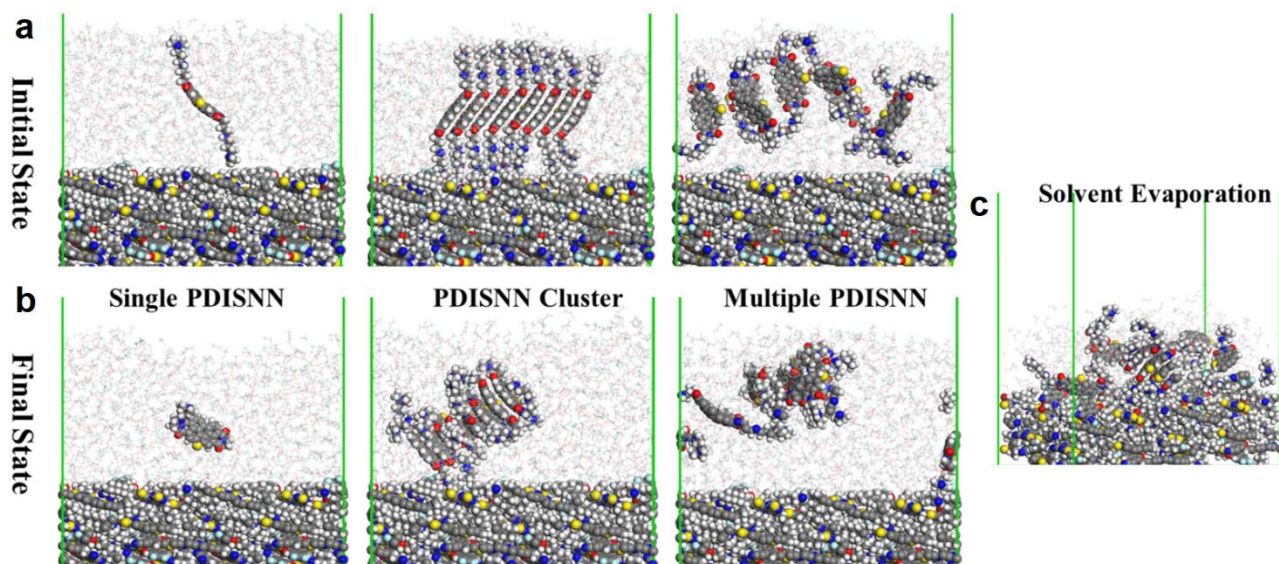
Supplementary Figure 17. Different polarization combination SFG spectra of the ITO substrate.



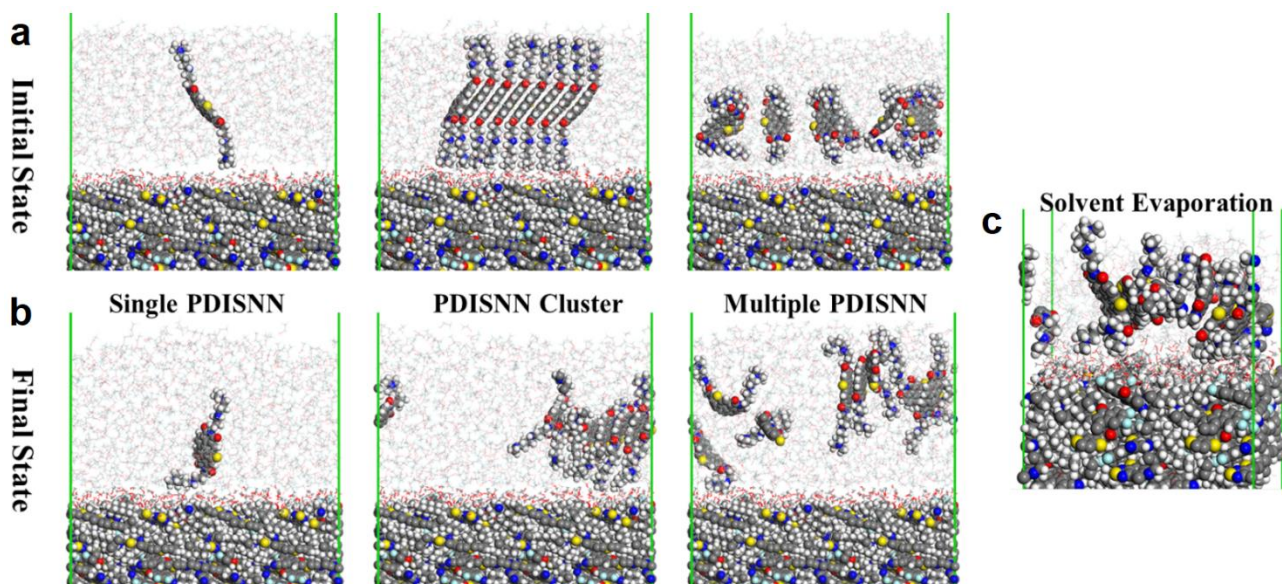
Supplementary Figure 18. SFG spectra of the ITO surface and ITO/active layer. The inset displays an expanded view of the spectrum between 1450 and 1600 cm⁻¹.



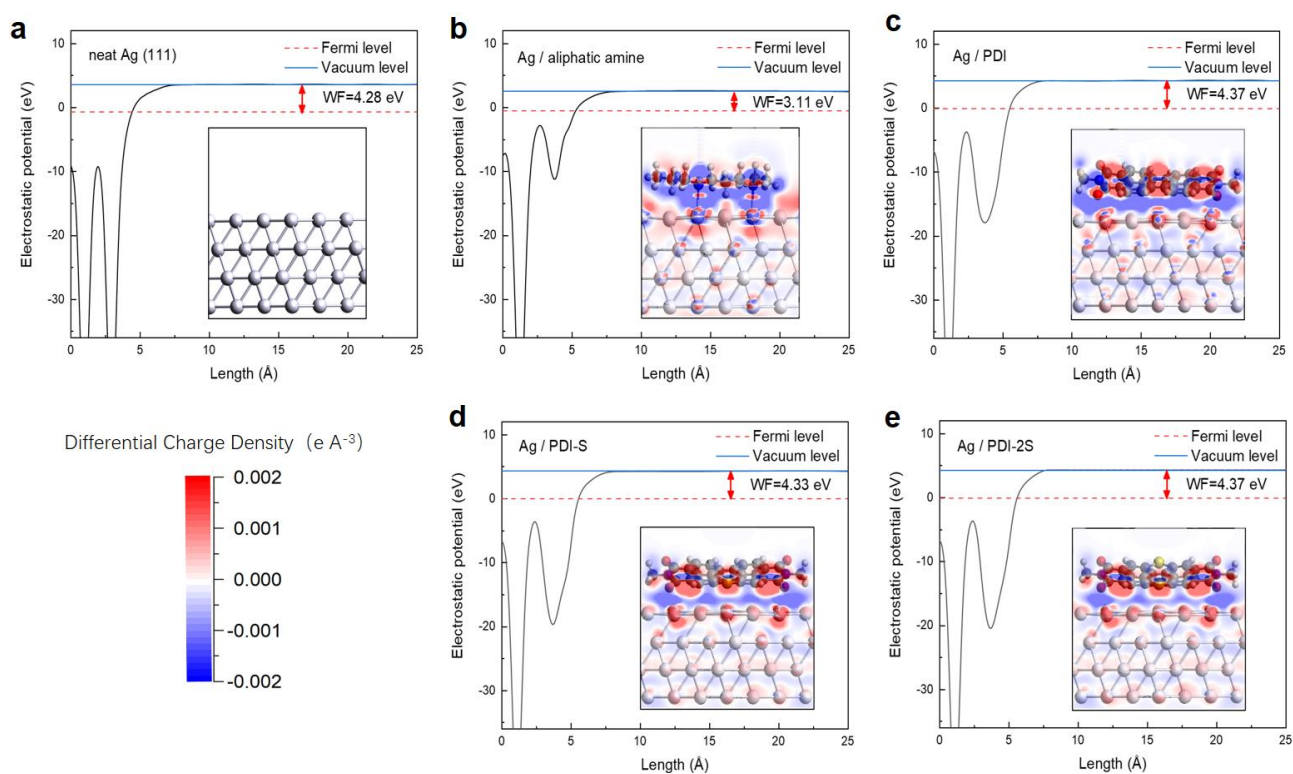
Supplementary Figure 19. Molecular orientation of the interlayers. **a**, Angle-dependent near-edge X-ray absorption fine structure for three different film deposition methods. **b**, 2-D GIWAXS patterns for samples prepared via Method I and Method III. **c**, The integrated orientation distribution for samples prepared via Method III. The summary of the integrated orientation distribution for each samples are indicated.



