Supporting Information

The role of the solvent and the size of the nanotube in the non-covalent dispersion of carbon nanotubes with short organic oligomers - A DFT Study

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Table S1. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using B97D with 6-31G(d) and 6-31++G(d,p) basis sets. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | B97D/6-31G(d) | B97D/6-31++G(d,p) |
|-----------------|---------------|-------------------|
|                 | Isolated      | With (6,5) SWCNT  | Isolated      | With (6,5) SWCNT |
| R_{1-2}         | 1.407         | 1.408             | 1.409         | 1.408            |
| R_{2-3}         | 1.404         | 1.405             | 1.406         | 1.404            |
| R_{3-4}         | 1.403         | 1.403             | 1.405         | 1.403            |
| R_{4-5}         | 1.468         | 1.469             | 1.469         | 1.469            |
| R_{5-6}         | 1.405         | 1.404             | 1.406         | 1.404            |
| R_{6-7}         | 1.405         | 1.405             | 1.406         | 1.404            |
| R_{7-8}         | 1.408         | 1.408             | 1.409         | 1.406            |
| Bond Angle (A)  |               |                   |               |                   |
| A_{1-2-3}       | 120.7         | 120.7             | 120.7         | 120.7            |
| A_{2-3-4}       | 118.7         | 118.8             | 118.7         | 118.9            |
| A_{3-4-5}       | 131.1         | 131.2             | 131.1         | 131.2            |
| A_{4-5-6}       | 131.1         | 131.2             | 131.1         | 131.3            |
| A_{5-6-7}       | 118.7         | 118.7             | 118.7         | 118.7            |
| A_{6-7-8}       | 120.7         | 120.7             | 120.6         | 120.8            |
| Dihedral Angle (|Dh|) |               |                   |               |                   |
| D_{1-2-3-4}     | 0.0           | 0.0               | 0.0           | 0.1              |
| D_{2-3-4-5}     | 180.0         | 180.0             | 180.0         | 179.4            |
| D_{3-4-5-6}     | 0.0           | 0.1               | 0.0           | 0.6              |
| D_{4-5-6-7}     | 180.0         | 179.9             | 180.0         | 178.5            |
| D_{5-6-7-8}     | 0.0           | 0.1               | 0.0           | 0.3              |
Table S2. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using B97D with 6-31G(d) and 6-31++G(d,p) basis sets. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | B97D/6-31G(d) | B97D/6-31++G(d,p) |
|-----------------|---------------|-------------------|
|                 | Isolated  | With (6,5) SWCNT | With (8,7) SWCNT | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
| R₁₂             | 1.777    | 1.767       | 1.768       | 1.776    | 1.768       | 1.768       |
| R₂₃             | 1.782    | 1.795       | 1.796       | 1.782    | 1.793       | 1.794       |
| R₃₄             | 1.795    | 1.782       | 1.780       | 1.793    | 1.782       | 1.780       |
| R₄₅             | 1.349    | 1.353       | 1.353       | 1.352    | 1.355       | 1.355       |
| Bond Angle (A)  |           |               |             |           |               |             |
| A₁₂₃            | 116.7    | 118.7       | 118.8       | 116.8    | 118.8       | 118.9       |
| A₂₃₄            | 97.0     | 96.1        | 95.5        | 97.0     | 96.3        | 95.7        |
| A₃₄₅            | 123.9    | 124.1       | 124.2       | 123.9    | 123.8       | 124.1       |
| Dihedral Angle (|Dh|) |           |               |             |           |               |             |
| D₁₂₃₄           | 179.8    | 176.2       | 172.3       | 179.8    | 177.7       | 173.5       |
| D₂₃₄₅           | 179.9    | 164.4       | 159.4       | 179.9    | 166.0       | 160.9       |
Table S3. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using B97D with 6-31G(d) and 6-31++G(d,p) basis sets. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | B97D/6-31G(d) | B97D/6-31++G(d,p) |
|----------------|---------------|-------------------|
|                | Isolated      | With (6,5) SWCNT  | With (8,7) SWCNT |
| R_{1,2}        | 1.376         | 1.378             | 1.377            |
| R_{2,3}        | 1.406         | 1.406             | 1.406            |
| R_{3,4}        | 1.401         | 1.401             | 1.401            |
| R_{4,5}        | 1.411         | 1.410             | 1.410            |
| R_{5,6}        | 1.376         | 1.378             | 1.379            |
| Bond Angle (A) |               |                   |                  |
| A_{1,2,3}      | 116.0         | 116.4             | 116.2            |
| A_{2,3,4}      | 120.8         | 120.6             | 120.6            |
| A_{3,4,5}      | 120.0         | 120.1             | 120.1            |
| A_{4,5,6}      | 124.9         | 124.3             | 124.3            |
| Dihedral Angle (|Dh|) |               |                   |                  |
| D_{1,2,3,4}    | 180.0         | 176.2             | 176.3            |
| D_{2,3,4,5}    | 0.0           | 1.0               | 0.7              |
| D_{3,4,5,6}    | 180.0         | 175.0             | 174.5            |

The labeling of atoms is shown in Figure 1.
