Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

On the chirality-dependent adsorption behavior of volatile organic compounds on carbon nanotubes

Bin Li and Changwen Mi*

Jiangsu Key Laboratory of Engineering Mechanics, School of Civil Engineering, Southeast University, Nanjing, Jiangsu 210096, China

E-mail: mi@seu.edu.cn

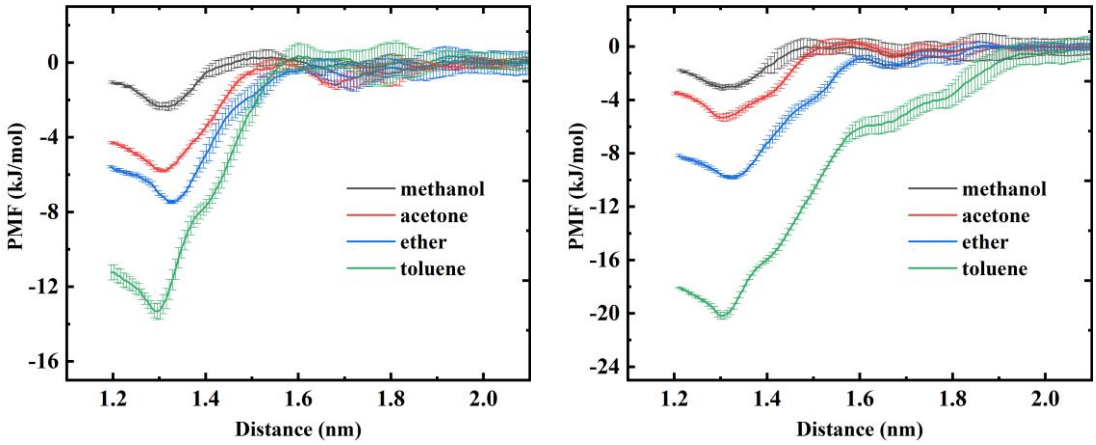

Fig. S1 PMF profiles corresponding to pulling one VOC molecule from the surface of CNT (14,14) for simulation systems having 1 VOC molecule and 20 VOC molecules, respectively.

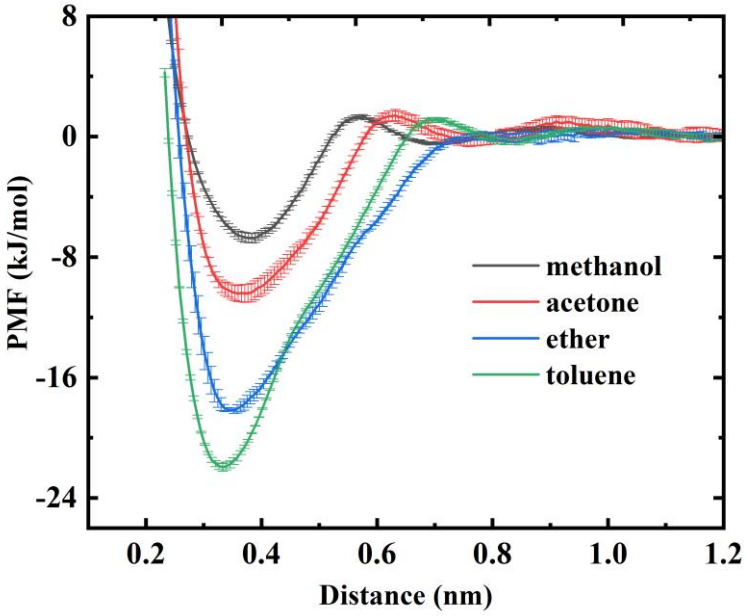

Fig. S2 PMF profiles of four VOC species corresponding to pulling a single molecule from the surface of graphene.

