Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Influence of Heteroatoms on the Charge Mobility of Anthracene Derivatives

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Surface modification of SiO_2 substrates: OTS device substrates we used highly doped n-type Si wafers with a 250 nm dry thermal oxide gate dielectric. These wafers were cleaned in piranha solution (highly corrosive and oxidizing 7:3 mixture of H_2SO_4 and H_2O_2) for 30 min, rinsed with deionized water and dried under a nitrogen stream. For OTS treatment, the wafer was treated with OTS by immersing the cleaned wafer substrate in 0.1 M solution of OTS in toluene at 60 °C for 30 min, and rinsing with toluene and blown dry with nitrogen. The semiconductor layer was deposited over the treated surface through shadow mask.

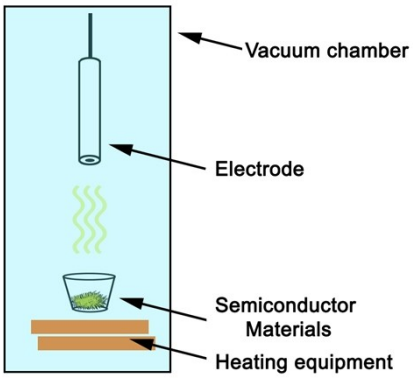

Figure S1. The simplified graph of the evaporating methods for the GCE (Φ=3mm).

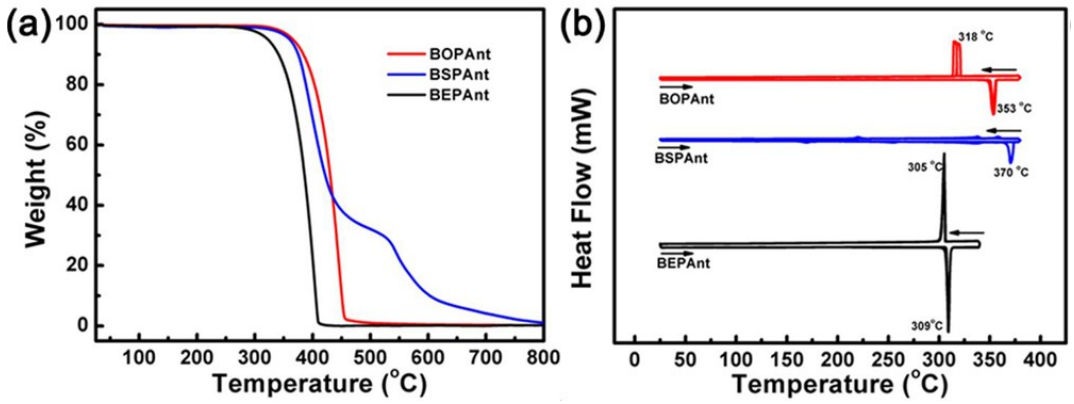

Figure S2. TGA (a) and DSC (b) plots of BOPAnt, BSPAnt and BEPAnt (scan rate: 10 °C/min).

Table S1. Single Crystal Data of Three Semiconductors

	BOPAnt		BSPAnt		BEPAnt	
Crystal system	Orthorhombic		Triclinic		Monoclinic	
Space group	P b c a		P-1		P 21/c	
Unit cell dimensions	a = 7.44 Å	α = 90°	a = 6.03 Å	α =92.83°	a = 22.66 Å	α =90°
	b = 6.16 Å	β = 90°	b = 7.68 Å	β = 96.55°	b = 7.72 Å	β = 92.45°
	c = 42.30 Å	γ = 90°	c = 22.61 Å	γ = 90.10°	c = 6.04 Å	γ = 90°
Z	4		2		2	
Volume	1938.71(15) Å^3		1040.09(11) Å^3		1056.00(7) Å^3	
Packing D	2.06 / nm^3		1.92 / nm^3		1.89 / nm^3	

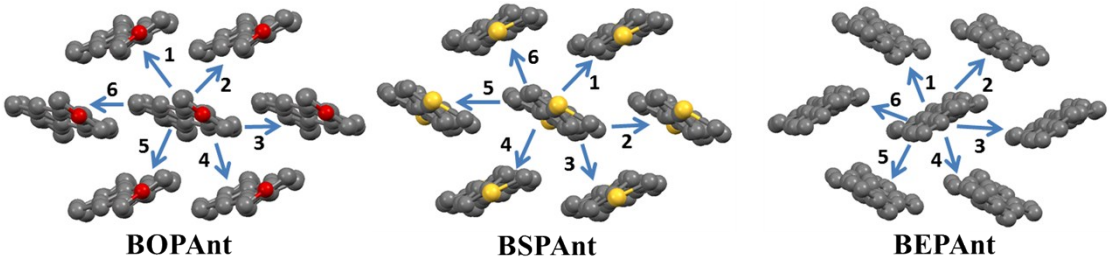

Table S2. the hole and electron reorganization energy levels and the respected hole and electron couplings data

Semi-conductor	pathway	Distance (Å)	Hole coupling (eV)	Electron coupling (eV)	Hole reorganization (eV)	Electron reorganization (eV)	Hole drift mobility (cm^2/Vs)	Electron drift mobility (cm^2/Vs)
BOPAnt	1	4.83	0.07253	0.1692	0.2491	0.2246	0.2635	1.7141
	2	4.83	0.07252	0.1693				
	3	4.83	0.07257	0.1691				
	4	4.83	0.07254	0.1691				
	5	21.37	0.03190	0.0001				
	6	6.16	0.01334	0.0194				
BSPAnt	1	4.881	0.02144	0.03371	0.1829	0.4656	0.1075	0.0074
	2	4.889	0.01202	0.05132				
	3	4.89	0.02181	0.03693				
	4	23.501	0.00110	0.0004				
	5	22.722	0.01265	0.00253				
	6	23.501	0.00176	0.00081				

BEPAnt	1	6.043	0.02328	0.02772	0.1790	0.2190	0.1732 // [a] 0.6583 ⊥ [b]	0.0699 // [a] 1.2594 ⊥ [b]
	2	6.043	0.02328	0.02772				
	3	4.901	0.07939	0.13906				
	4	4.901	0.07939	0.13906				
	5	4.901	0.07939	0.13906				
	6	4.901	0.07939	0.13906				

[a] Based on BEPAnt crystal parallel aligned ethyl group (Figure S3a); [b]: Based on BEPAnt crystal vertically aligned ethyl group (Figure S3b).

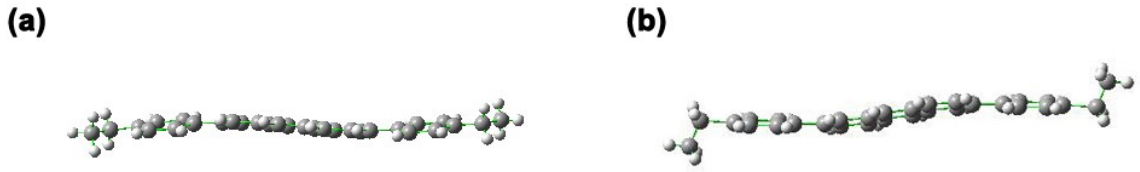

Figure S3. Two possible single crystal structure of BEPAnt: (a) Ethyl parallel to the plane; (b) Ethyl perpendicular to plane.