Table S4. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using wB97XD and B3LYP-D3 with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | wB97XD   | B3LYP-D3  |            |            |            |            |            |            |
|-----------------|-----------|-----------|------------|------------|------------|------------|------------|------------|
|                 | Isolated  | With (6,5)| With (8,7)| Isolated  | With (6,5)| With (8,7)| Isolated  | With (6,5)| With (8,7)|
| R₁-₂            | 1.395     | 1.395     | 1.395      | 1.399      | 1.400      | 1.399      | 1.399      | 1.400      | 1.399      |
| R₂-₃            | 1.393     | 1.393     | 1.393      | 1.397      | 1.398      | 1.398      |          |            |            |
| R₃-₄            | 1.391     | 1.391     | 1.391      | 1.395      | 1.396      | 1.396      |          |            |            |
| R₄-₅            | 1.470     | 1.471     | 1.471      | 1.468      | 1.469      | 1.468      |          |            |            |
| R₅-₆            | 1.391     | 1.391     | 1.391      | 1.395      | 1.396      | 1.396      |          |            |            |
| R₆-₇            | 1.393     | 1.393     | 1.393      | 1.397      | 1.397      | 1.397      |          |            |            |
| R₇-₈            | 1.395     | 1.395     | 1.395      | 1.399      | 1.400      | 1.399      |          |            |            |
| Bond Angle (A)  |            |           |            |            |            |            |            |            |
| A₁-₂-₃          | 120.6     | 120.6     | 120.6      | 120.6      | 120.6      | 120.5      |          |            |            |
| A₂-₃-₄          | 118.8     | 118.7     | 118.8      | 118.8      | 118.8      | 118.8      |          |            |            |
| A₃-₄-₅          | 131.0     | 131.1     | 131.1      | 131.0      | 131.1      | 131.0      |          |            |            |
| A₄-₅-₆          | 131.0     | 131.0     | 131.1      | 131.0      | 131.0      | 131.0      |          |            |            |
| A₅-₆-₇          | 118.8     | 118.8     | 118.7      | 118.8      | 118.9      | 118.8      |          |            |            |
| A₆-₇-₈          | 120.6     | 120.6     | 120.6      | 120.6      | 120.6      | 120.6      |          |            |            |
| Dihedral Angle (|Dh|) |            |           |            |            |            |            |            |            |
| D₁-₂-₃-₄        | 0.0       | 0.1       | 0.0        | 0.0        | 0.0        | 0.2        |          |            |            |
| D₂-₃-₄-₅        | 180.0     | 179.9     | 180.0      | 180.0      | 180.0      | 179.5      |          |            |            |
| D₃-₄-₅-₆        | 0.0       | 0.0       | 0.1        | 0.0        | 0.2        | 0.1        |          |            |            |
| D₄-₅-₆-₇        | 180.0     | 180.0     | 179.9      | 180.0      | 179.9      | 179.5      |          |            |            |
| D₅-₆-₇-₈        | 0.0       | 0.0       | 0.0        | 0.0        | 0.0        | 0.0        |          |            |            |
Table S5. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using wb97XD and B3LYP-D3 with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|----------------|----------|------------------|------------------|----------|------------------|------------------|
| R₁₋₂          | 1.768    | 1.761            | 1.760            | 1.775    | 1.767            | 1.768            |