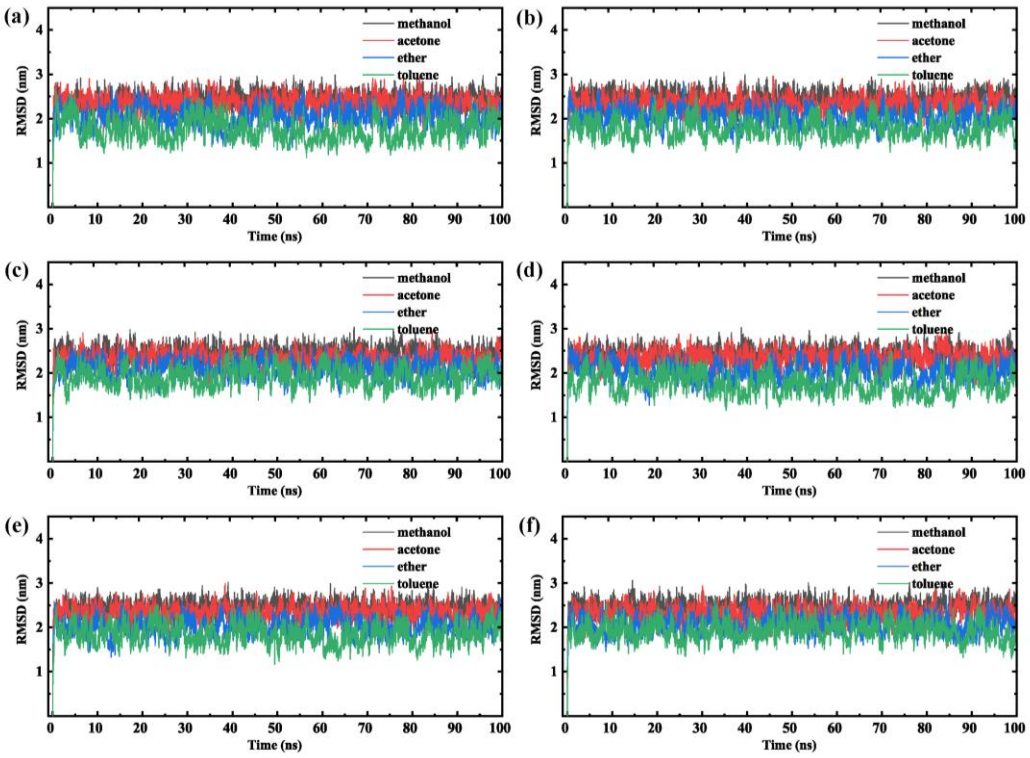

Fig. S3 The root mean square deviation for four VOC species with respect to their initial structures as a function of time. (a) CNT(6, 6), (b) CNT(10, 10), (c) CNT(14, 14), (d) CNT(10, 0), (e) CNT(17, 0) and (f) CNT(24, 0).

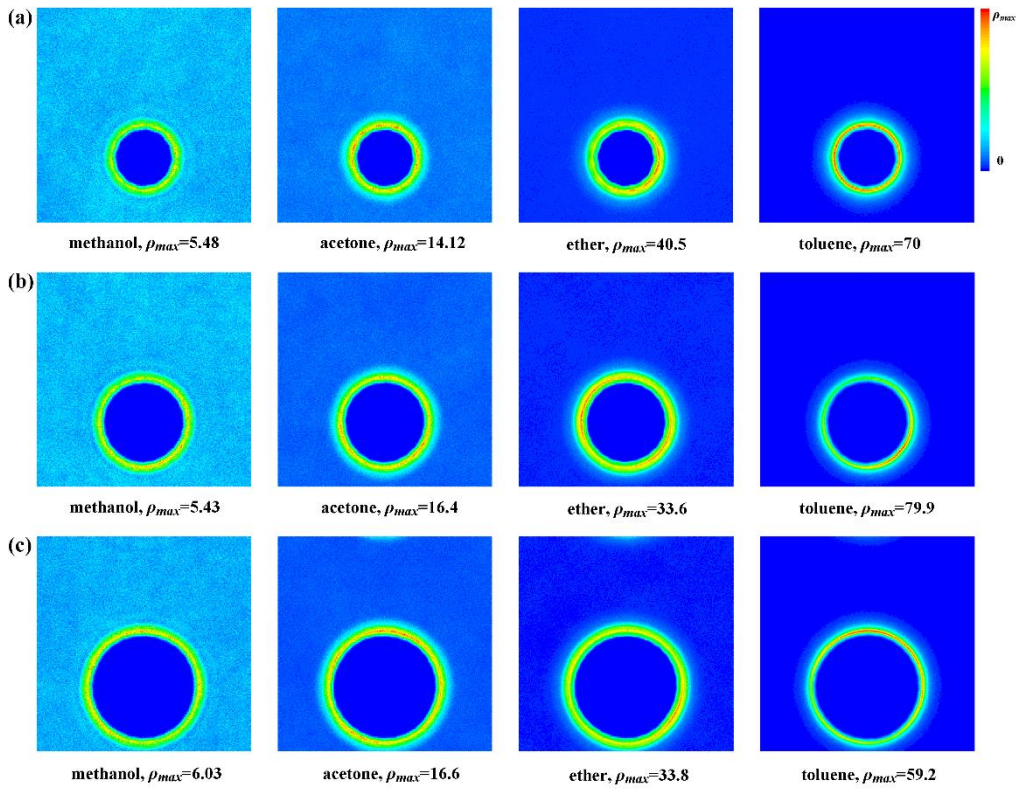

Fig. S4 The number densities of the four VOC species over the entire production simulation period. (a) CNT(6, 6), (b) CNT(10, 10) and (c) CNT(14, 14).

