

The effect of electron withdrawing substituent in asymmetric anthracene derivative semiconductors

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Table S1. Crystal data and structure refinement of TZ-Ant and F₅Ph-Ant. (CCDC No. 2033809, 2033782.)

Compound	TZ-Ant	F ₅ Ph-Ant
Empirical formula	C ₁₇ H ₁₁ NS	C ₂₀ H ₉ F ₅
Formula weight	261.33	344.27
Temperature/K	293(2)	293(2)
Crystal system	orthorhombic	orthorhombic
Space group	Pna2 ₁	Pna2 ₁
a/Å	24.3454(3)	12.26360(10)
b/Å	8.44650(10)	15.4509(2)
c/Å	6.09350(10)	7.56040(10)
α/°	90	90
β/°	90	90
γ/°	90	90
Volume/Å ³	1253.03(3)	1432.57(3)
Z	4	4
ρ _{calc} g/mm ³	1.385	1.596
μ /mm ⁻¹	2.132	1.199
F(000)	544.0	696.0
Crystal size/mm ³	0.4 × 0.3 × 0.2	0.3 × 0.3 × 0.3
Radiation	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range for data collection	7.262 to 134.064	9.206 to 134.136°
Index ranges	-27 ≤ h ≤ 29, -6 ≤ k ≤ 10, -7 ≤ l ≤ 7	-10 ≤ h ≤ 14, -18 ≤ k ≤ 16, -8 ≤ l ≤ 9
Reflections collected	7392 2231	9117 2484
Independent reflections	[R _{int} = 0.0221, R _{sigma} = 0.0202]	[R _{int} = 0.0196, R _{sigma} = 0.0173]
Data/restraints/parameters	2231/1/216	2484/1/226
Goodness-of-fit on F ²	1.075	1.064
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0265, wR ₂ = 0.0687	R ₁ = 0.0266, wR ₂ = 0.0677
Final R indexes [all data]	R ₁ = 0.0274, wR ₂ = 0.0698	R ₁ = 0.0271, wR ₂ = 0.0685
Largest diff. peak/hole / e Å ⁻³	0.12/-0.20	0.11/-0.19
Flack parameter	-0.003(11)	0.03(4)