| R₂₋₃          | 1.765    | 1.775            | 1.777            | 1.776    | 1.788            | 1.790            |
| R₃₋₄          | 1.778    | 1.769            | 1.768            | 1.790    | 1.780            | 1.777            |
| R₄₋₅          | 1.335    | 1.337            | 1.338            | 1.340    | 1.343            | 1.343            |
| Bond Angle (A)|          |                  |                  |          |                  |                  |
| A₁₋₂₋₃       | 116.6    | 118.9            | 119.1            | 116.4    | 118.8            | 118.9            |
| A₂₋₃₋₄       | 96.5     | 95.6             | 94.9             | 96.7     | 95.9             | 95.2             |
| A₃₋₄₋₅       | 123.7    | 123.9            | 124.0            | 123.8    | 123.8            | 124.1            |
| Dihedral Angle (|Dh|)|          |                  |                  |          |                  |                  |
| D₁₋₂₋₃₋₄     | 179.9    | 176.6            | 171.8            | 180.0    | 175.9            | 171.9            |
| D₂₋₃₋₄₋₅     | 179.9    | 165.1            | 159.8            | 179.9    | 164.9            | 159.7            |
Table S6. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using wB97XD and B3LYP-D3 with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | wB97XD | B3LYP-D3 |
|-----------------|---------|----------|
|                 | Isolated | With (6,5) SWCNT | With (8,7) SWCNT | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
| R_{1-2}         | 1.362    | 1.363    | 1.362    | 1.370    | 1.371    | 1.369    |
| R_{2-3}         | 1.374    | 1.394    | 1.394    | 1.402    | 1.398    | 1.398    |
| R_{3-4}         | 1.390    | 1.390    | 1.390    | 1.394    | 1.394    | 1.393    |
| R_{4-5}         | 1.397    | 1.397    | 1.397    | 1.402    | 1.402    | 1.402    |
| R_{5-6}         | 1.362    | 1.363    | 1.362    | 1.370    | 1.370    | 1.369    |
| Bond Angle (A)  |         |          |          |          |          |          |
| A_{1-2-3}       | 116.1    | 116.9    | 116.4    | 116.0    | 116.8    | 116.3    |
| A_{2-3-4}       | 121.0    | 120.7    | 120.9    | 121.0    | 120.7    | 120.9    |
| A_{3-4-5}       | 119.9    | 120.0    | 120.0    | 119.9    | 120.0    | 120.0    |
| A_{4-5-6}       | 124.8    | 124.2    | 124.5    | 124.9    | 124.4    | 124.6    |
| Dihedral Angle (|Dh|) |         |          |          |          |          |          |
| D_{1-2-3-4}     | 180.0    | 176.9    | 177.8    | 180.0    | 177.3    | 177.8    |
| D_{2-3-4-5}     | 0.0      | 0.6      | 0.6      | 0.0      | 0.7      | 0.7      |
| D_{3-4-5-6}     | 180.0    | 176.6    | 177.2    | 180.0    | 176.7    | 177.1    |
Table S7. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) and those using B97D/6-31++G(d,p) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|----------------|----------|------------------|------------------|
| R\(_{1-2}\)    | 0.001    | 0.000            | 0.001            |
| R\(_{2-3}\)    | 0.000    | 0.001            | 0.000            |
| R\(_{3-4}\)    | 0.001    | 0.001            | 0.000            |
| R\(_{4-5}\)    | 0.001    | 0.000            | 0.000            |
| R\(_{5-6}\)    | 0.000    | 0.001            | 0.001            |
| R\(_{6-7}\)    | 0.001    | 0.001            | 0.001            |
| R\(_{7-8}\)    | 0.002    | 0.002            | 0.001            |
| Bond Angle (A) |          |                  |                  |
| A\(_{1-2-3}\)  | 0.0      | 0.1              | 0.0              |
| A\(_{2-3-4}\)  | 0.0      | 0.1              | 0.1              |