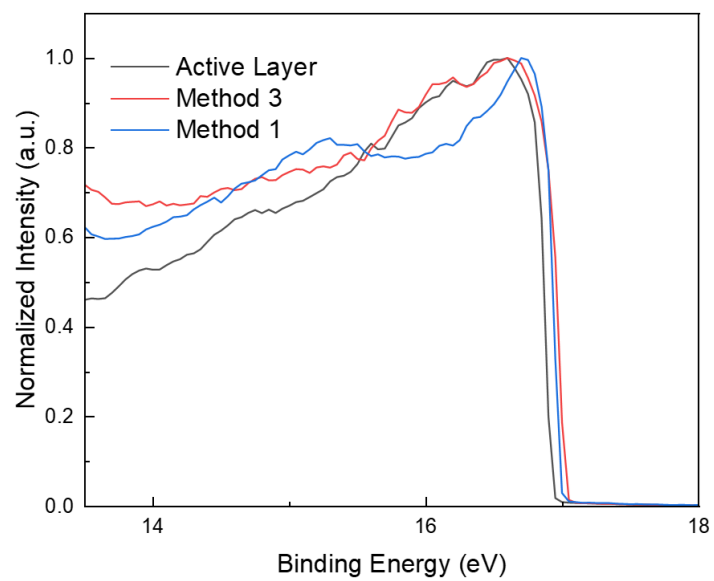
Supplementary Figure 20. MD simulation of PDISNN without methanol layer on the L8-BO substrate. **a**, Initial state of single molecule, molecular clusters and multiple molecules in the trifluoroethanol solution on the L8-BO substrate. **b**, Final state of single molecule, molecular clusters and multiple molecules in the trifluoroethanol solution on the L8-BO substrate. **c**, Most of the solvent molecules are evaporated for the final state of multiple molecules.



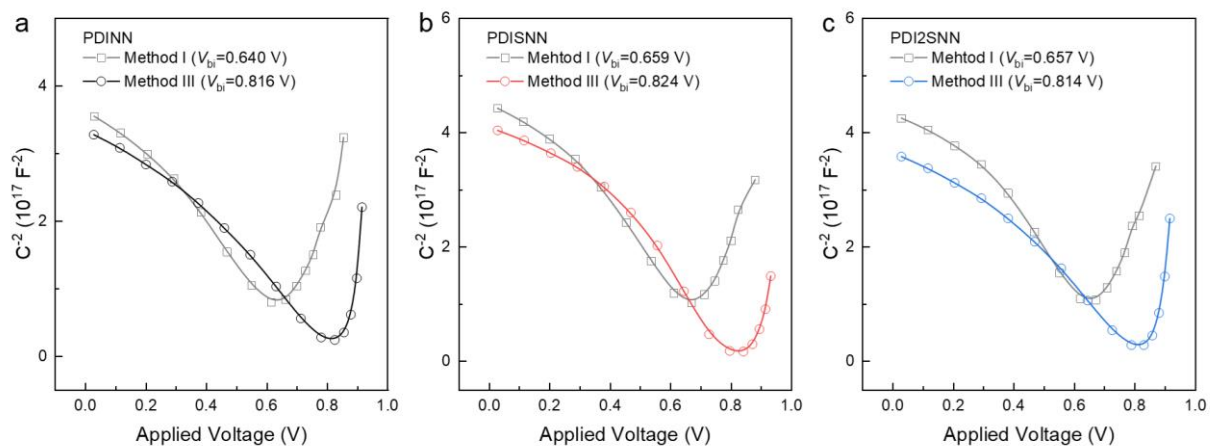
Supplementary Figure 21. MD simulation of PDISNN with methanol layer on the L8-BO substrate. **a**, The initial state of single molecule, molecular clusters and multiple molecules in the trifluoroethanol solution on the L8-BO substrate. **b**, The final state of single molecule, molecular clusters and multiple molecules in the trifluoroethanol solution on the L8-BO substrate. **c**, Most of the solvent molecules are evaporated for the final state of multiple molecules.



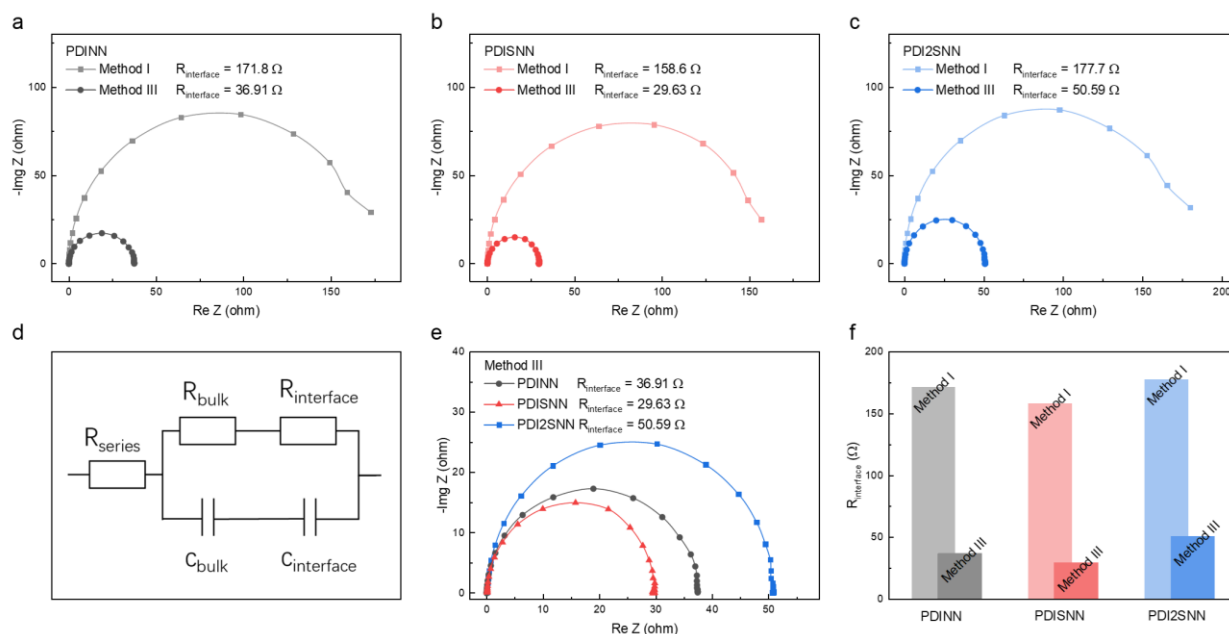
Supplementary Figure 22. The work functions of all models. **a**, neat Ag with four layers. **b**, NH-Ag system. **c**, PDI-Ag system. **d**, PDI-S-Ag system. **e**, PDI-2S-Ag system. The dashed line indicates the Fermi level, E_F . The insets display the electron density difference between different PDI-CIL fragments and silver, the blue and red regions represent electron depletion and accumulation, respectively



