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Supplementary Information

Crystalline organic thin films for crystalline OLEDs (I): orientation of phenanthroimidazole derivatives

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1. Growth process of single crystal

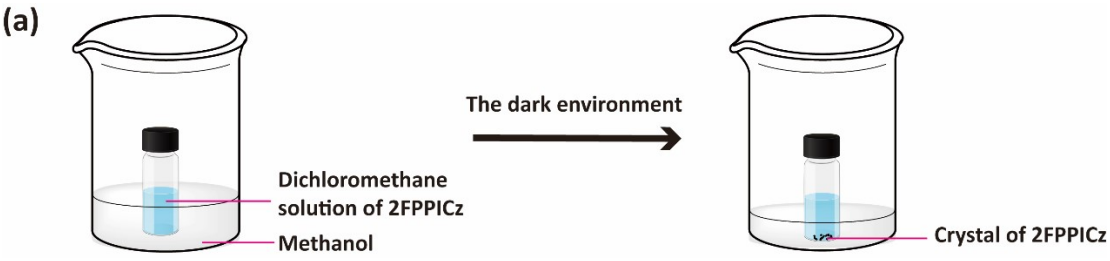

Fig. S1 Growth process of 2FPPICz single crystal by solvent diffusion method.

2. ^{19}F NMR spectra of 2FPPICz.

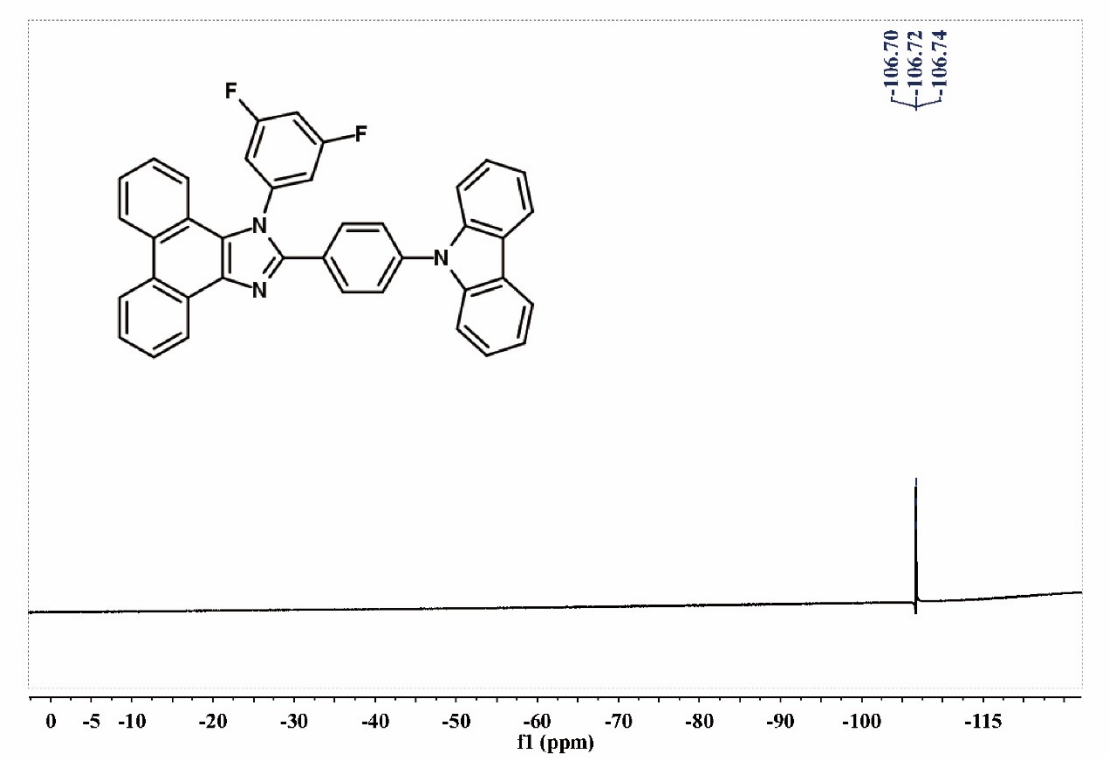

Fig. S2 ^{19}F NMR spectra of 2FPPICz.

^{19}F NMR (500 MHz, DMSO-d_6) δ -106.69 ─ -106.76.

