Supplemental material

1. New force field parameters

We have derived new force field potentials describing the interaction between the BNNT and a silane coupling agent covalently bonded to the tube by one of its oxygens. The form of the proposed potentials and their fitted parameters are summarized in Tabs. 1S, 2S, and 3S. The data was generated with DFT calculations, using the functional B3LYP and basis set 6-31++G(d,p), implemented in the software Gaussian [37]. This ab initio method allowed us to compute the full system's potential energy for a given set of bond lengths and bond and dihedral angles. The ab initio data was then fitted to analytical expressions for the bond, angle, and torsional potentials, with the form reported in Tabs. 1S, 2S and 3S, resulting in the parameter values shown in the tables.

Table 1S. Bond stretching potentials

Bonds	$V_{bonds} = K_r (r - r_0)^2$	
	r_0 / Å	K_r / eV
B-O	1.472	13.283
Si-O	1.629	17.602
C-Si	1.880	8.988
O-H	0.975	26.521

Table 2S. Bond angle potentials

Angles	$V_{angles} = K_\theta (\theta - \theta_0)^2$	
	θ_0 / degrees	K_θ / eV
O-B-N	118.676	3.934
B-O-Si	134.850	1.462
O-Si-O	113.414	3.080
O-Si-C	109.558	3.075
Si-O-H	116.953	1.094
C-C-Si	116.134	2.379

Table 3S. Dihedral angle potentials

Dihedrals	$V_{dihedrals} = \sum_{i=1,m} K_i \left[1.0 + \cos\left(n_i\phi - d_i\right)\right]$															
	m	K_1	n_1	d_1	K_2	n_2	d_2	K_3	n_3	d_3	K_4	n_4	d_4	K_5	n_5	d_5
Si-O-B-N	5	-0.039	2	41.28	-0.018	1	12.3	0.003	3	130.9	0.075	4	174.4	0.0753	4	-37.65
B-O-Si-O	3	0.098	3	0.0426	-0.089	1	0.069	0.071	0	-9.449	--	--	--	--	--	--
C-Si-O-B	3	0.099	3	5.825	0.091	1	-50.19	-0.02	0	-0.936	--	--	--	--	--	--
O-Si-O-H	4	-0.064	2	-75.21	0.005	1	58.38	0.02	3	94.23	0.013	4	114.6			
H-O-Si-C	3	0.117	0	-9.215	7.331	1	1.399	-7.404	1	0.266	--	--	--	--	--	--
O-Si-C-C	3	0.031	3	0.815	0.0006	1	0.260	0.0001	0	0.594	--	--	--	--	--	--
Si-C-C-C	4	0.04	2	-7.06	0.093	1	-14.68	0.0655	3	-7.66	-0.037	0	-9.802	--	--	--

2. **Estimation of the van der Waals interaction frequency between the BNNT and PE.**

To estimate the phonon frequency associated to the van der Waals interaction between BNNT and PE, we have calculated in the simulations the van der Waals potential energy U_{LJ} as a function of the distance between them, as shown in Fig. 1S. Then, the phonon or vibration frequency was estimated by the formula

$$\omega = \sqrt{K / m^*} \tag{1}$$

where K is a force constant calculated by harmonic approximation

$$U_{LJ} = \frac{1}{2} K (r - r_0)^2 \tag{2}$$

and m^* is the reduced mass between BNNT and polyethylene

$$\frac{1}{m^*} = \frac{1}{m_{BNNT}} + \frac{1}{m_{PE}} \tag{3}$$

yielding about 5.95THz.

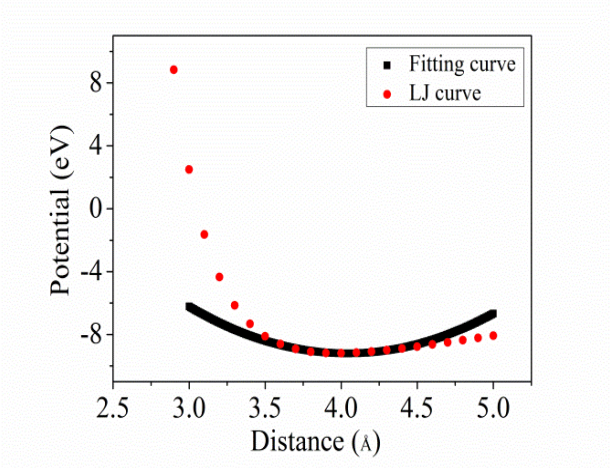

Figure 1S. The interface potential between the BNNT and polyethylene. The red dots are the original simulation data and the black line is the fitting curve.