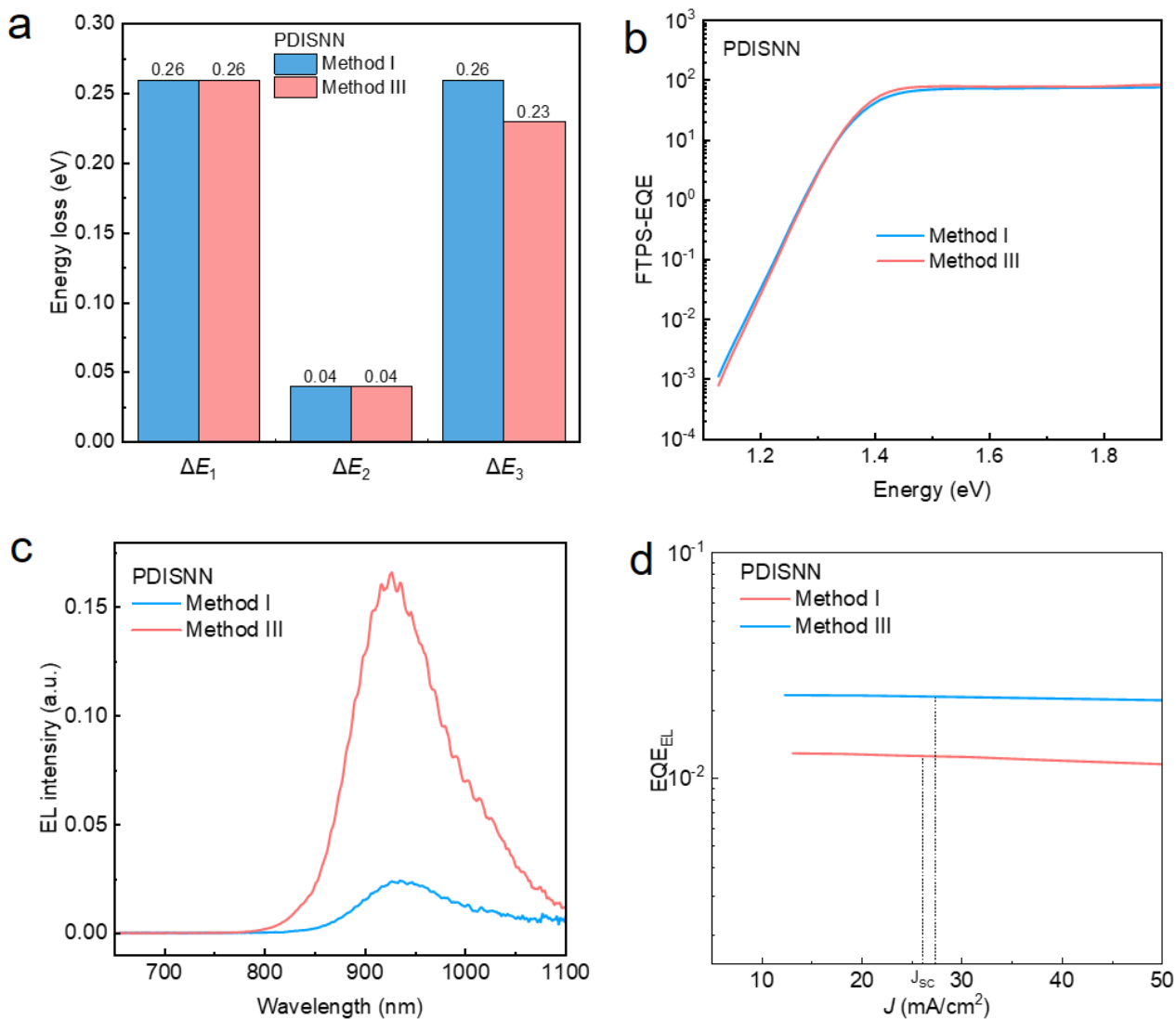
Supplementary Figure 23. Ultraviolet photoelectron spectroscopy for the samples under different fabrication methods.



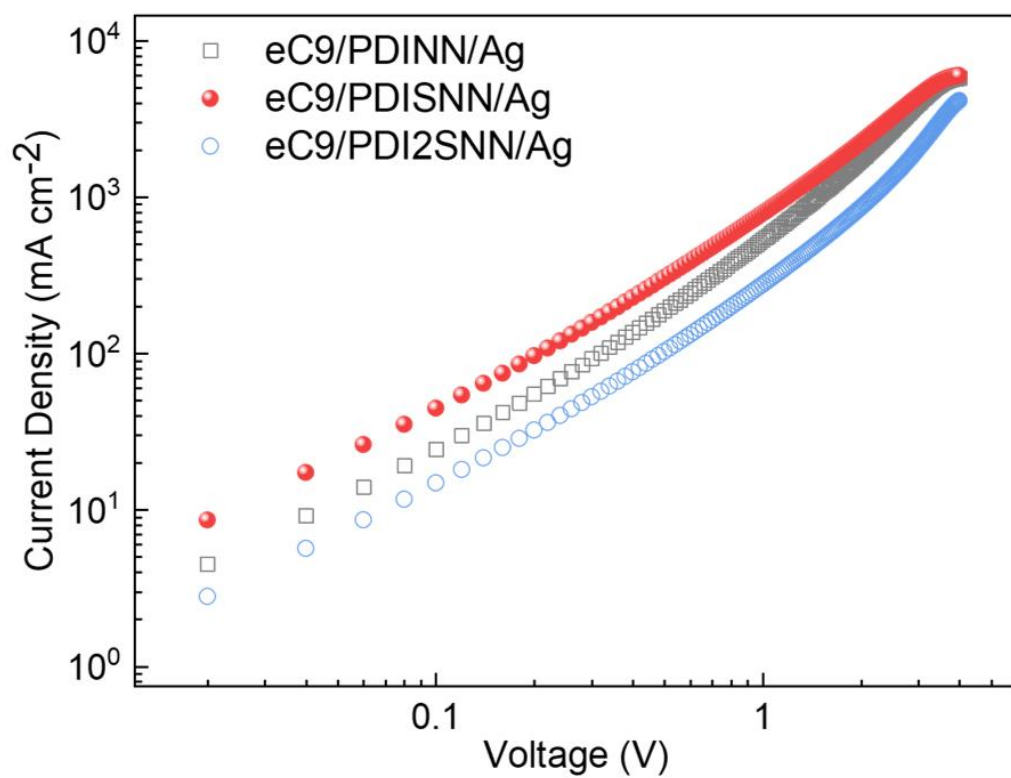
Supplementary Figure 24. Built-in potential measurement at 21.5 kHz in the dark. a, Mott-Schottky characteristics of the PDINN based devices. **b,** Mott-Schottky characteristics of the PDISNN based devices. **c,** Mott-Schottky characteristics of the PDI2SNN based devices.



