

Investigation of the Interfacial Binding between Single-walled Carbon Nanotubes and Heterocyclic Conjugated Polymers

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The specifications of investigated SWCNTs are given in Table S1.

Table S1. Specifications of each SWCNT utilized in MD simulations.

SWCNT type	H atoms	C atoms	Diameter (Å)	Length (Å)
(4,4)	16	704	5.49	110
(6,6)	24	1056	8.18	110
(8,8)	32	1408	10.88	110
(10,10)	40	1760	13.58	110
(12,12)	48	2112	16.29	110
(14,14)	56	2464	19.00	110
(16,16)	64	2816	21.71	110
(18,18)	72	3168	24.42	110
(20,20)	80	3520	27.13	110

Calculation of the alignment angle

The schematic view of the alignment angle θ has been given in Figure 6. As this figure shows for each aromatic ring on the polymer, we consider a vector as an indicative of aromatic ring orientation.

Since the aromatic rings are absolutely planar in xy plane, we can suppose this in the same direction of the longitudinal axis of CNT (X axis) as follows

$$y = mx + c \quad (1)$$

which m is the slope of the equation (1) and is computed according to the formulation below

$$m = \frac{|y_2 - y_1|}{|x_2 - x_1|} \quad (2)$$

where x and y are the coordinations of the spotted atoms in Figure 6.

The alignment angle is then evaluated as

$$\theta = \tan^{-1} m \quad (3)$$