| A\(_{3-4-5}\)  | 0.0      | 0.1              | 0.1              |
| A\(_{4-5-6}\)  | 0.0      | 0.1              | 0.1              |
| A\(_{5-6-7}\)  | 0.0      | 0.1              | 0.0              |
| A\(_{6-7-8}\)  | 0.1      | 0.1              | 0.0              |
| Dihedral Angle (|Dh|) |          |                  |                  |
| D\(_{1-2-3-4}\)| 0.0      | 0.1              | 0.0              |
| D\(_{2-3-4-5}\)| 0.0      | 0.6              | 0.0              |
| D\(_{3-4-5-6}\)| 0.0      | 0.5              | 0.1              |
| D\(_{4-5-6-7}\)| 0.0      | 1.4              | 0.2              |
| D\(_{5-6-7-8}\)| 0.0      | 0.2              | 0.0              |
Table S8. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) and those using B97D/6-31++G(d,p) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|-----------------|----------|------------------|------------------|
| R₁-₂            | 0.000    | 0.000            | 0.001            |
| R₂-₃            | 0.000    | 0.001            | 0.001            |
| R₃-₄            | 0.002    | 0.000            | 0.001            |
| R₄-₅            | 0.002    | 0.001            | 0.001            |
| Bond Angle (A)  |          |                  |                  |
| A₁-₂-₃          | 0.0      | 0.0              | 0.0              |
| A₂-₃-₄          | 0.0      | 0.0              | 0.0              |
| A₃-₄-₅          | 0.0      | 0.0              | 0.0              |
| Dihedral Angle (|Dh|) |          |                  |                  |
| D₁-₂-₃-₄        | 0.4      | 0.6              | 0.2              |
| D₂-₃-₄-₅        | 1.3      | 0.2              | 0.4              |

Table S9. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) and those using B97D/6-31++G(d,p) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|-----------------|----------|------------------|------------------|
| R₁-₂            | 0.002    | 0.002            | 0.003            |
| R₂-₃            | 0.001    | 0.000            | 0.000            |
| R₃-₄            | 0.002    | 0.001            | 0.001            |
| R₄-₅            | 0.000    | 0.000            | 0.000            |
| R₅-₆            | 0.002    | 0.003            | 0.005            |
| Bond Angle (A)  |          |                  |                  |
| A₁-₂-₃          | 0.0      | 0.3              | 0.1              |
| A₂-₃-₄          | 0.1      | 0.0              | 0.2              |
| A₃-₄-₅          | 0.0      | 0.0              | 0.1              |
| A₄-₅-₆          | 0.2      | 0.1              | 0.5              |
| Dihedral Angle (|Dh|) |          |                  |                  |
| D₁-₂-₃-₄        | 0.0      | 0.5              | 0.9              |
| D₂-₃-₄-₅        | 0.0      | 0.6              | 0.1              |
| D₃-₄-₅-₆        | 0.0      | 0.5              | 2.1              |
Table S10. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using B97D/6-31G(d) in PCM with chloroform and hexane solvents. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Chloroform | Hexane |
|-----------------|------------|--------|
|                 | Isolated   | With (6,5) SWCNT | With (8,7) SWCNT | Isolated   | With (6,5) SWCNT | With (8,7) SWCNT |
| R_{1-2}         | 1.408      | 1.409   | 1.408 | 1.408      | 1.408   | 1.408   |
| R_{2-3}         | 1.405      | 1.405   | 1.405 | 1.405      | 1.405   | 1.405   |
| R_{3-4}         | 1.404      | 1.404   | 1.404 | 1.404      | 1.404   | 1.404   |
