Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

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

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Calculation of the alignment angle

As mentioned before, the dihedral angle is the angle between two planes. In each simulation step, the method used to compute the dihedral angle between the plane of the cation ring and the longitudinal axis of the nanotube is as follows:

In the plane of the cation ring, using the positions of the three points on it, (NB, CP2, and CP1), an equation was defined for axis S1 (vertical to the plane of the cation ring) as below:

$$aX + bY + cZ + d = 0 \qquad (S1)$$

Using this equation and the mathematical relations, the equation of the axis which is set on the plane of the cation ring and vertical to the previous axis, is calculated as below:

$$A_1x + B_1y + C_1z + D_1 = 0 \qquad (S2)$$

Furthermore, in nanotube molecules, the mass centers of the hydrogen atoms at the two ends of the nanotube and its carbon atom of central cell were computed and three points- in center and at the two ends of the nanotube- were obtained. Afterwards, using these three points, the main axis of the nanotube was defined as:

$$A_2x + B_2y + C_2z + D_2 = 0 \qquad (S3)$$

The indices1 and 2 in the relations S1 and S2, indicate the plane of the cation ring and nanotube, respectively.

Since the longitudinal axis of nanotube is parallel to the surfaces of all its rings, for all existing cations in the system, the dihedral angle between cation ring and this axis was calculated as:

$$\cos\theta^{-1} = \frac{A_1.A_2 + B_1.B_2 + C_1.C_2}{\sqrt[2]{A_1^2 + B_1^2 + C_1^2} + \sqrt[2]{A_2^2 + B_2^2 + C_2^2}} \qquad \text{(S4)}$$

The considered nanotubes in dihedral angle calculations, were (6, 6) armchair-type CNT. It is important to notice that this method can't be used for (m, n) nanotube because its axis will be calculated in a tilted position, but for two other kinds, (n, n) - and (o, n)-type, the obtained results are very accurate.