Electronic Supplementary Information

Covalent-organic framework as a template to assemble carbon nanotubes into a high-density membrane: computational demonstration

Zhongqiao Hu and Jianwen Jiang*

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

Table S1. Lennard-Jones parameters and atomic charges. The LJ parameters for COF-8 and $CHCl_3$ atoms are adopted from the Amber force field (ref. 1), except for B atom that is from ref. 2. The parameters for C atom in CNT are from ref. 3.

Species	Atoms	σ (nm)	ε (kJ/mol)	q (e)
COF-8	B	0.3960	0.1423	+0.5029
	O	0.2960	0.8786	–0.4193
	C1	0.3400	0.3598	–0.0676
	C2	0.3400	0.3598	+0.3381
	C3	0.3400	0.3598	+0.1563
	C4	0.3400	0.3598	–0.2403
	H	0.2650	0.0657	+0.1120
$CHCl_3$	C	0.2789	0.2466	–0.3847
	Cl	0.3564	1.3598	+0.0396
	H	0.3011	0.6897	+0.2659
CNT	C	0.3400	0.3598	0

Table S2. Parameters of bond stretching and bending potentials for $CHCl_3$.

Stretching		
i-j	k_r [10^5 kJ/(mol·nm^2)]	r_0 (nm)
C-Cl	1.9447	0.1758
C-H	2.8451	0.1100

Bending		
i-j-k	k_θ (10^2 kJ/mol)	θ_0 (degree)
Cl-C-H	3.1882	107.68
Cl-C-Cl	6.5019	111.30

(1) Cornell, W. D.; Cieplak, P.; Bayly, C. I.; Gould, I. R.; Merz, K. M.; Ferguson, D. M.; Spellmeyer, D. C.; Fox, T.; Caldwell, J. W.; Kollman, P. A. A 2nd Generation Force-Field for the Simulation of Proteins, Nucleic-Acids, and Organic-Molecules. *J. Am. Chem. Soc.* **1995**, *117*, 5179-5197.

(2) Tafi, A.; Agamennone, M.; Tortorella, P.; Alcaro, S.; Gallina, C.; Botta, M. Amber Force Field Implementation of the Boronate Function to Simulate the Inhibition of Beta-Lactamases by Alkyl and Aryl Boronic Acids. *Eur. J. Med. Chem.* **2005**, *40*, 1134-1142.

(3) Hummer, G.; Rasaiah, J. C.; Noworyta, J. P. Water Conduction through the Hydrophobic Channel of a Carbon Nanotube. *Nature* **2001**, *414*, 188-190.