

Supplementary Information for:

Effects of fluorine substitution on the intermolecular interactions, energetics and packing behaviour of N-benzyl substituted diketopyrrolopyrroles

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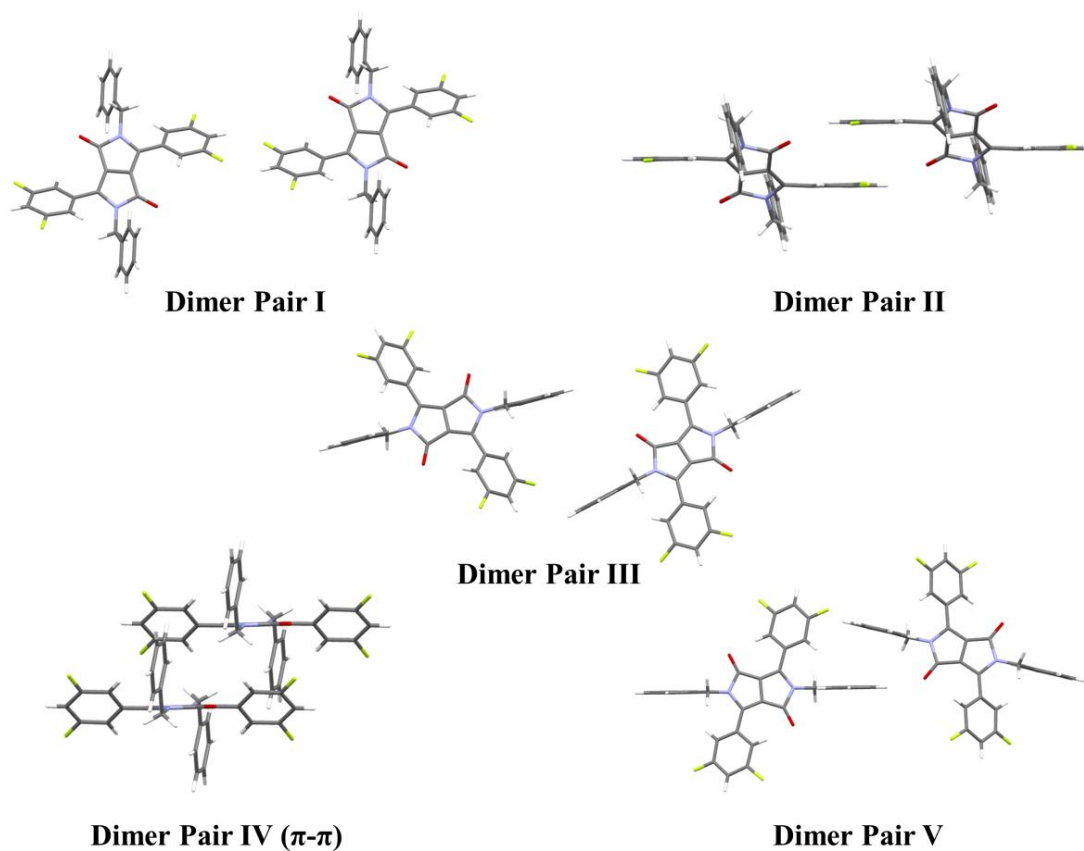
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## SI1 Nearest neighbour dimer pairs

**Table S1.1** Number of equivalent molecules and site for different dimer pairs of *HFHBDPP*

Dimer pair	No eq. molecules	Site <sup>a</sup>
<b>I</b>	2	(-2,1/2,1)
<b>II</b>	2	(-1,1/2,1)
<b>III</b>	2	(-1,1,1/2)
<b>IV (<math>\pi</math>-<math>\pi</math>)</b>	2	(1,1/2,0)
<b>V</b>	2	(0,1,-1/2)

<sup>a</sup> Around the monomer at (0,1/2,0)