| R_{4-5}         | 1.469      | 1.470   | 1.470 | 1.469      | 1.469   | 1.469   |
| R_{5-6}         | 1.404      | 1.404   | 1.404 | 1.404      | 1.404   | 1.404   |
| R_{6-7}         | 1.405      | 1.405   | 1.405 | 1.405      | 1.405   | 1.405   |
| R_{7-8}         | 1.408      | 1.408   | 1.408 | 1.408      | 1.408   | 1.408   |
| Bond Angle (A)  |            |         |       |            |         |         |
| A_{1-2-3}       | 120.7      | 120.7   | 120.7 | 120.7      | 120.7   | 120.7   |
| A_{2-3-4}       | 118.7      | 118.7   | 118.7 | 118.7      | 118.7   | 118.7   |
| A_{3-4-5}       | 131.0      | 131.2   | 131.3 | 131.1      | 131.2   | 131.3   |
| A_{4-5-6}       | 131.0      | 131.1   | 131.2 | 131.1      | 131.2   | 131.1   |
| A_{5-6-7}       | 118.7      | 118.7   | 118.7 | 118.7      | 118.7   | 118.7   |
| A_{6-7-8}       | 120.7      | 120.7   | 120.7 | 120.7      | 120.7   | 120.7   |
| Dihedral Angle (|Dh|) |            |         |       |            |         |         |
| D_{1-2-3-4}     | 0.0        | 0.1     | 0.1   | 0.0        | 0.1     | 0.3     |
| D_{2-3-4-5}     | 180.0      | 179.9   | 179.7 | 180.0      | 180.0   | 179.0   |
| D_{3-4-5-6}     | 0.0        | 0.1     | 0.3   | 0.0        | 0.0     | 0.5     |
| D_{4-5-6-7}     | 180.0      | 180.0   | 180.0 | 180.0      | 180.0   | 179.6   |
| D_{5-6-7-8}     | 0.0        | 0.0     | 0.0   | 0.0        | 0.0     | 0.0     |
Table S11. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using B97D/6-31G(d) in PCM with chloroform and hexane solvents. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Chloroform | Hexane |
|-----------------|------------|--------|
|                 | Isolated   | With (6,5) SWCNT | With (8,7) SWCNT | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
| R<sub>1-2</sub> | 1.776      | 1.769     | 1.769     | 1.776     | 1.768     | 1.768     |
| R<sub>2-3</sub> | 1.784      | 1.795     | 1.796     | 1.783     | 1.795     | 1.796     |
| R<sub>3-4</sub> | 1.796      | 1.785     | 1.783     | 1.796     | 1.784     | 1.782     |
| R<sub>4-5</sub> | 1.349      | 1.351     | 1.351     | 1.349     | 1.352     | 1.352     |
| Bond Angle (A) |            |           |           |           |           |           |
| A<sub>1-2-3</sub> | 116.8      | 118.5     | 118.7     | 116.7     | 118.6     | 118.8     |
| A<sub>2-3-4</sub> | 97.1       | 96.0      | 95.3      | 97.0      | 96.0      | 95.4      |
| A<sub>3-4-5</sub> | 124.0      | 124.1     | 124.2     | 123.9     | 124.1     | 124.2     |
| Dihedral Angle (|Dh|) |            |           |           |           |           |           |
| D<sub>1-2-3-4</sub> | 179.9      | 175.4     | 171.8     | 179.8     | 175.8     | 172.1     |
| D<sub>2-3-4-5</sub> | 179.9      | 163.9     | 159.0     | 179.9     | 164.2     | 159.4     |
Table S12. Selected bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using B97D/6-31G(d) in PCM with chloroform and hexane solvents. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Chloroform | Hexane |
|-----------------|------------|--------|
|                 | Isolated   | With (6,5) SWCNT | With (8,7) SWCNT | Isolated   | With (6,5) SWCNT | With (8,7) SWCNT |
| R₁₂             | 1.375      | 1.377   | 1.375 | 1.376 | 1.377 | 1.375 |
| R₂₃             | 1.408      | 1.406   | 1.407 | 1.407 | 1.406 | 1.406 |
| R₃₄             | 1.402      | 1.400   | 1.400 | 1.401 | 1.400 | 1.400 |
| R₄₅             | 1.411      | 1.410   | 1.410 | 1.411 | 1.410 | 1.410 |
| R₅₆             | 1.375      | 1.376   | 1.375 | 1.376 | 1.376 | 1.375 |