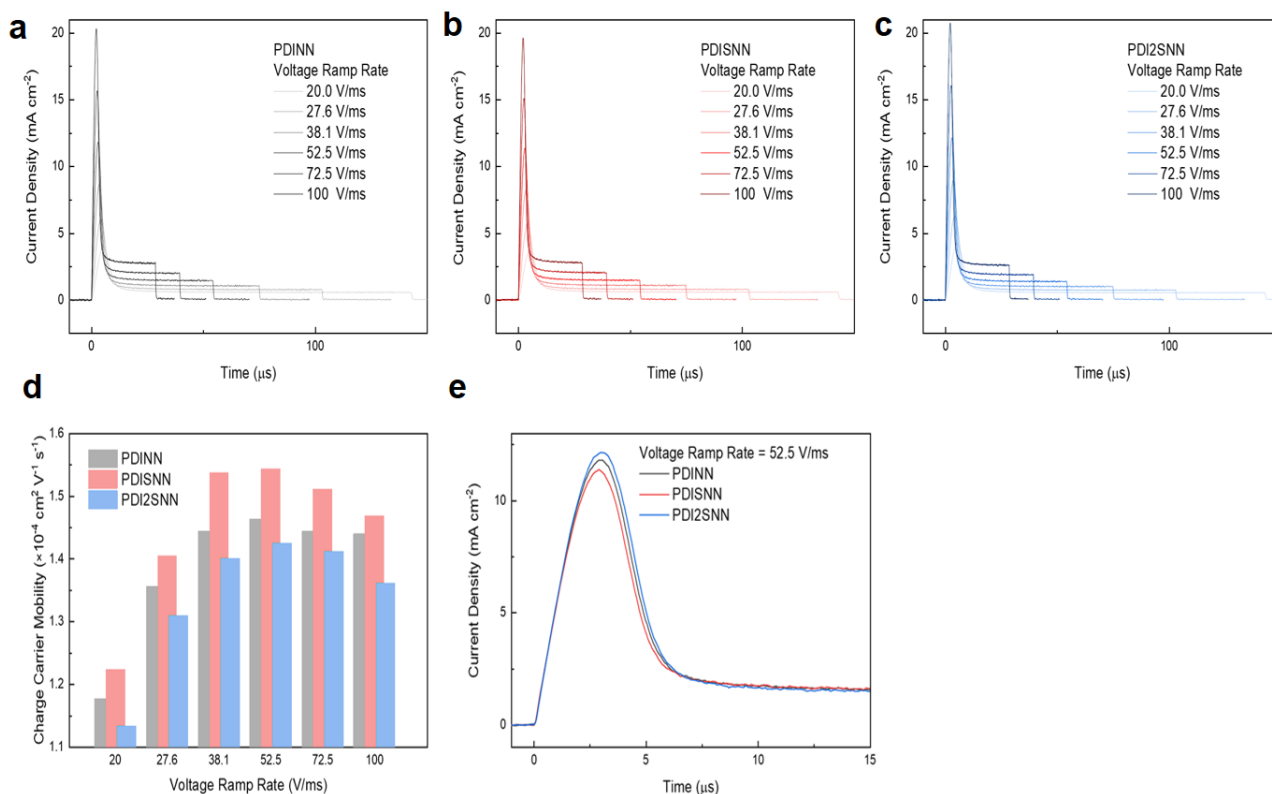
Supplementary Figure 25. Electrochemical impedance spectroscopy measurements of different PDIs interlayers. a, Nyquist plots of cells based on PDINN. **b**, Nyquist plots of cells based on PDISNN. **c**, Nyquist plots of cells based on PDI2SNN. **d**, Equivalent-circuit model fitted for impedance spectra. **e**, Comparison of the impedance spectra of cells based on three PDIs that were deposited through TFE solutions on methanol-treated active layer. **f**, Comparison of the interface resistance of corresponding CILs.



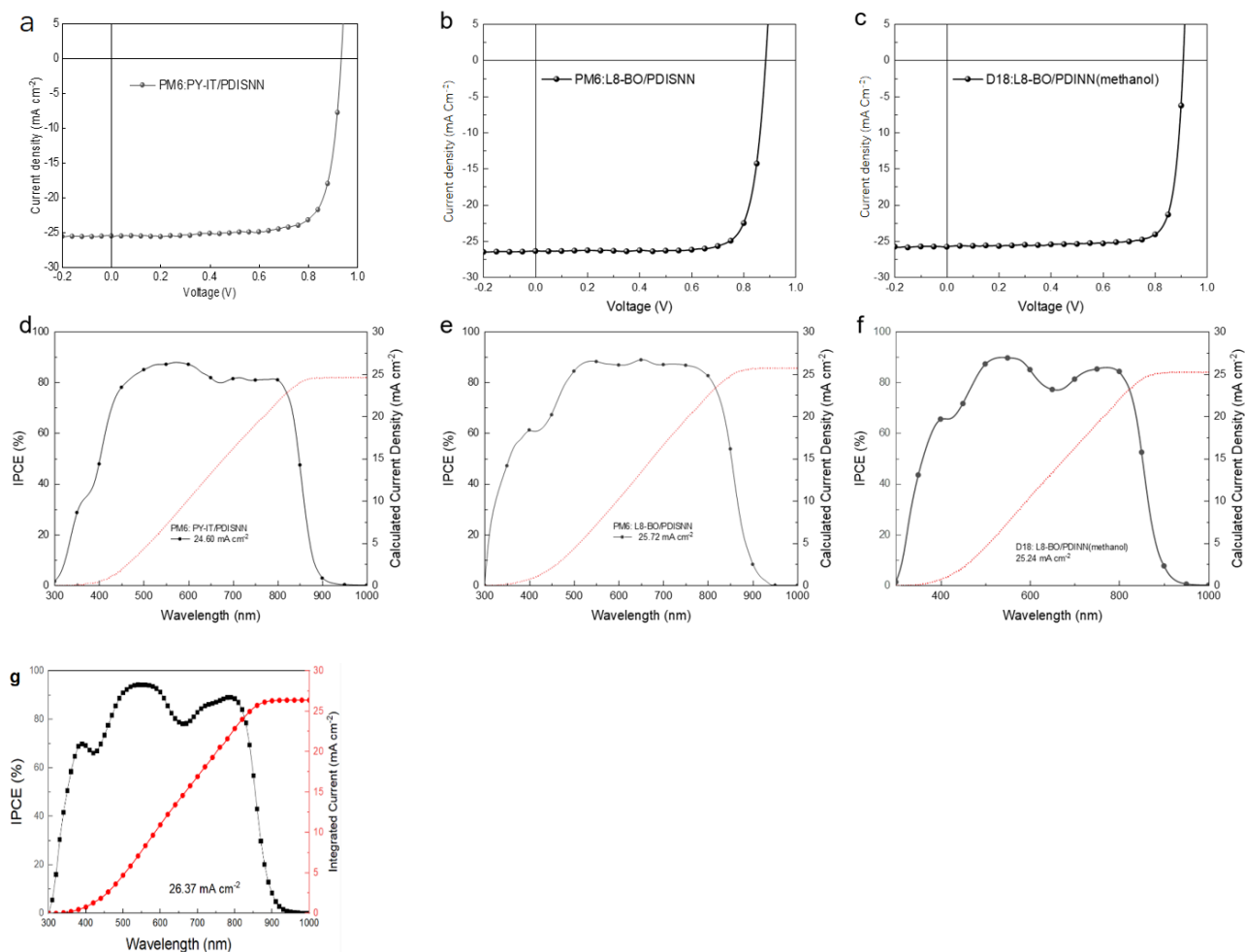
Supplementary Figure 26. Energy loss for method I and method III. **a**, Comparison of energy loss. **b**, FTPS-EQE curves. **c**, Electroluminescence intensity. **d**, EQE_{EL} curves of the devices based on PDISNN deposited through Method I and III. Given that Method I and Method III are exclusively based on a controlled active layer, we propose that the observed changes in V_{OC} losses primarily originate from the interface, specifically driven by the self-assembly behavior of the interlayer. Based on the observations, we propose that Method III promotes improved interfacial contact. The self-assembly of the interlayer on the active layer enhances the interfacial dipole, as confirmed by KPFM, effectively suppressing nonradiative recombination and energy loss. This work also underscores the critical role of interfacial engineering in modulating nonradiative recombination and energy loss, offering valuable insights for optimizing the performance of OSCs.