3. Morphologies of *p*-6P thin films with different thickness

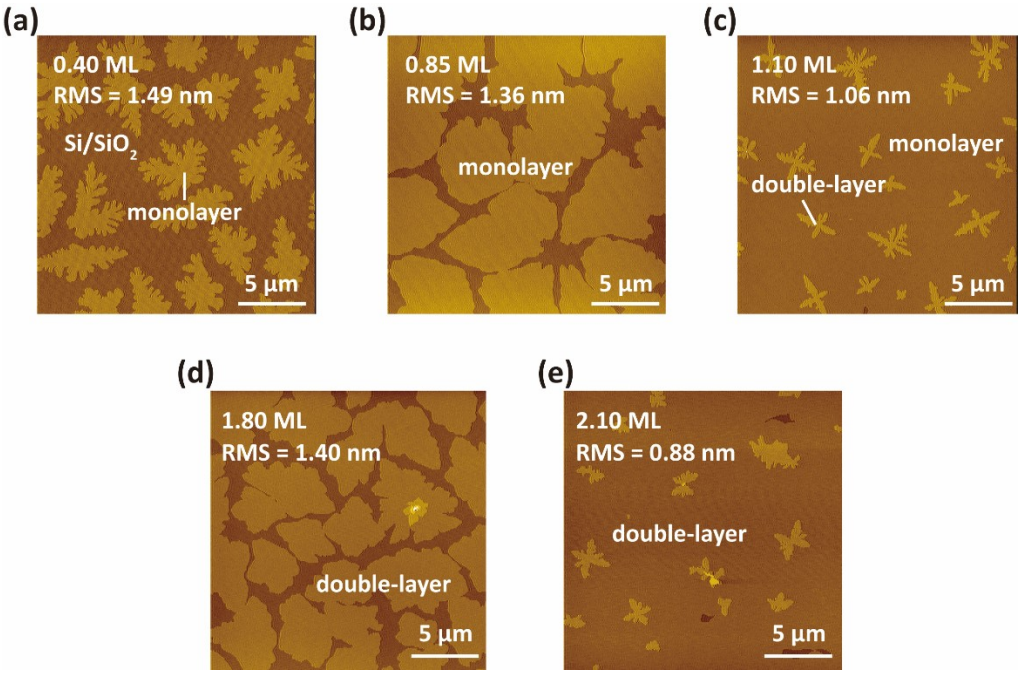

Fig. S3 Morphologies of *p*-6P thin films with different thicknesses. RMS surface roughness values are displayed in each figure.

4. SAED pattern and the corresponding electron micrograph of *p*-6P double-layer

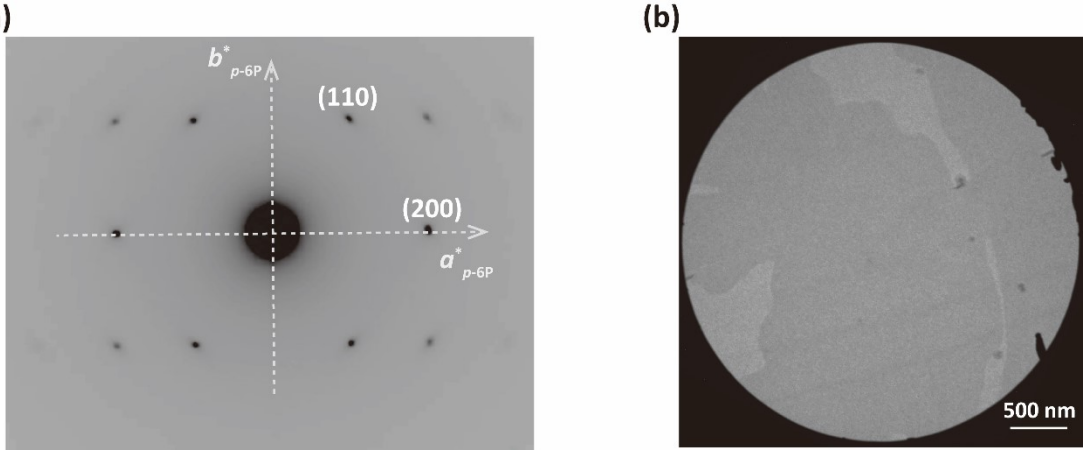

Fig. S4 SAED pattern (a) and the corresponding electron micrograph (b) of *p*-6P double-layer