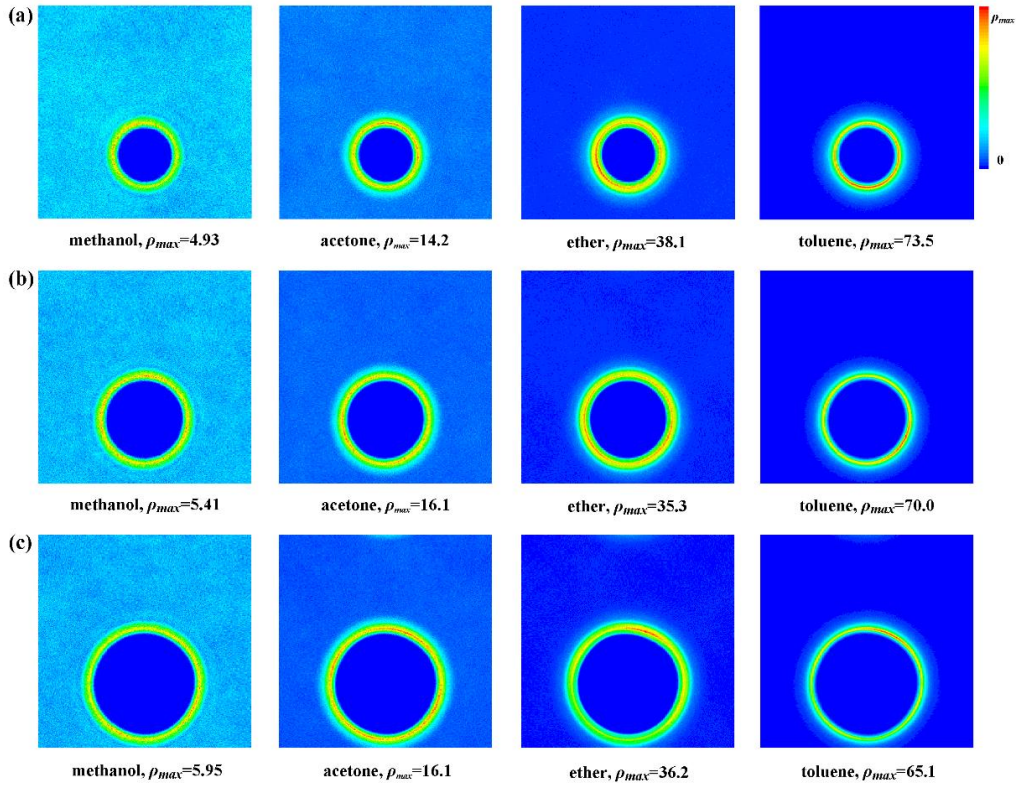

Fig. S5 The number densities of the four VOC species over the entire production simulation period (in nm^{-3}). (a) CNT(10, 0), (b) CNT(17, 0) and (c) CNT(24, 0).