| Bond Angle (A)  |            |         |       |       |       |       |
| A₁₂⁻³⁻⁴         | 116.0      | 116.8   | 116.2 | 116.0 | 116.7 | 116.2 |
| A₂₃⁻⁴⁻⁵         | 120.9      | 120.5   | 120.8 | 120.9 | 120.5 | 120.8 |
| A₃₄⁻⁵⁻⁶         | 120.0      | 120.1   | 120.0 | 120.0 | 120.1 | 120.0 |
| A₄₅⁻⁶⁻⁷         | 124.9      | 124.3   | 124.6 | 124.9 | 124.4 | 124.7 |
| Dihedral Angle (|Dh|) |            |         |       |       |       |       |
| D₁₂⁻³⁻⁴⁻⁵       | 180.0      | 176.0   | 177.5 | 180.0 | 175.9 | 177.4 |
| D₂₃⁻⁴⁻⁵⁻⁶       | 0.0        | 0.4     | 0.6   | 0.0   | 0.4   | 0.6   |
| D₃₄⁻⁵⁻⁶⁻⁷       | 180.0      | 175.7   | 176.9 | 180.0 | 175.6 | 176.8 |
Table S13. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) without a solvent and those obtained using B97D/6-31G(d) in PCM/chloroform and in PCM/hexane respectively for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Chloroform | Hexane |
|-----------------|------------|--------|
|                 | Isolated   | With (6,5) SWCNT | With (8,7) SWCNT | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
| R₁-₂            | 0.001      | 0.001   | 0.000       | 0.001      | 0.000     | 0.000       |
| R₂-₃            | 0.001      | 0.000   | 0.000       | 0.001      | 0.000     | 0.000       |
| R₃-₄            | 0.001      | 0.000   | 0.001       | 0.001      | 0.000     | 0.001       |
| R₄-₅            | 0.001      | 0.001   | 0.000       | 0.001      | 0.000     | 0.001       |
| R₅-₆            | 0.001      | 0.000   | 0.000       | 0.001      | 0.000     | 0.000       |
| R₆-₇            | 0.000      | 0.000   | 0.000       | 0.000      | 0.000     | 0.000       |
| R₇-₈            | 0.000      | 0.000   | 0.000       | 0.000      | 0.000     | 0.000       |
| Bond Angle (A)  |            |         |             |            |         |             |
| A₁-₂-₃          | 0.0        | 0.0     | 0.0         | 0.0        | 0.0      | 0.0         |
| A₂-₃-₄          | 0.0        | 0.1     | 0.1         | 0.0        | 0.1      | 0.1         |
| A₂-₃-₄-₅        | 0.1        | 0.0     | 0.1         | 0.0        | 0.0      | 0.0         |
| A₃-₄-₅-₆        | 0.1        | 0.1     | 0.1         | 0.0        | 0.0      | 0.0         |
| A₅-₆-₇          | 0.0        | 0.0     | 0.0         | 0.0        | 0.0      | 0.0         |
| A₆-₇-₈          | 0.0        | 0.0     | 0.0         | 0.0        | 0.0      | 0.0         |
| Dihedral Angle (|Dh|) |            |         |             |            |         |             |
| D₁-₂-₃-₄        | 0.0        | 0.1     | 0.1         | 0.0        | 0.1      | 0.3         |
| D₂-₃-₄-₅        | 0.0        | 0.1     | 0.2         | 0.0        | 0.0      | 0.9         |
| D₃-₄-₅-₆        | 0.0        | 0.0     | 0.1         | 0.0        | 0.1      | 0.2         |
| D₄-₅-₆-₇        | 0.0        | 0.1     | 0.6         | 0.0        | 0.1      | 0.2         |
| D₅-₆-₇-₈        | 0.0        | 0.1     | 0.1         | 0.0        | 0.1      | 0.1         |
Table S14. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) without a solvent and those obtained using B97D/6-31G(d) in PCM/chloroform and in PCM/hexane respectively for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Chloroform | Hexane |
|----------------|------------|--------|
|                | Isolated  | With (6,5) SWCNT | With (8,7) SWCNT | Isolated  | With (6,5) SWCNT | With (8,7) SWCNT |
| R₁-2           | 0.001     | 0.002   | 0.001   | 0.001     | 0.001   | 0.000   |