5. Carrier transporting characteristics

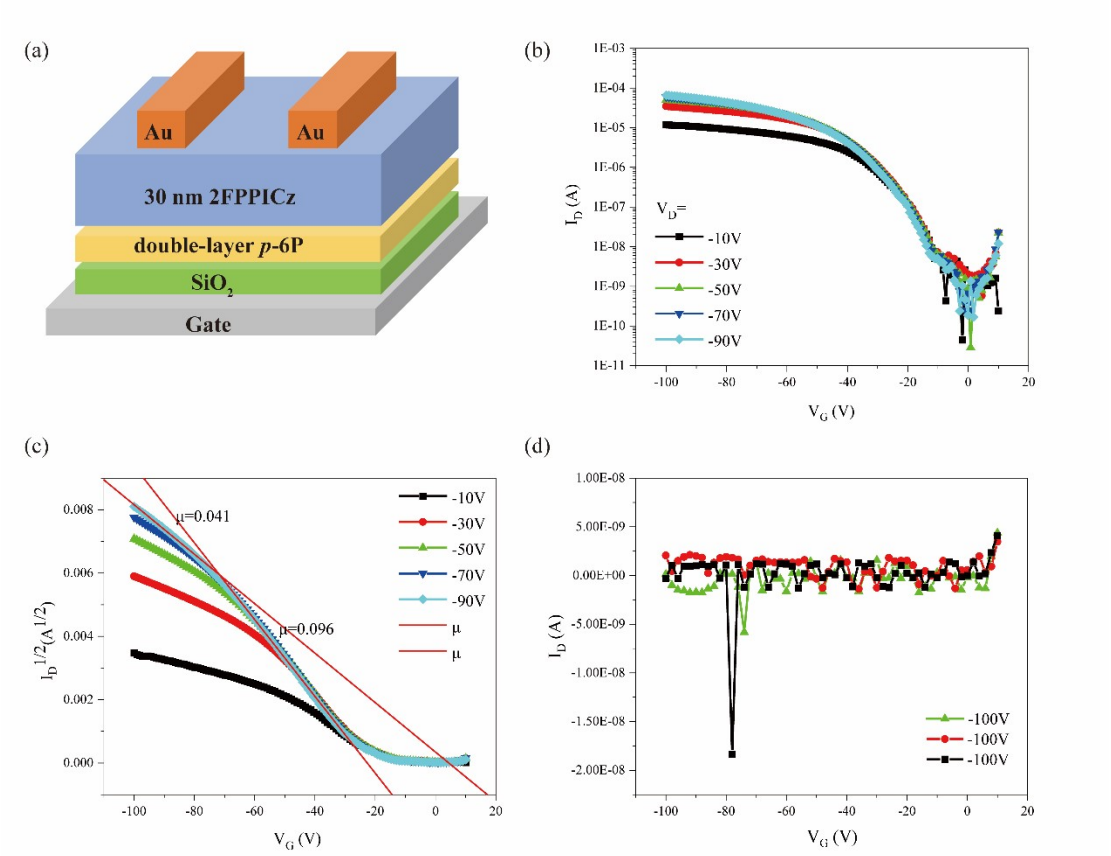

Fig. S5 (a) Device configuration of the *p*-6P/2FPPICz. (b-c) The hysteresis characteristics of the crystalline *p*-6P /2FPPICz OTFT in transfer curves (b) and the typical $I_D^{1/2}$ vs. V_G plot (c). (d) The transfer curve of amorphous OTFT.

