Supplementary Data (Table S1)

Table 1 Average bond length, angles, and torsion of Py with n=1 units optimized by B3LYP/3-21G*, B3LYP/6-31G* and SCC-DFTB calculation.

Method	a (Å)	b (Å)	c (Å)	α (°)	β (°)	Torsion1(°)	Torsion2(°)
B3LYP/3-21G*	1.39	1.01	-	-	-	-	-
B3LYP /6-31G*	1.38	1.01	-	-	-	-	-
SCC-DFTB	1.37	1.04	-	-	-	-	-

Table 2 Average bond length, angles, and torsion of Py with n=2 units optimized by B3LYP/3-21G*, B3LYP/6-31G* and SCC-DFTB calculation.

Method	a (Å)	b (Å)	c (Å)	α (°)	β (°)	Torsion1(°)	Torsion2(°)
B3LYP/3-21G*	1.39	1.01	1.44	122.67	130.52	176.58	176.48
B3LYP /6-31G*	1.38	1.01	1.45	122.00	132.10	179.80	179.80
SCC-DFTB	1.38	1.04	1.46	122.17	131.03	177.94	178.20

Table 3 Average bond length, angles, and torsion of Py with n=3 units optimized by B3LYP/3-21G*, B3LYP/6-31G* and SCC-DFTB calculation.

Method	a (Å)	b (Å)	c (Å)	α (°)	β (°)	Torsion1(°)	Torsion2(°)
B3LYP/3-21G*	1.39	1.01	1.44	122.80	130.50	175.71	175.51
B3LYP /6-31G*	1.38	1.01	1.44	122.00	131.74	179.30	179.40
SCC-DFTB	1.38	1.04	1.46	122.20	130.98	178.87	178.80

Table 4 Average bond length, angles, and torsion of Py with n=4 units optimized by B3LYP/3-21G*, B3LYP/6-31G* and SCC-DFTB calculation.

Method	a (Å)	b (Å)	c (Å)	α (°)	β (°)	Torsion1(°)	Torsion2(°)
B3LYP/3-21G*	1.39	1.01	1.44	122.69	130.54	172.53	171.31
B3LYP /6-31G*	1.38	1.01	1.44	121.80	131.70	177.20	177.30
SCC-DFTB	1.38	1.04	1.46	122.15	131.03	179.00	179.04

Table 5 Average bond length, angles, and torsion of Py with n=5 units optimized by B3LYP/3-21G*, B3LYP/6-31G* and SCC-DFTB calculation.

Method	a (Å)	b (Å)	c (Å)	α (°)	β (°)	Torsion1(°)	Torsion2(°)
B3LYP/3-21G*	1.39	1.01	1.44	122.70	130.54	172.27	171.32
B3LYP /6-31G*	1.38	1.01	1.44	121.76	131.61	176.69	174.40
SCC-DFTB	1.38	1.04	1.46	122.15	131.00	179.45	179.43