| R₂-3           | 0.002     | 0.000   | 0.000   | 0.001     | 0.000   | 0.000   |
| R₃-4           | 0.001     | 0.003   | 0.003   | 0.001     | 0.002   | 0.002   |
| R₄-5           | 0.000     | 0.002   | 0.002   | 0.000     | 0.001   | 0.001   |
| Bond Angle (A) |            |         |         |            |         |         |
| A₁-2-3         | 0.1       | 0.2     | 0.1     | 0.0       | 0.1     | 0.0     |
| A₂-3-4         | 0.1       | 0.1     | 0.2     | 0.0       | 0.1     | 0.1     |
| A₃-4-5         | 0.1       | 0.0     | 0.0     | 0.0       | 0.0     | 0.0     |
| Dihedral Angle (|Dh|) |            |         |         |            |         |         |
| D₁-2-3-4       | 0.1       | 0.8     | 0.5     | 0.0       | 0.4     | 0.2     |
| D₂-3-4-5       | 0.0       | 0.5     | 0.4     | 0.0       | 0.2     | 0.0     |

Table S15. Differences between bond lengths (R) (in Å), bond angles (A), and dihedral angles (|Dh|) (in degrees) obtained using B97D/6-31G(d) without a solvent and those obtained using B97D/6-31G(d) in PCM/chloroform and in PCM/hexane respectively for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs. The labeling of atoms is shown in Figure 1.

| Bond Length (R) | Chloroform | Hexane |
|----------------|------------|--------|
|                | Isolated  | With (6,5) SWCNT | With (8,7) SWCNT | Isolated  | With (6,5) SWCNT | With (8,7) SWCNT |
| R₁-2           | 0.001     | 0.001   | 0.002   | 0.000     | 0.001   | 0.002   |
| R₂-3           | 0.002     | 0.000   | 0.001   | 0.001     | 0.000   | 0.000   |
| R₃-4           | 0.001     | 0.001   | 0.001   | 0.000     | 0.001   | 0.001   |
| R₄-5           | 0.000     | 0.000   | 0.000   | 0.000     | 0.000   | 0.000   |
| R₅-6           | 0.001     | 0.002   | 0.004   | 0.000     | 0.002   | 0.004   |
| Bond Angle (A) |            |         |         |            |         |         |
| A₁-2-3         | 0.0       | 0.4     | 0.0     | 0.0       | 0.3     | 0.0     |
| A₂-3-4         | 0.1       | 0.1     | 0.2     | 0.1       | 0.1     | 0.2     |
| A₃-4-5         | 0.0       | 0.0     | 0.1     | 0.0       | 0.0     | 0.1     |
| A₄-5-6         | 0.0       | 0.0     | 0.3     | 0.0       | 0.1     | 0.4     |
| Dihedral Angle (|Dh|) |            |         |         |            |         |         |
| D₁-2-3-4       | 0.0       | 0.2     | 1.2     | 0.0       | 0.3     | 1.1     |
| D₂-3-4-5       | 0.0       | 0.6     | 0.1     | 0.0       | 0.6     | 0.1     |
| D₃-4-5-6       | 0.0       | 0.7     | 2.4     | 0.0       | 0.6     | 2.3     |
**Table S16.** HOMO and LUMO energies (in eV) for isolated FLU, DDTF, BDOB, and SWCNTs obtained using B3LYP/6-31G(d) without a solvent and with chloroform and hexane solvents.

| No solvent | Isolated molecules | SWCNT |   |   |   |   |
|------------|--------------------|-------|---|---|---|---|
|            | FLU | DDTF | BDOB | (6,5) | (8,7) |   |   |
| E\text{HOMO} | -5.72 | -5.19 | -5.18 | -4.41 | -4.70 |   |   |
| E\text{LUMO} | -0.77 | -0.95 | 0.15 | -2.55 | -2.28 |   |   |
| **Chloroform** |   |   |   |   |   |   |   |
| E\text{HOMO} | -5.80 | -5.36 | -5.36 | -4.48 | -4.78 |   |   |
| E\text{LUMO} | -0.84 | -1.07 | -0.05 | -2.62 | -2.36 |   |   |
| **Hexane** |   |   |   |   |   |   |   |
| E\text{HOMO} | -5.76 | -5.28 | -5.27 | -4.43 | -4.72 |   |   |
| E\text{LUMO} | -0.80 | -1.01 | 0.05 | -2.58 | -2.31 |   |   |

**Table S17.** HOMO and LUMO energies (in eV) for interacting FLU, DDTF, and BDOB with (6,5) and (8,7) SWCNTs obtained using B3LYP/6-31G(d)//B3LYP-D3/6-31G(d) without a solvent.