Supplementary Figure 27. J - V curves of electron-only devices.



Supplementary Figure 28. Photo-CELIV measurements of the OSCs. **a**, Photo-CELIV curves of the OSCs based on PDINN at different voltage ramp rate. **b**, Photo-CELIV curves of the OSCs based on PDISNN at different voltage ramp rate. **c**, Photo-CELIV curves of the OSCs based on PDI2SNN at different voltage ramp rate. **d**, Histogram and summary of calculated fast carrier mobilities of PDIs-based cells at different voltage ramp rate. **e**, The expanded view of the Photo-CELIV curves at voltage ramp rate of 52.5 V/ms.



Supplementary Figure 29. Device performance. **a**, $J-V$ curve of PM6: PYIT. **b**, $J-V$ curve of PM6: L8BO with method I. **c**, $J-V$ curve of PM6: L8BO method III. **d**, IPCE spectra of PM6: PYIT. **e**, IPCE spectra of PM6: L8BO with method I. **f**, IPCE spectra of PM6: L8BO with method III. **g**, IPCE spectra and integrated current densities of D18: L8BO devices with method III.



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Organic Solar Cells
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MODEL/TYPE D18: L8-B0/PDISNN
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Beijing University of Chemical
Technology
委托单位
APPLICANT



Wuxi Institute of Inspection, Testing and Certification

国家太阳能光伏产品质量检验检测中心

National Center of Inspection on Solar Photovoltaic Products Quality

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无锡市检验检测认证研究院

Wuxi Institute of Inspection, Testing and Certification

国家太阳能光伏产品质量检验检测中心

National Center of Inspection on Solar Photovoltaic Products Quality

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国家太阳能光伏产品质量检验检测中心
National Center of Inspection on Solar Photovoltaic Products Quality
无锡市检验检测认证研究院
Wuxi Institute of Inspection, Testing and Certification
检验检测报告
TEST REPORT

No: 2025DMWA20739

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产品名称 Sample Description	有机太阳能电池 Organic Solar Cells	规格型号 Model/Type	D18: L8-B0/PDISNN
标称生产单位 Nominal Producer	—	商 标 Trade Mark	—
委托单位名称/地址/邮编 Applicant Name Add./P.C.	北京化工大学\北京市朝阳区 北三环东路15号\— Beijing University of Chemical Technology\15, North Third Ring East Road, Chaoyang District, Beijing, China\—		
样品数量 Sample Quantity	3片(其中2片备样) 3 pieces (2 spare samples)	样品状态 Condition of Sample	符合检验要求 Commission Test
标称生产日期/批号 Nominal Date of Production /Lot No.	—/—	样品接收日期 Date of Sample Receiving	2025-04-30
检验检测日期 Testing Date(s)	2025-04-30	检验检测地点 Testing Location	本机构·新华路 CPVT·Xinhua Road
检验检测依据 Test In Accordance With	IEC 60904-1:2020 Photovoltaic devices-Part 1: Measurement of photovoltaic current-voltage characteristics		
判定依据 Decide In Accordance With	—		
检验结论 Conclusion	—		
备 注 Remarks:	—		

批准: 王美娟
Approved by 王美娟

审核: 曹月娟
Reviewed by 曹月娟

主检: 蒋非洲
Tested by 蒋非洲

No:2025DMWA20739

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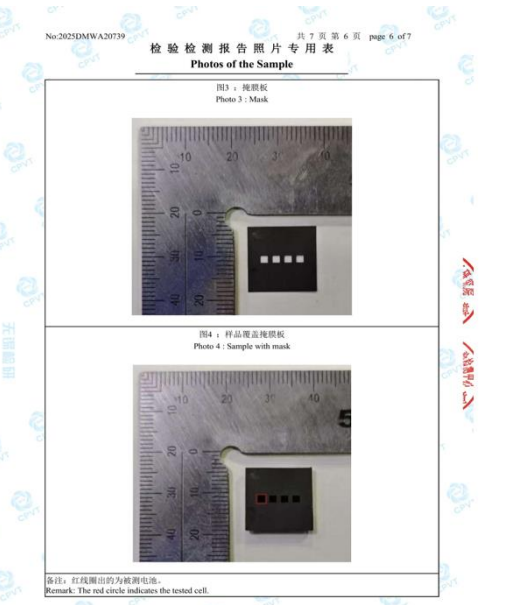
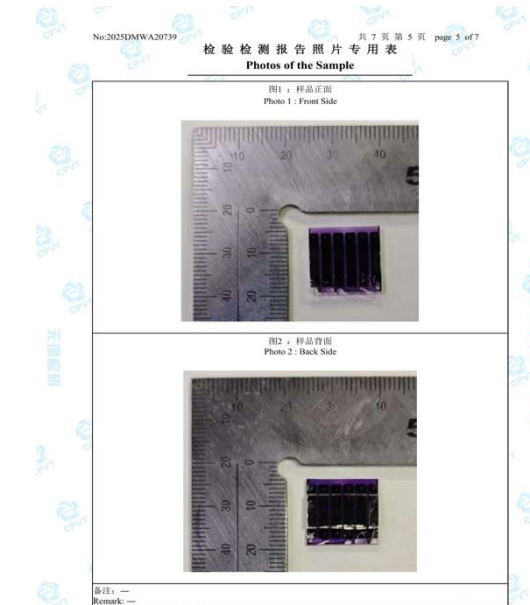
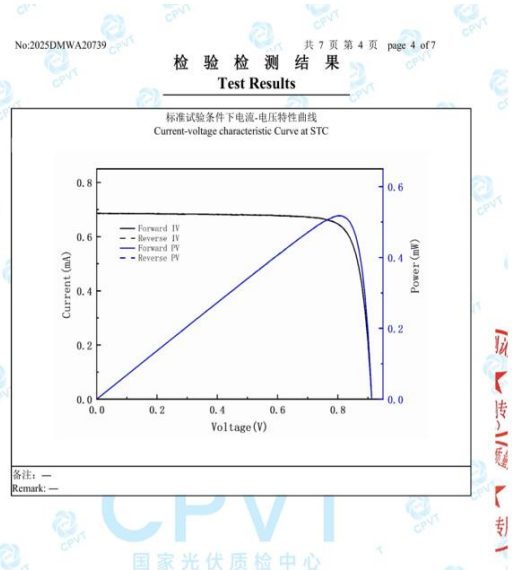
检验检测结果

Test Results

序号 Clause	检验项目 Test Item(s)	单位 Unit	技术要求 Technical requirements	结果 Results	单项评价 Verdict Pass/Fail
1	电流-电压特性的测量 (正扫) Current-voltage characteristic measurement (Forward scan)	—	在标准试验条件下(样品温度: 25℃±2℃, 辐照度: 1000W/m², 标准太阳光谱辐照度分布符合 IEC 60904-3 规定), 测量样品随负荷变化的电流-电压特性。 At STC (module temperature: 25℃±2℃, irradiance: 1000W/m², standard solar spectral irradiance distribution corresponds to IEC60904-3), measure the current-voltage characteristics of the cell with the variation of load.	—	—
1.1	开路电压 Voc Open-circuit voltage, Voc	V	—	0.9123	—
1.2	短路电流 Isc Short-circuit current, Isc	mA	—	0.6864	—
1.3	最大功率 Pmax Maximum-power, Pmax	mW	—	0.5180	—
1.4	最大功率点电压 Vmp Maximum-power voltage, Vmp	V	—	0.8100	—
1.5	最大功率点电流 Imp Maximum-power current, Imp	mA	—	0.6395	—
1.6	填充因子 FF, % Fill factor FF, %	—	—	82.72	—
1.7	转换效率 η, % Conversion efficiency η, %	—	$\eta = \frac{P_{max}}{1000W/m^2 \times S} \times 100\%$ S为掩膜板面积/Area S is determined by mask	20.65	—

备注: 1.测试过程中引入光谱失配修正, 光谱失配修正因子为: 1.011
2.正扫描方向为-0.2V~1V, 步进 0.01V, 延迟时间: 0s; 短路电流密度 $J_{sc} = \frac{I_{sc}}{S} = 27.37 \text{ mA/cm}^2$, 计算短路电流密度及转换效率所用面积为掩膜板面积, S=2.508 mm²。
Remark: 1.The test process takes into account spectra mismatch correction.The spectra mismatch correction factor is 1.011.
2.Forward sweep direction: -0.2V~1V, step: 0.01V, delay time: 0s. $J_{sc} = \frac{I_{sc}}{S} = 27.37 \text{ mA/cm}^2$
The area used to calculate J_{sc} and Conversion efficiency is determined by mask, S=2.508 mm².