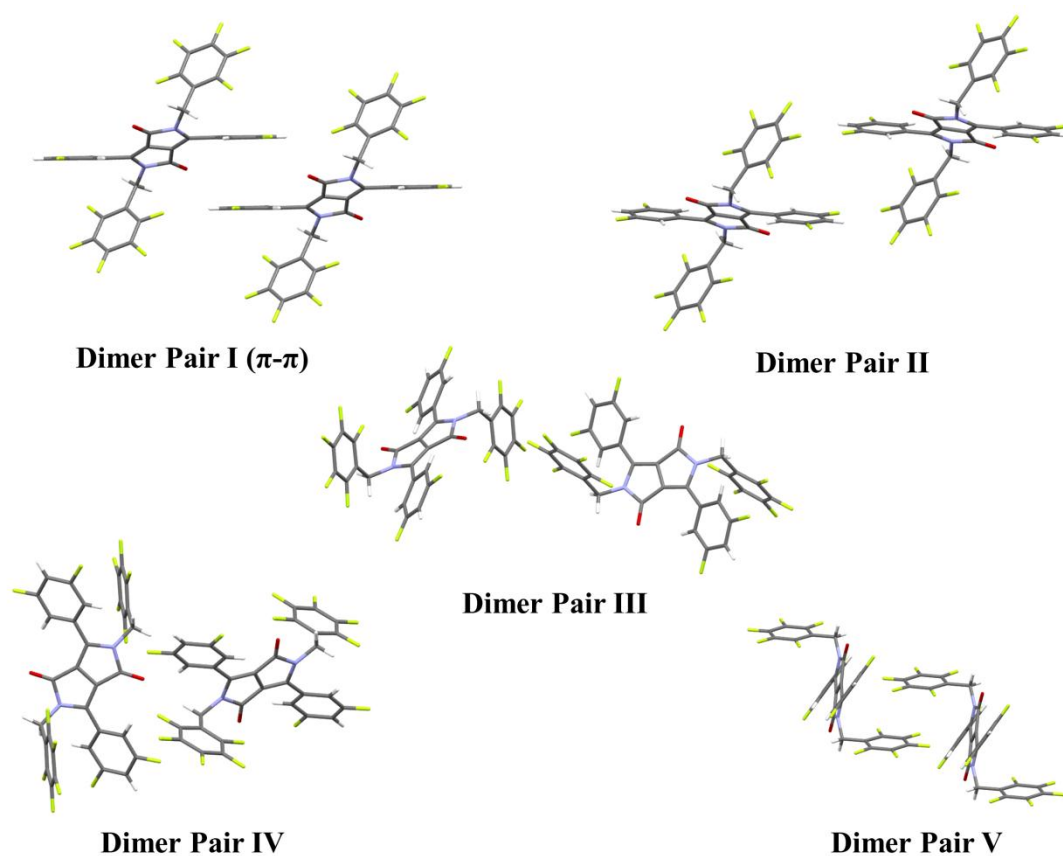


**Figure S1.1** Capped stick illustration of the different nearest neighbour dimers of *HFHBDPP*.

**Table S1.2** Number of equivalent molecules and site for different dimer pairs of *HFFBDPP*

Dimer pair	No eq. molecules	Site <sup>a</sup>
I ( $\pi$ - $\pi$ )	2	(0,1,0)
II	2	(-1,1,0)
III	2	(1,-1/2,-1/2)
IV	4	(0,1/2,-1/2)
V	2	(-1,0,0)

<sup>a</sup> Around the monomer at (0,0,0)

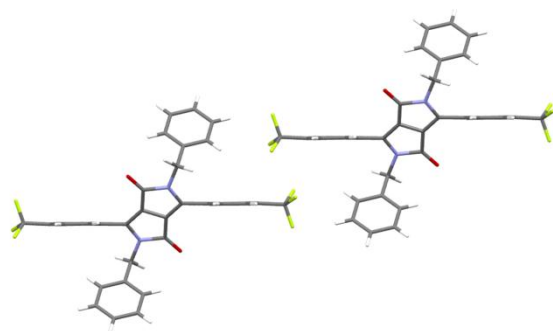


**Figure S1.2** Capped stick illustration of the different nearest neighbour dimers of *HFFBDPP*.

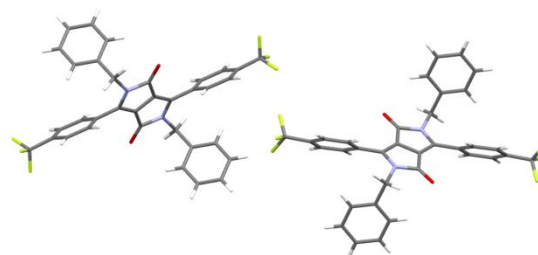
**Table S1.3** Number of equivalent molecules and site for different dimer pairs of *THHBDPP*

