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Supplementary Materials

The Influence of Side Chains on the Structures and Properties of Functionalized Pentacenes

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1. Detailed Phase Transition Information Extracted from DSC

Table S1. Transition temperatures and corresponding enthalpies (+ for endo, - for exo) upon heating of functionaized pentacenes

	Transition 1 Temperature (Enthalpy)	**Transition 2** Temperature (Enthalpy)	**Transition 3** Temperature (Enthalpy)	**Transition 4** Temperature (Enthalpy)	**Transition 5** Temperature (Enthalpy)
6-P	142 °C (-160 J/g)	-----	-----	-----	-----
7-P	156 °C (-130 J/g)	-----	-----	-----	-----
8-P	124 °C (-113 J/g)	-----	-----	-----	-----
10-P	155±50 °C (-122 J/g)	-----	-----	-----	-----
12-P	128 °C (+, N/A*)	131 °C (-, N/A*)	-----	-----	-----
2-Si	142 °C (+5 J/g)	227 °C (+, N/A*)	230 °C (-, N/A*)	-----	-----
3-Si	124°C (+26 J/g)	260°C (+, N/A*)	265°C (-, N/A*)	-----	-----
4-Si	53 °C (+7 J/g)	142 °C (+50 J/g)	195±35 °C (-36 J/g)	-----	-----
4II-Si	219 °C (+, N/A*)	225 °C (-, N/A*)	-----	-----	-----
6-Si	51 °C (+12 J/g)	74 °C (+10 J/g)	83 °C (+9 J/g)	100 °C (+18 J/g)	190±40 °C (-67 J/g)
8-Si	69 °C (+72 J/g)	200±60 °C (-45 J/g)	-----	-----	-----

* Sometime the enthalpy values were hard to determine, since more than one transitions (or reactions) were concurring. For example, melting and degradation of 2-Si, 3-Si, and 12-P happened at similar temperature respectively, which complicated the enthalpy estimation and precise peak locating.

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2. UV-vis Molar Extinction Coefficients

Molar extinction coefficient ε=A/(c*l), where A is the absorption, c is the concentration (mol/l), and l is the length (cm). For the experiments in this work, l was kept at 1 cm, and c is about 30 mg/liter.

Table S2. Molar extinction coefficients ε (in liter · mol^{-1} · cm^{-1}) of functionalized pentacenes at selected wavelengths λ (in nm)

	Peak 1 ε_1 (λ_1)	**Peak 2** ε_2 (λ_2)	**Peak 3** ε_3 (λ_3)	**Peak 4** ε_4 (λ_4)
6-P	19591 (630)	9795 (580)	3509 (537)	1462 (437)
7-P	16487 (632)	8243 (583)	3111 (541)	1400 (438)
8-P	22097 (630)	12203 (578)	6101 (537)	5277 (434)
10-P	3121 (623)	2754 (572)	2570 (535)	N/A
12-P	2022 (615)	1416 (568)	607 (527)	N/A
2-Si	24847 (640)	12424 (590)	4073 (545)	3462 (440)
3-Si	19809 (640)	9798 (590)	3408 (545)	2769 (440)
4-Si	34912 (640)	17345 (590)	6226 (545)	5114 (440)
4II-Si	38469 (640)	18679 (590)	6671 (545)	5337 (440)
6-Si	32785 (640)	16151 (590)	5786 (545)	4339 (440)
8-Si	29094 (640)	14287 (590)	5195 (545)	4156 (440)

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3. Single Crystal Analysis

All the functionalized pentacenes mentioned in this paper were crystallized from hexanes. For alkynyl pentacenes, the compound in hexanes was first heated at 35-40°C in a hot water bath, cooled to room temperature before cooled at 0°C. The solution-grown crystals were filtered, and washed with cold hexanes before analyzed by X-ray crystallography. For the diisopropylsilyl pentacenes, the procedure was the same as that of alkynyl pentacenes except that the material in hexanes were heated at an elevated temperature (~75°C) before they were cooled. Due to thermal instability, alkynyl pentacenes were heated at lower temperature.

Crystal structures were refined in Full-matrix SHELXL on F2, X, Y, Z, Uij, etc as per any normal small molecule structure. In all seven compounds the molecules lie about inversion centers. In 6-P and 2-Si, the asymmetric unit has two independent half molecules. The crystallographic data including structure refinement information of the functionalized pentacenes were available in Table S3 and attached cif files. The structures will be deposited in Cambridge database.

Table S3. Crystallographic data of functionalized pentacenes (6-P, 7-P, 8-P, 2-Si, 4-Si, 6-Si, and 8-Si).

	6-P	**7-P**	**8-P**	**2-Si**	**4-Si**	**6-Si**	**8-Si**
Formula	$C_{34}H_{30}$	$C_{36}H_{34}$	$C_{38}H_{38}$	$C_{42}H_{50}Si_2$	$C_{46}H_{58}Si_2$	$C_{50}H_{66}Si_2$	$C_{54}H_{74}Si_2$
Molecular Weight	438.58	466.63	494.68	611.0	667.10	723.21	779.31
Crystal System	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic	Orthorhombic	Triclinic
Space Group	P 21/c	P 21/n	P -1	P –1	P 21/c	P bca	P -1
a (Å)	19.8513 (4)	12.3212 (3)	6.6368 (1)	10.6177 (2)	8.8840 (2)	10.3715 (2)	8.8577 (1)
b (Å)	5.3006 (1)	5.1420 (2)	8.3446 (2)	13.6171 (3)	22.3240 (5)	15.4649 (2)	11.1290 (1)
c (Å)	22.6989 (5)	20.8030 (7)	13.7421 (3)	14.0829 (3)	10.7970 (3)	27.5066 (4)	12.5975 (1)
α	90	90	105.5261 (9)	75.154 (1)	90	90	101.9194 (4)
β	93.5526 (8)	101.1599 (12)	100.2523 (9)	73.915 (1)	110.146 (1)	90	93.8211 (4)
γ	90	90	92.7360 (9)	71.123 (1)	90	90	101.2905 (4)
Z	4	2	1	2	2	4	1
T (K)	90.0 (2)	90.0 (2)	90.0 (2)	90.0 (2)	90.0 (2)	90.0 (2)	90.0 (2)
λ (Å)	0.71073	0.71073	0.71073	1.54178	0.71073	1.54178	0.71073
Volume ($Å^3$)	2383.88 (8)	1293.07 (7)	717.92 (3)	1819.86 (7)	2010.32 (9)	4411.90 (12)	1184.10 (2)
Mu (mm^{-1})	0.069	0.067	0.064	1.071	0.118	0.950	0.109
S	0.980	0.975	0.993	1.028	1.049	1.037	1.006