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检 验 检 测 结 果					
Test Results					
序号 Clause	检验项目 Test item(s)	单位 Unit	技术要求 Technical requirements	结果 Results	单项评价 Verdict Pass/Fail
2	电流-电压特性的测量 (反扫) Current-voltage characteristic measurement (Reverse Scan)	—	在标准试验条件下 (样品温度: 25℃±2℃, 辐照度: 1000W/m ² , 标准太阳光谱辐照分布符合 IEC 60904-3 规定), 测量样品随负载 变化的电流-电压特性。 At STC (module temperature: 25℃±2℃, irradiance: 1000W/m ² , standard solar spectral irradiance distribution corresponds to IEC60904-3), measure the current- voltage characteristics of the cell with the variation of load.	—	—
2.1	开路电压 Voc Open-circuit voltage, Voc	V	—	0.9121	—
2.2	短路电流 Isc Short-circuit current, Isc	mA	—	0.6856	—
2.3	最大功率 Pmax Maximum-power, Pmax	mW	—	0.5171	—
2.4	最大功率点电压 Vmp Maximum-power voltage, Vmp	V	—	0.8000	—
2.5	最大功率点电流 Imp Maximum-power current, Imp	mA	—	0.6464	—
2.6	填充因子 FF, % Fill factor FF, %	—	—	82.69	—
2.7	转换效率 η, % Conversion efficiency η, %	—	$\eta = \frac{P_{max}}{1000W/m^2 \times S} \times 100\%$ S 为掩膜板面积/Area S is determined by mask	20.62	—
备注: 1.测试过程中引入光谱失配修正, 光谱失配修正因子为: 1.011 2.反扫扫描方向为 1V~0.2V, 步速: 0.01V, 延迟时间: 0s; 短路电流密度 $J_{sc} = \frac{I_{sc}}{S} = 27.34 \text{ mA/cm}^2$, 计算短路电流密度及转换效率所用面积为掩膜板面积, S=2.508 mm ² . Remark: 1. The test process takes into account spectra mismatch correction. The spectra mismatch correction factor is 1.011. 2. Reverse sweep direction: 1V~0.2 V, step: 0.01V, delay time: 0s, $J_{sc} = \frac{I_{sc}}{S} = 27.34 \text{ mA/cm}^2$ The area used to calculate J_{sc} and Conversion efficiency is determined by mask, S=2.508 mm ² .					



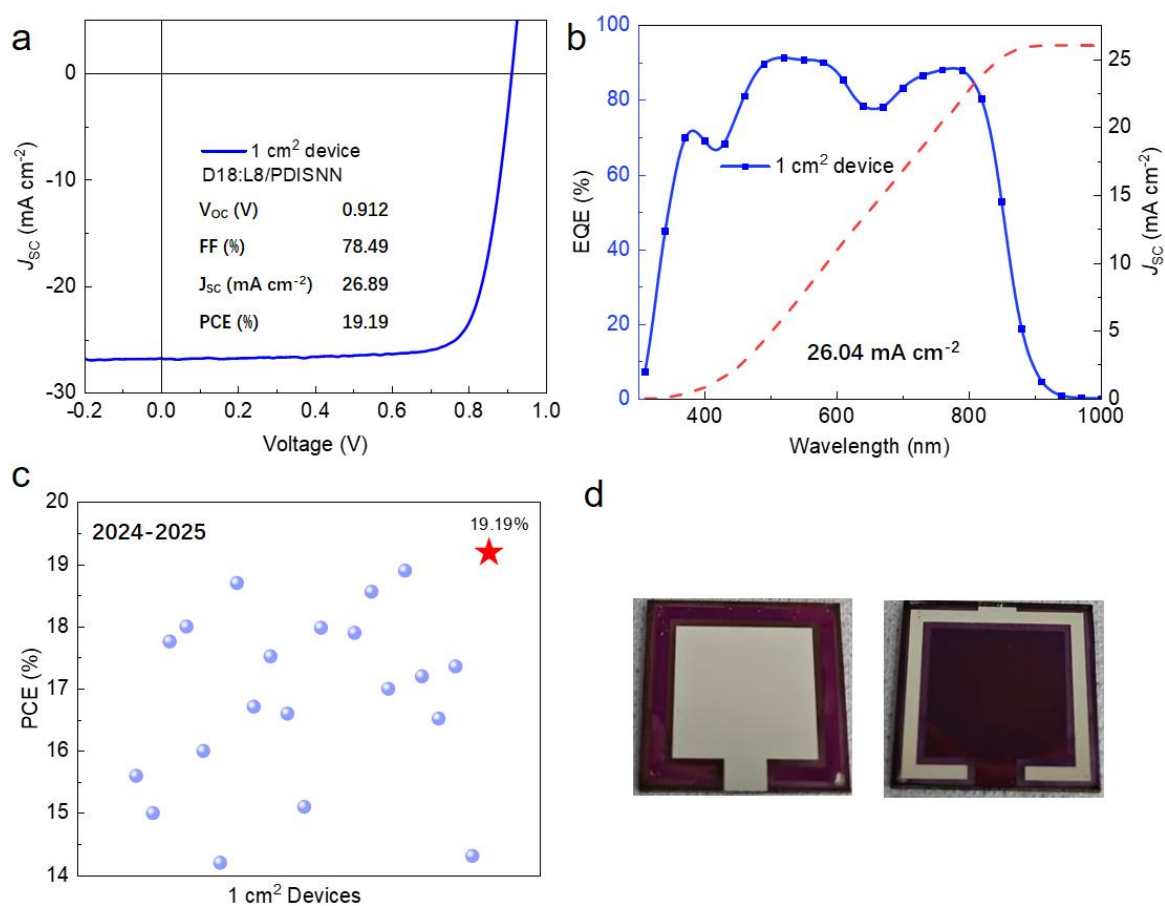
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附录 1: 试验仪器设备清单
Annex 1: List of measurement equipment