Dimer pair	No eq. molecules	Site <sup>a</sup>
I	2	(-1/2,0,1/2)
II	4	(-1/2,1/2,1)
III	2	(1/2,1,1/2)
IV	2	(1/2,1/2,0)

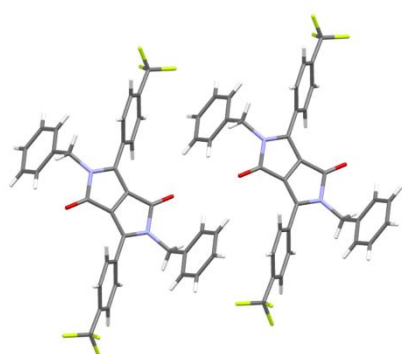
<sup>a</sup> Around the monomer at (1/2,0,1/2)



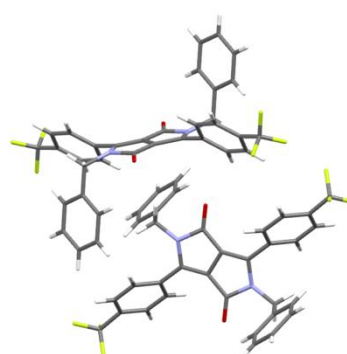
**Dimer Pair I**



**Dimer Pair II**



**Dimer Pair III**



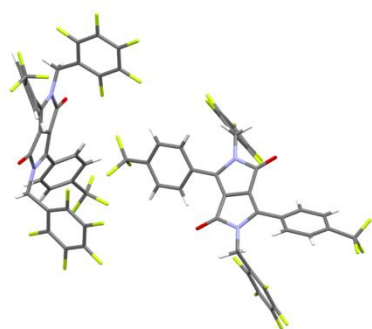
**Dimer Pair IV**

**Figure S1.3** Capped stick illustration of the different nearest neighbour dimers of *THHBDPP*.

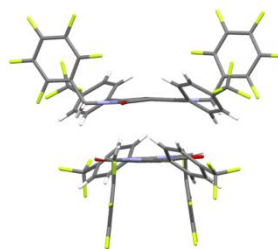
**Table S1.4** Number of equivalent molecules and site for different dimer pairs of *THFBDPP*

Dimer pair	No eq. molecules	Site <sup>a</sup>
I	2	(1/12,8/12,1/2)
II	2	(8/12,-1/12,1/2)
III	2	(1/12,1/12,3/2)
IV	2	(1/12,5/12,-1/2)

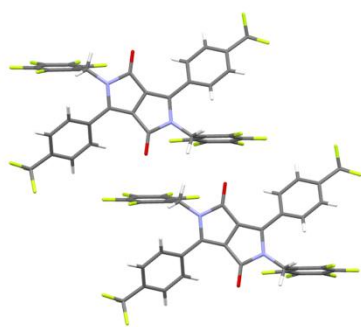
<sup>a</sup> Around the monomer at (1/2,1/12,1/2)



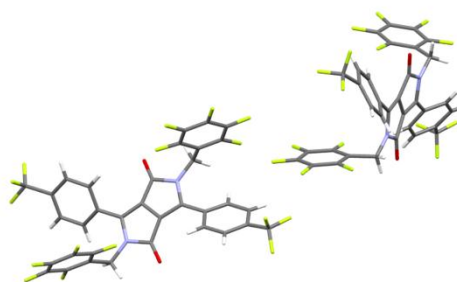
**Dimer Pair I**



**Dimer Pair II**



**Dimer Pair III**



**Dimer Pair IV**

**Figure S1.4** Capped stick illustration of the different nearest neighbour dimers of *THFBDPP*.