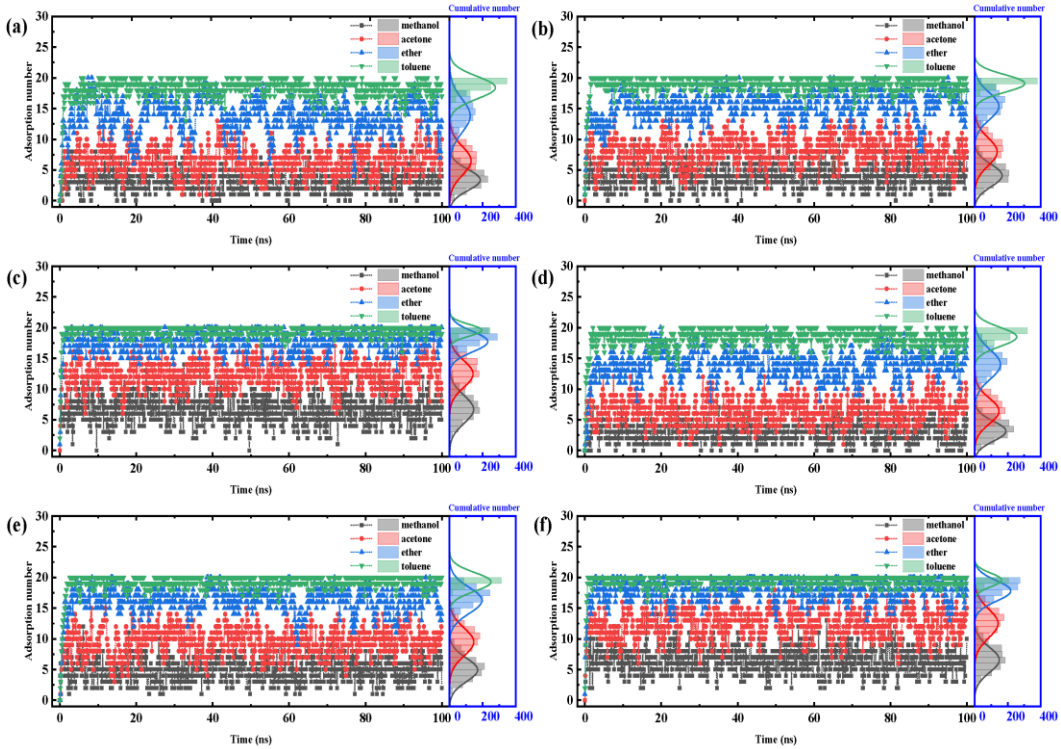

Fig. S6 The molecule number of the four VOC species adsorbed on the surface of CNTs over the entire production simulation period. (a) CNT(6, 6), (b) CNT(10, 10), (c) CNT(14, 14), (d) CNT(10, 0), (e) CNT(17, 0) and (f) CNT(24, 0).

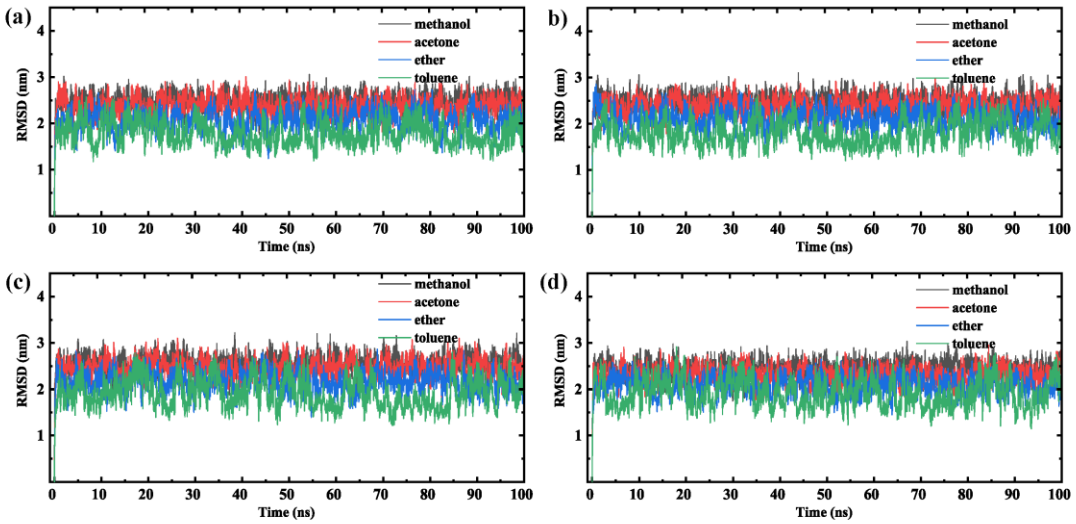

Fig. S7 The root mean square deviation of VOC molecules with respect to their initial structures as a function of time. (a) CNT(8, 7), (b) CNT(13, 0), (c) CNT(10, 6) and (d) CNT(14, 0).