6. The major intermolecular interactions in crystal of 2FPPICz

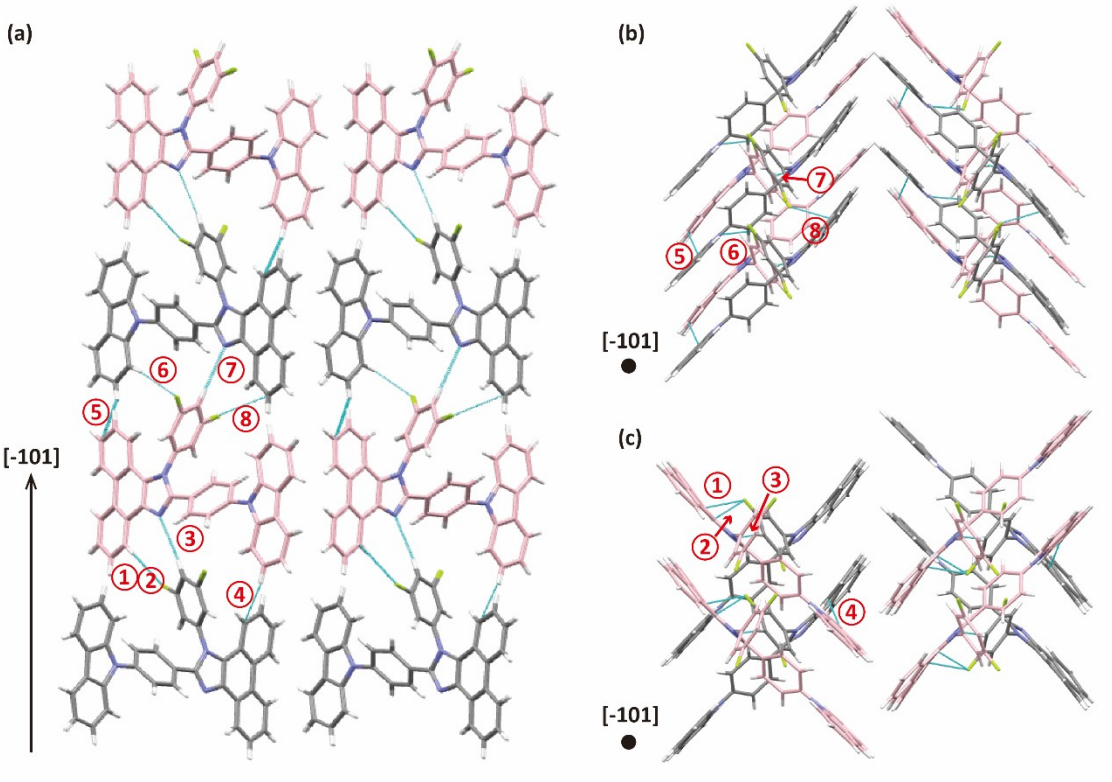

Fig. S6 (a) The intermolecular interaction of 2FPPICz molecules in crystalline films, and the [-101] direction is perpendicular to the substrate. (b-c) The corresponding top views of the [-101] direction. (①⑧ n-π interactions; ②⑥ C-H…F hydrogen bonds; ③⑦ C-H…N hydrogen bonds; ④⑤ C-H…π interactions.)

7. DFT calculated the transition dipole moment of 2FPPICz

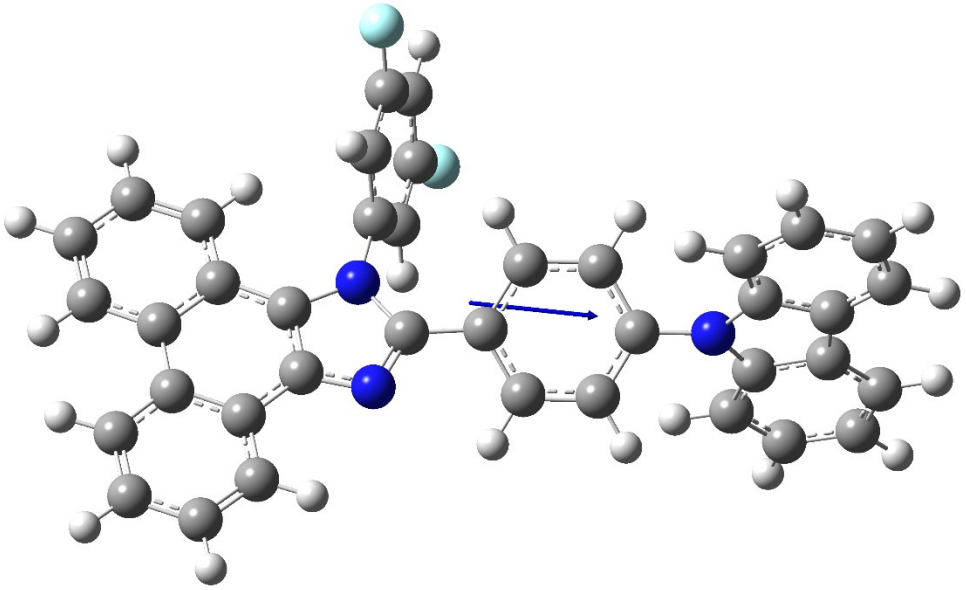

Fig. S7 Density functional theory (DFT) calculated the transition dipole moment of 2FPPICz. The blue arrow represents the direction of ground to excited state transition electric dipole moments.

8. In-plane parameters of *p*-6P and 2FPPICz

	p-6P(double-layer)	2FPPICz
$d_{(010)}$ (Å)	5.58 ± 0.04	5.59 ± 0.04
$d_{(100)}$ (Å)	7.96 ± 0.04	—
$d_{(101)}$ (Å)	—	12.95 ± 0.04

Table S1 The interplanar spacing of *p*-6P double-layer and 2FPPICz.

Table S2 Crystal data and structure refinement for **2FPPICz**

CCDC number	2106623	
Empirical weight	C39 H23 F2 N3	
Formula weight	571.63	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P n	
Unit cell dimensions	a = 22.3845(9) Å	α = 90°.
	b = 5.4788(2) Å	β = 112.382(2)°.
	c = 23.6129(10) Å	γ = 90°.
Volume	2677.73(19) $Å^3$	
Z	4	
Density(calculated)	1.418 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	1192	
Crystal size	0.7 x 0.1 x 0.1 mm^3	
Theta range for data collection	2.59 to 29.19°	
Index ranges	-31<=h<=31, -7<=k<=7, -32<=l<=32	
Reflections collected	57264	
Independent reflections	15060 [R(int) = 0.0767]	
Completeness to theta = 29.19°	99.8%	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15060/2/794	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0825, wR2 = 0.2019	
R indices (all data)	R1 = 0.1203, wR2 = 0.2311	
Largest diff. peak and hole	1.119 and -0.490 e.Å-3	

8. Crystallographic Report Tables