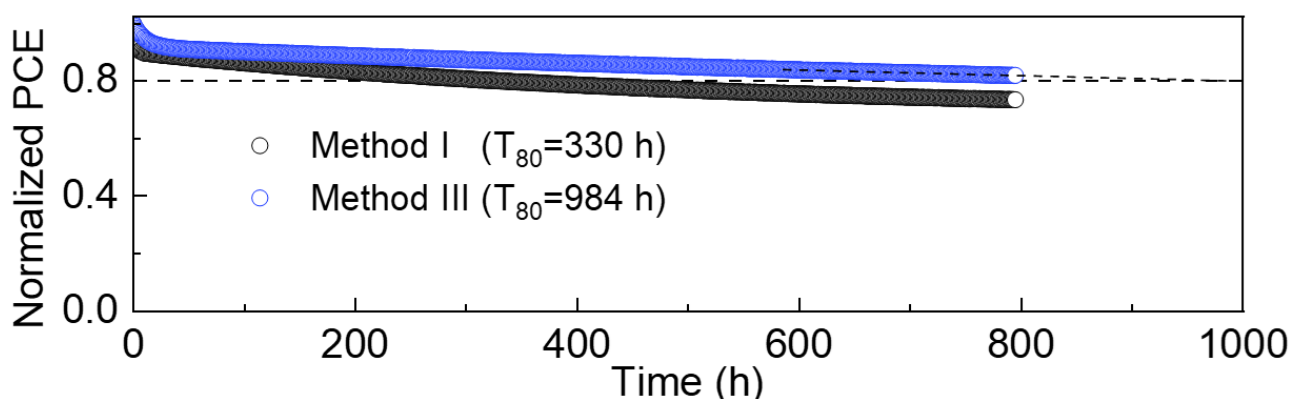
序号 No.	仪器设备名称 Equipment	编号 Code	设备有效期至 Calibration Expire Date
1	稳态太阳辐射模拟器 Steady state solar Simulator	0121-07	2025-12
2	数字源表 Digital source meter	EV21-40	2025-09

注: 测试期间, 所有仪器、设备均在校准有效期内。
NOTE: During test date, all the equipment are in the calibration date.

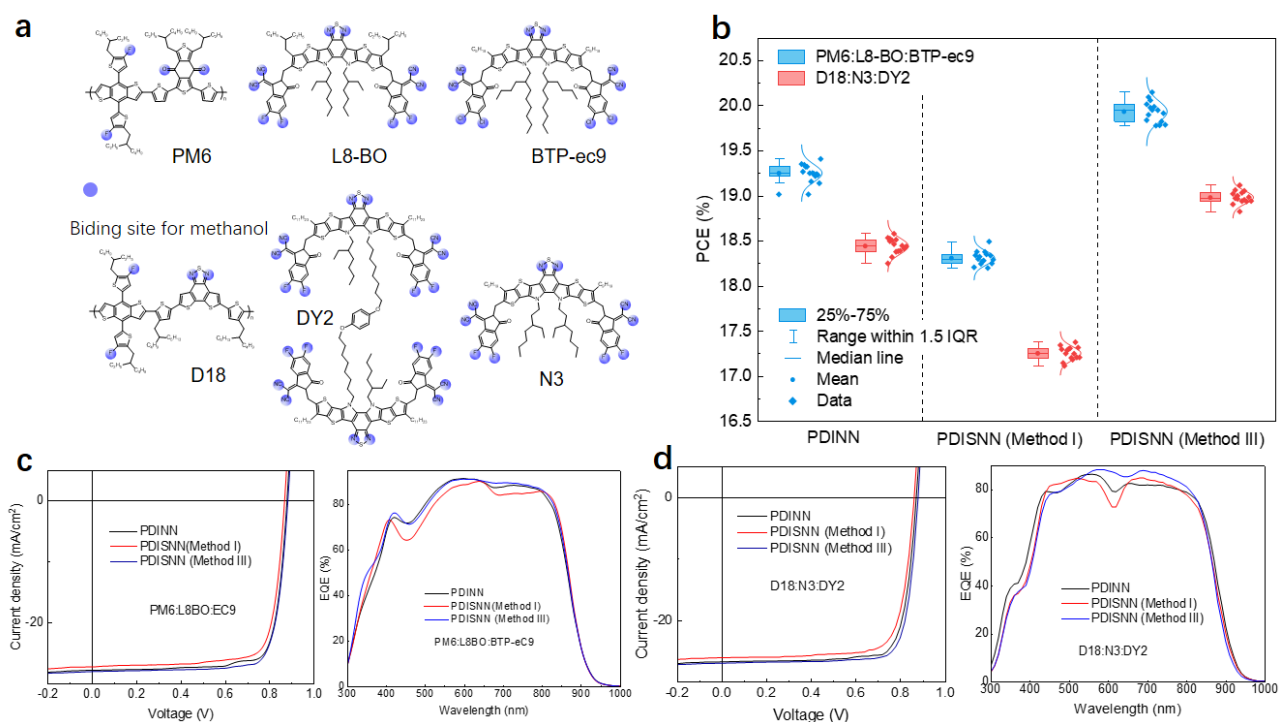
Supplementary Figure 30. Scanning copy of the certified efficiency for the D18: L8-BO/PDISNN based device from National Center of Inspection on Solar Photovoltaic Products Quality



Supplementary Figure 31. Device performance of 1-cm² device of D18:L8-BO devices fabricated by method III. a, J-V curves. b, EQE curves. c, Summary of reported high PCEs of large area binary devices (1 cm²). d, Photograph of the 1-cm² device.



Supplementary Figure 32. Enhanced operational stability achieved by Method III compared to Method I. The long-term stability of encapsulated devices was evaluated using a multi-channel solar cell performance decay test system (PVL-6001M-32A, Suzhou D&R Instruments Co. Ltd.) at a simulated intensity of 100 mW cm^{-2} (spectral region: 410–850 nm). In our test, the glass encapsulated devices were exposed to continuous white LED light (D&R Light, L-W5300KA-150, Suzhou D&R Instruments Co. Ltd.) while being stored in the air at approximately 25°C , with the MPP recalibrated every hour based on the measured J–V characteristic curves. The initial illumination intensity was adjusted to match the J_{SC} measured under standard conditions by AM1.5G. The initial efficiencies are 15.5% for the device prepared by method I and 20.4% for the device prepared by method III.



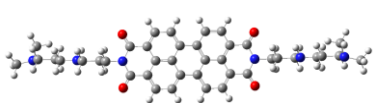
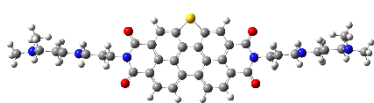
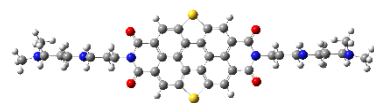
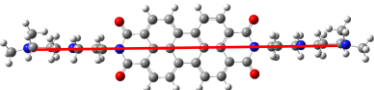
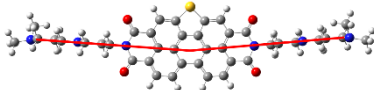
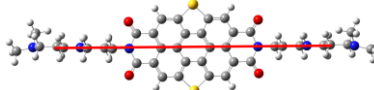
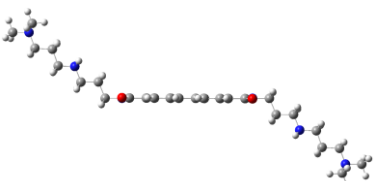
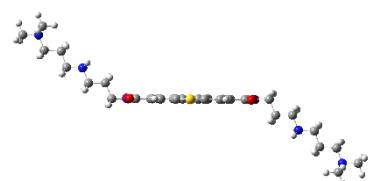
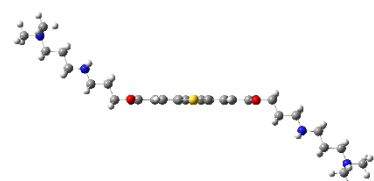
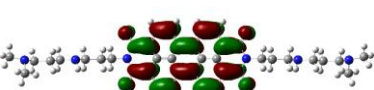
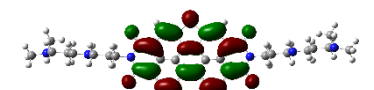
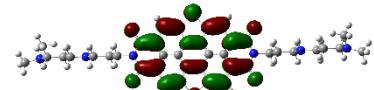
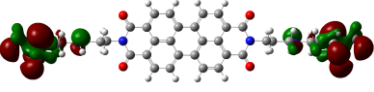
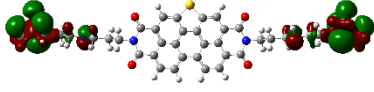
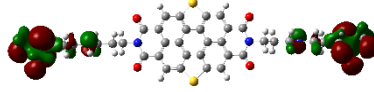
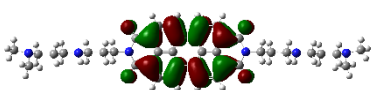
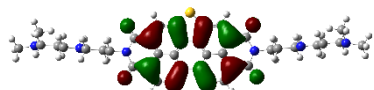
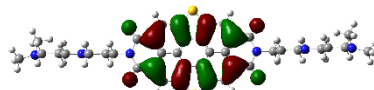
Supplementary Figure 33. Ternary devices. **a**, Molecular structures used in ternary devices. **b**, Comparison of PDISNN-based cathode interlayer performance with and without methanol pretreatment, and against the methanol-treated PDINN benchmark. For the box plots, the central line represents the median, the bounds of the box represent the interquartile range (25th and 75th percentiles) and the whiskers extend to the minimum and maximum values within 1.5 times the interquartile range. Outliers are shown as individual points. **c**, Champion J–V characteristics of PM6:L8BO:BTP-Ec9 (1:1:0.2, w/w) with 2PACz as interlayer. **d**, Champion J–V characteristics of D18:N3:DY2 (1:1:0.3, w/w) with PEDOT: PSS as interlayer under simulated AM 1.5G solar light (100 mW cm⁻²) and their corresponding EQE curves.