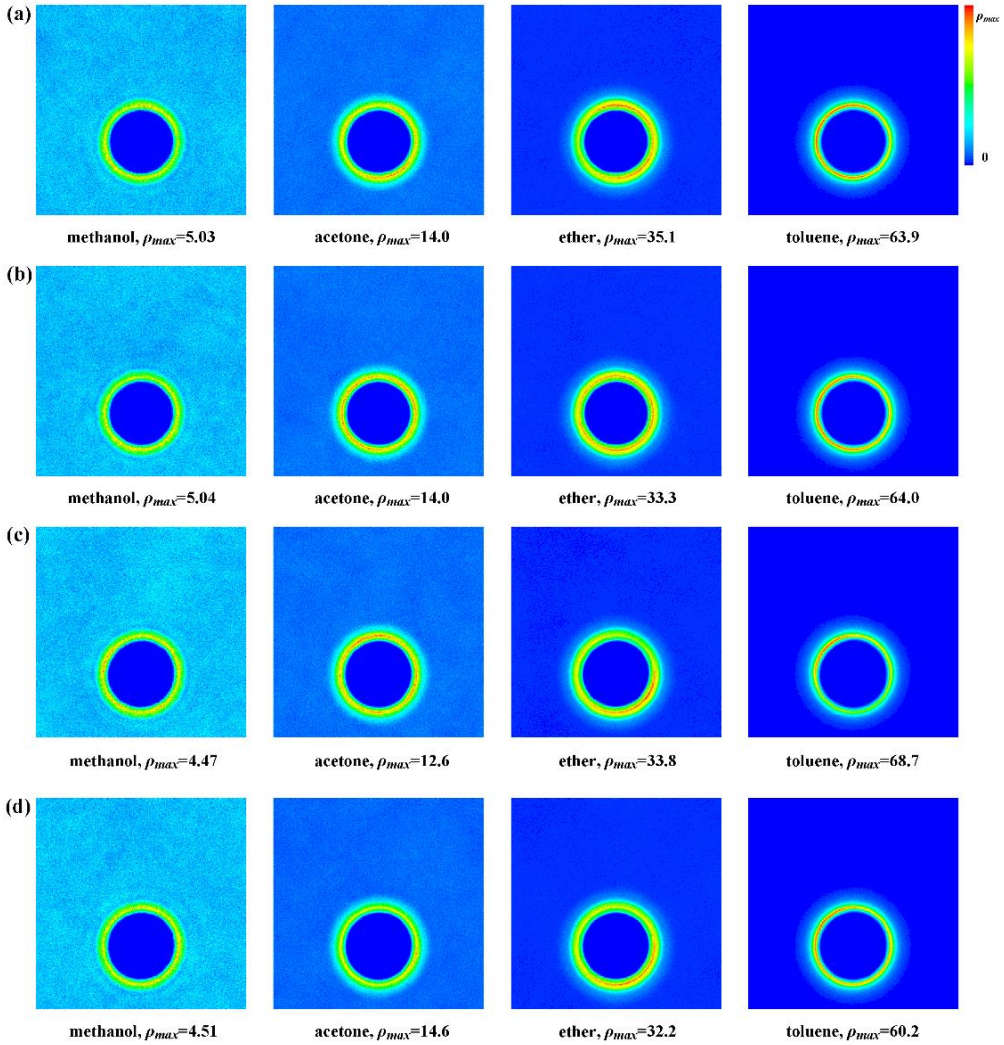

Fig. S8 The number densities of the four VOC species over the entire production simulation period (in nm^{-3}). (a) CNT(8, 7), (b) CNT(13, 0), (c) CNT(10, 6) and (d) CNT(14, 0).