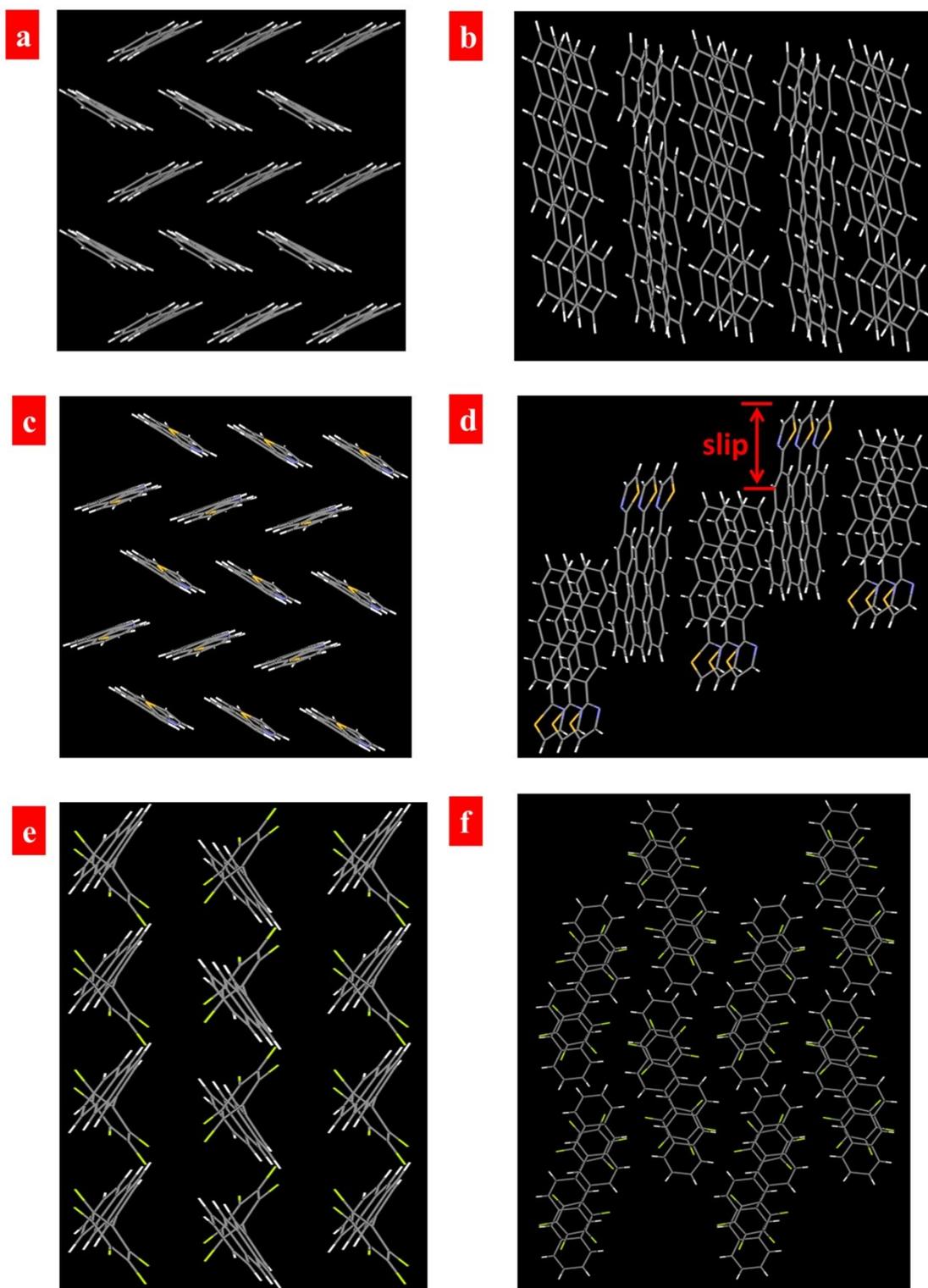


Figure S1 Comparison of molecular packing for Ph-Ant(a,b), TZ-Ant(c,d) and F₅Ph-Ant(e,f).

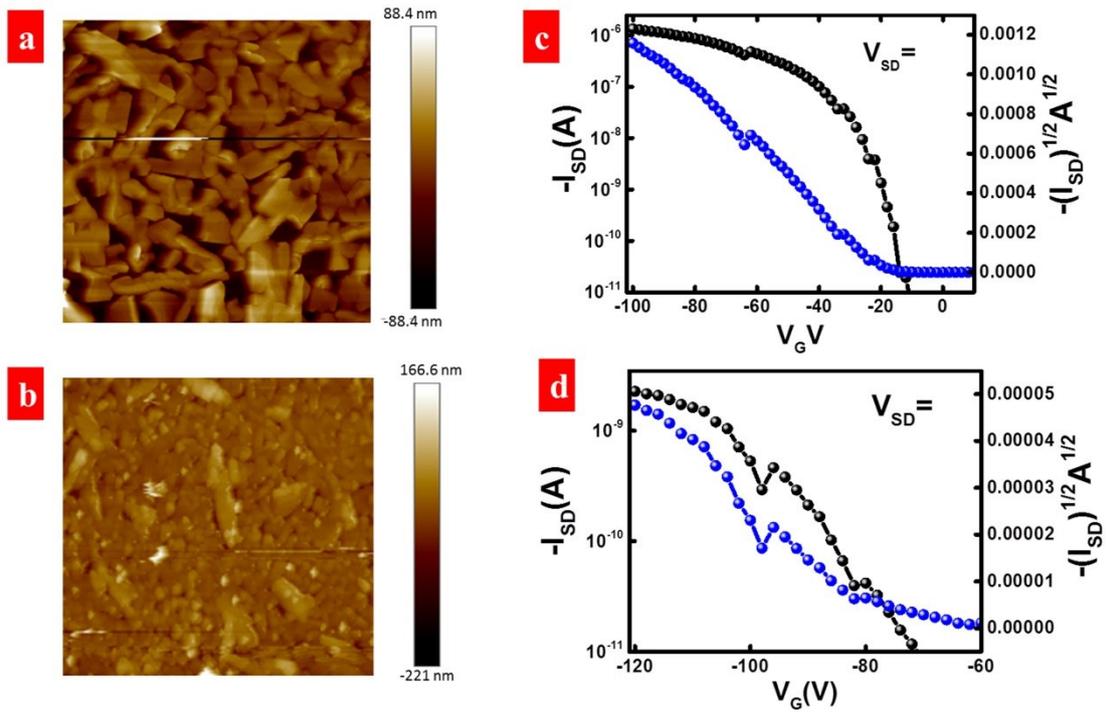


Figure S2. Atomic force microscopy image of a thin film of Ph-Ant (a) and TZ-Ant (b) in the tapping mode and transfer characteristics of devices based on Ph-Ant (c) and TZ-Ant (d)

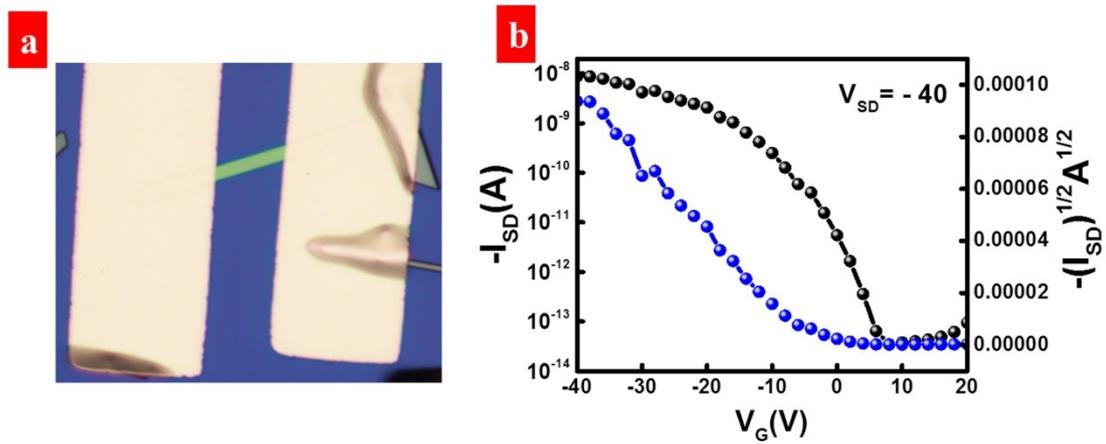


Figure S3. Single crystal based transistor of TZ-Ant and transfer characteristics of devices based on TZ-Ant