Supplementary Table

Supplementary Table 1. Summary of d-spacing (Å) and CCL length (Å) for PDIs in in-plane and out-of-plane directions.

In-Plane		q (Å ⁻¹)	d-spacing (Å)	CCL length (Å)
π - π stacking	PDINN	1.755	3.58	41.35
	PDISNN	1.811	3.47	50.41
	PDI2SNN	1.745	3.60	43.12
Out-of-Plane		q (Å ⁻¹)	d-spacing (Å)	CCL length (Å)
Lamellar stacking	PDINN	0.288	21.80	149.24
	PDISNN	0.298	21.04	119.55
	PDI2SNN	0.301	20.87	52.12

Supplementary Table 2. Molecular structures of PDINN, PDISNN and PDI2SNN. Their Geometries are optimized by Gaussian 09 at B3LYP/6-31G (d, p) level.

	PDINN	PDISNN	PDI2SNN
Front View			
Angle	 180°	 171° “V”type	 180°
Side View			
Dihedral	0.11° 0.15°	S side 0.02° Other side 0.07°	0.02 ° 0.02 °
LUMO	 -3.45 eV	 -3.42 eV	 -3.46 eV
HOMO & HOMO-1	 -5.63 eV	 -5.63 eV	 -5.63 eV
HOMO-2	 -5.98 eV	 -6.14 eV	 -6.31 eV
Optical gap	2.53 eV	2.72 eV	2.85 eV

Supplementary Table 3. the impact of the time interval between methanol pretreatment and spin-coating the TFE solution of CILs on the device performance.

Active layer	Time (min)	V_{oc} [V]	FF [%]	J_{sc} [mA cm ⁻²]	PCE [%]
PM6: L8-BO	0.5	0.885	78.49	26.37	18.32 [18.08±0.16]
	1	0.884	77.30	26.50	18.10 [17.94±0.13]
	5	0.882	78.72	26.41	18.32 [17.98±0.20]
	10	0.888	78.98	26.38	18.50 [18.00±0.29]
	30	0.880	78.24	26.48	18.23 [17.96±0.15]

Supplementary Table 4 Photovoltaic parameters of devices based on PDISNN-CIL that was deposited through different methods, measured under the illumination of AM 1.5G at 100 mW cm⁻². Average values and standard deviation data were calculated from 10 devices.

CILs	Method	V_{oc} [V]	FF [%]	J_{sc} [mA cm ⁻²]	PCE [%]	
PDISNN	TFE	0.81	71.06	25.98	14.98	[14.36±0.35]
	Methanol-TFE	0.85	78.40	27.23	18.25	[17.85±0.19]
	Ethanol-TFE	0.83	67.50	25.19	14.12	[13.65±0.37]
	IPA-TFE	0.79	65.38	24.93	12.87	[12.54±0.25]
	TFE-Methanol	0.83	74.04	26.01	16.04	[15.74±0.20]
	TFE-Ethanol	0.83	70.47	25.65	15.00	[14.48±0.29]
	TFE-IPA	0.83	69.12	25.37	14.47	[13.59±0.44]

Supplementary Table 5. Photovoltaic parameters of devices (PM6: Y6) based on PDINN that was deposited through different methods, measured under the illumination of AM 1.5G at 100 mW cm⁻². Average values and standard deviation data were calculated from 8 devices.

CIL	Method	V_{oc} [V]	FF [%]	J_{sc} [mA cm ⁻²]	PCE [%]
PDINN	Methanol	0.855	74.94	25.69	16.46
	<i>n</i> -hexane	0.747	68.12	24.97	12.71

Supplementary Table 6. Energy loss for method I and method III.

Devices	E_g (eV)	qV_{OC}^{SQ} (eV)	qV_{OC}^{rad} (eV)	ΔE_1 (eV) ΔV_{OC}^{SQ}	ΔE_2 (eV) ΔV_{OC}^{rad}	ΔE_3 (eV) $\Delta E_{non-rad}$	ΔE_{total} (eV)	eV_{OC} (eV) calculated
Method III	1.38	1.12	1.08	0.26	0.04	0.23	0.53	0.85
Method 1	1.38	1.12	1.08	0.26	0.04	0.26	0.56	0.82

Supplementary Table 7. Summarized certified parameters.

FF (%)	PCE (%)	Ref.
78.35	19.24	4
76.3	20.0	5
79.8	19.0	6
79.16	18.93	7
80.5	18.93	8
79.56	20.1	9
79.0	18.7	10
81.0	17.9	11
79.5	18.45	12
79.92	19.57	13
79.3	19.45	14
80.31	19.54	15
82.01	20.16	16
82.2	20.4	17
80.9	20.5	17

Supplementary Table 8. Photovoltaic parameters of PM6:L8BO:BTP-Ec9 (1:1:0.2, w/w) with 2PACz as interlayer and D18:N3:DY2 (1:1:0.3, w/w) with PEDOT: PSS as interlayer under simulated AM 1.5G solar light (100 mW cm⁻²).

Active Layer	PDI-interlayer	V _{oc} (V)	J _{sc} (mA cm ⁻²)	FF (%)	PCE (%)	J _{cal} (mA cm ⁻²)
PM6:L8BO:BTP-eC9	PDINN	0.878	27.74	79.70	19.41	26.75
		(0.875±0.003)	(27.55±0.08)	(79.55±0.11)	(19.25±0.10)	
	PDISNN (NO Methanol)	0.867	27.05	78.86	18.50	26.14
		(0.863±0.003)	(26.95±0.06)	(78.74±0.12)	(18.32±0.08)	
	PDISNN	0.881	27.98	81.73	20.15	27.01
		(0.877±0.003)	(27.86±0.09)	(81.61±0.11)	(19.94±0.12)	
D18:N3:DY2	PDINN	0.870	26.72	79.93	18.58	25.74
		(0.868±0.002)	(26.63±0.07)	(79.83±0.12)	(18.29±0.07)	
	PDISNN (NO Methanol)	0.861	26.18	77.10	17.38	25.22
		(0.858±0.003)	(26.13±0.05)	(76.97±0.13)	(17.26±0.07)	
	PDISNN	0.878	26.93	80.86	19.12	25.94
		(0.876±0.002)	(26.85±0.06)	(80.75±0.10)	(18.98±0.07)	

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