| No solvent | With (6,5) SWCNT |   |   |   |   | With (8,7) SWCNT |   |   |   |
|------------|------------------|---|---|---|---|------------------|---|---|---|
|            | FLU | DDTF | BDOB | FLU | DDTF | BDOB | FLU | DDTF | BDOB | FLU | DDTF | BDOB |
| E\text{HOMO} | -5.73 | -4.97 | -5.27 | -5.72 | -4.90 | -5.21 |   |   |   |   |   |   |
| E\text{LUMO} | -0.77 | -0.52 | 0.12 | -0.75 | -0.58 | 0.13 |   |   |   |   |   |   |
Figure S1. Representative (partially) optimized structures of FLU molecule interacting with (6,5) SWCNT (left) and (8,7) SWCNT (right) obtained using B97D/6-31G(d); (a) side view, (b) front view, and (c) top view with the oligomers highlighted (similar results are obtained with B97D/6-31++G(d,p) and other D-DFT methods with 6-31G(d) basis set).
Figure S2. Representative (partially) optimized structures of DDTF molecule interacting with (6,5) SWCNT (left) and (8,7) SWCNT (right) obtained using B97D/6-31G(d); (a) side view, (b) front view, and (c) top view with the oligomers highlighted (similar results are obtained with B97D/6-31++G(d,p) and other D-DFT methods with 6-31G(d) basis set).
Figure S3. Representative (partially) optimized structures of BDOB molecule interacting with (6,5) SWCNT (left) and (8,7) SWCNT (right) obtained using B97D/6-31G(d); (a) side view, (b) front view, and (c) top view with the oligomers highlighted (similar results are obtained with B97D/6-31++G(d,p) and other D-DFT methods with 6-31G(d) basis set).
Figure S4. (a) bond lengths (in Å), (b) bond angles, and (c) dihedral angles (in degrees) for the isolated FLU and for FLU interacting with (6,5) and (8,7) SWCNTs obtained using B97D, wB97XD, and B3LYP-D3 with 6-31G(d) basis set.
| Bond Length (Å) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|----------------|----------|------------------|------------------|
| B97D           |          |                  |                  |
| wB97XD         |          |                  |                  |
| B3LYP-D3       |          |                  |                  |

| Bond Angle (°) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|----------------|----------|------------------|------------------|
| B97D           |          |                  |                  |
| wB97XD         |          |                  |                  |
| B3LYP-D3       |          |                  |                  |
Figure S5. (a) bond lengths (in Å), (b) bond angles, and (c) dihedral angles (in degrees) for the isolated DDTF and for DDTF interacting with (6,5) and (8,7) SWCNTs obtained using B97D, wB97XD, and B3LYP-D3 with 6-31G(d) basis set.
| Bond Length (Å) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|----------------|----------|------------------|------------------|
|                | B97D     | wB97XD           | B3LYP-D3         |
| 1-2            |          |                  |                  |
| 2-3            |          |                  |                  |
| 3-4            |          |                  |                  |
| 4-5            |          |                  |                  |
| 5-6            |          |                  |                  |

| Bond Angle (deg) | Isolated | With (6,5) SWCNT | With (8,7) SWCNT |
|------------------|----------|------------------|------------------|
|                  | B97D     | wB97XD           | B3LYP-D3         |
| 1-2-3            |          |                  |                  |
| 2-3-4            |          |                  |                  |
| 3-4-5            |          |                  |                  |
| 4-5-6            |          |                  |                  |
Figure S6. (a) bond lengths (in Å), (b) bond angles, and (c) dihedral angles (in degrees) for the isolated BDOB and for BDOB interacting with (6,5) and (8,7) SWCNTs obtained using B97D, wB97XD, and B3LYP-D3 with 6-31G(d) basis set.