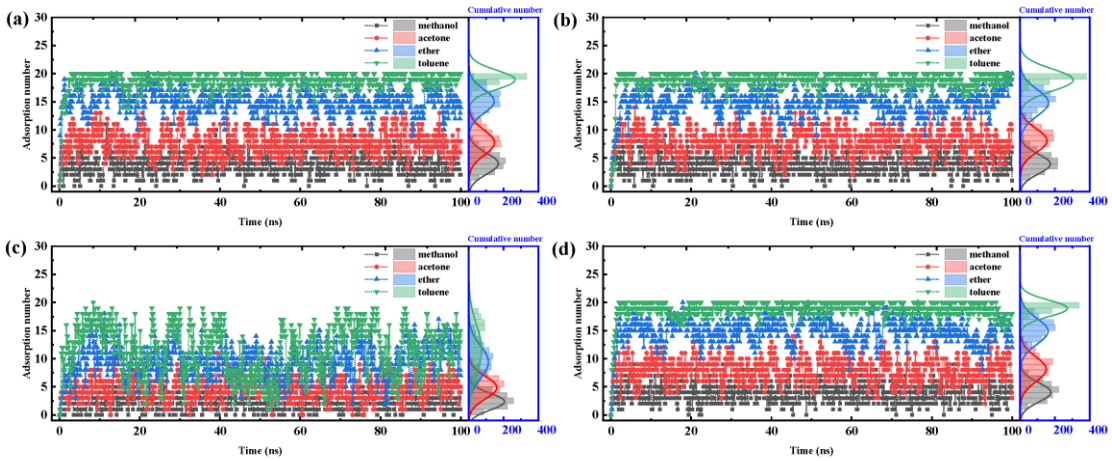

Fig. S9 The molecule number of the four VOC species adsorbed on the surface of CNTs over the entire production simulation period. (a) CNT(8, 7), (b) CNT(13, 0), (c) CNT(10, 6) and (d) CNT(14, 0).

Table S1 Average distance between the center of mass of VOC molecules and CNTs/graphene surface (in Å)

System	methanol		acetone		ether		toluene	
CNTs	d_{avg}	d^*	d_{avg}	d^*	d_{avg}	d^*	d_{avg}	d^*
(10,0)	4.24±0.84	3.49	4.21±0.54	3.58	4.26±0.59	3.62	4.22±0.86	3.45
(17,0)	4.14±0.71	3.59	4.15±0.71	3.62	4.28±0.55	3.74	4.07±0.59	3.52
(24,0)	4.23±0.64	3.57	4.22±0.57	3.59	4.24±0.59	3.76	4.04±0.50	3.46
(6,6)	4.26±0.60	3.55	4.20±0.56	3.70	4.32±0.53	3.73	4.25±0.77	3.49
(10,10)	4.27±0.55	3.65	4.24±0.52	3.62	4.21±0.61	3.75	4.09±0.60	3.49
(14,14)	4.15±0.83	3.56	4.21±0.61	3.60	4.27±0.61	3.79	3.95±0.54	3.54
(8,7)	4.19±0.78	3.46	4.24±3.56	3.56	4.31±0.65	3.60	4.13±0.62	3.43
(13,0)	4.13±0.52	3.64	4.17±0.59	3.63	4.38±0.71	3.50	4.13±0.63	3.76
(10,6)	4.00±0.46	3.63	4.11±0.55	3.55	4.28±0.60	3.72	4.08±0.60	3.54
(14,0)	4.26±0.77	3.54	4.12±0.51	3.62	4.35±0.67	3.73	4.09±0.57	3.50
Graphene	4.09±0.53	3.83	4.08±0.48	3.88	4.17±0.45	3.52	3.90±0.43	3.33

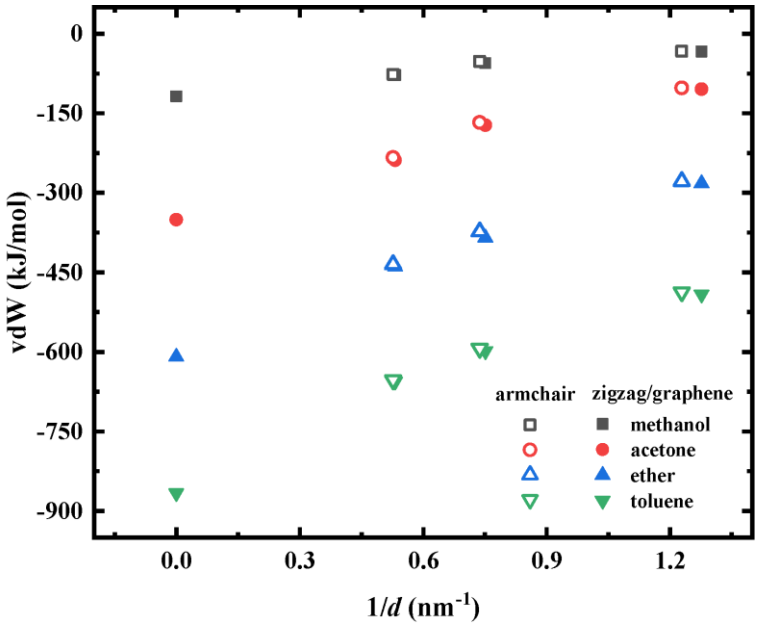

Fig. S10 The vdW interaction energies between four types of VOC molecules and CNTs/graphene, extracted from the total energies in the adsorbed states.