Supporting Information

A novel T-C_3N and seawater desalination

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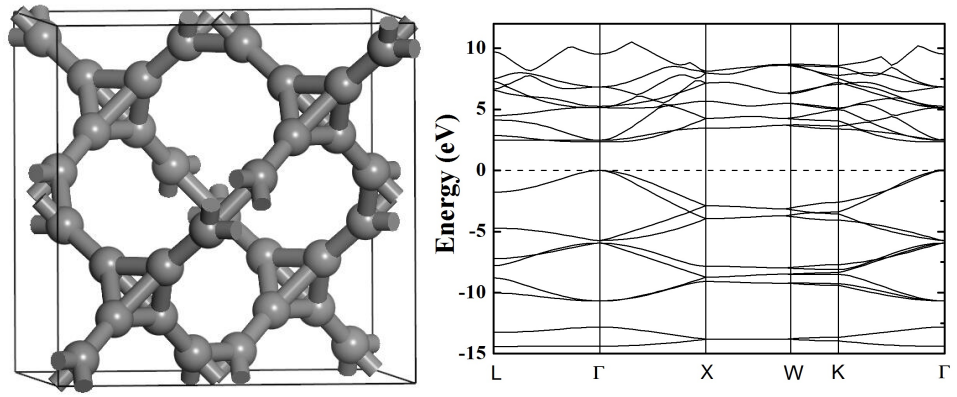
1 Pristine T-carbon



(a) T-carbon **(b) Band maps**

Figure ESI-1 (a) Sketch for the pristine T-carbon, and (b) its band maps calculated at PBE-D3 level. The Fermi level has been shifted to zero.

Table ESI-1 The lattice constant (l), bond length (d), Young's modulus (Y), bulk modulus (B), shear modulus (G), band gap (E_g) of T-carbon and cubic diamond. Note that the bond lengths of the intertetrahedron C−C bonds are listed in parentheses. Note again that the theoretical values listed here are all obtained from computer simulations at GGA level. The huge band gap reported in the experimental work for T-carbon is actually obtained from a G_0W_0 calculation. However, the convergence of this calculation is doubtful. We will discuss this point in another work.

		l (Å)	d (Å)	Y (GPa)	B (GPa)	G (GPa)	E_g (eV)
T-carbon	This work	7.473	1.492 (1.408)	126	166	46	2.201
	Theor.[1]	7.520	1.502 (1.417)	-	169	70	2.25
	Theor.[2]	7.49	1.500 (1.416)	-	161	48	2.25
	Exp.[3]	7.80	1.56 (1.47)	-	-	-	5.10
c-diamond	This work	3.557	1.540	1159	452	540	4.198
	Theor.[1]	3.566	1.544	-	464	-	4.16
	Theor.[4]	-	1.547	1116.4	434.9	520.6	-
	Exp.[5, 6, 7, 8]	3.567	1.54	1100	443	478.0	5.45

2 B doping in T-carbon

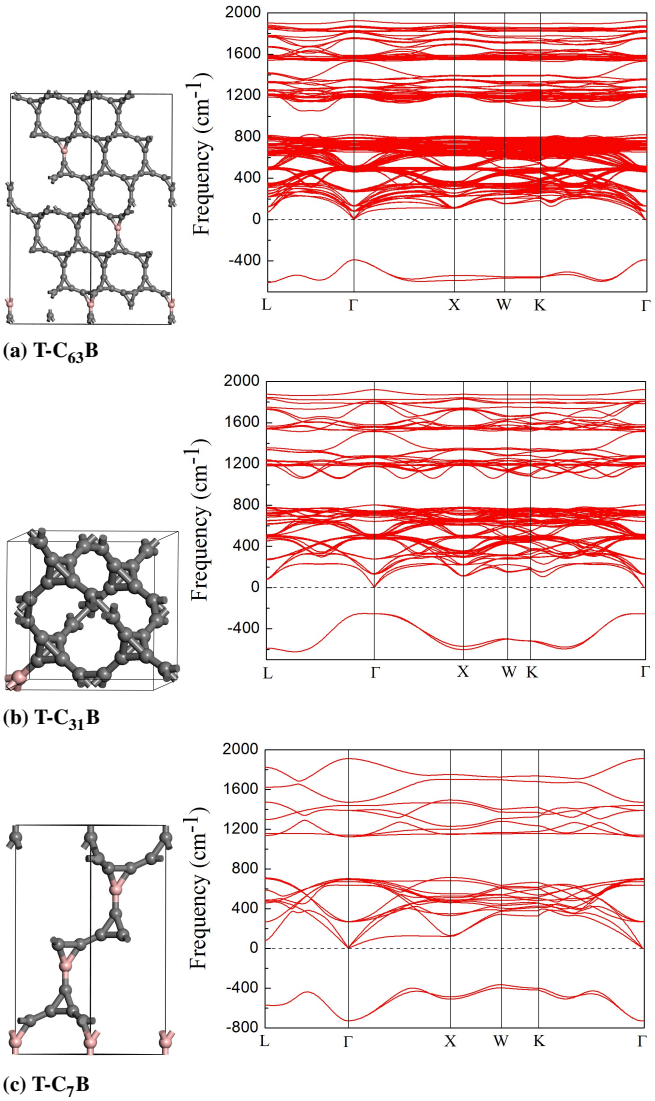
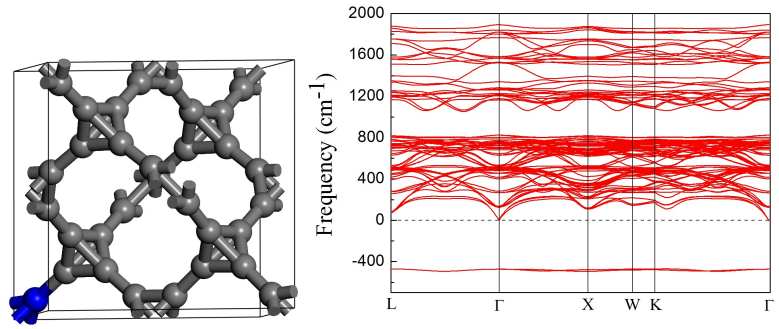
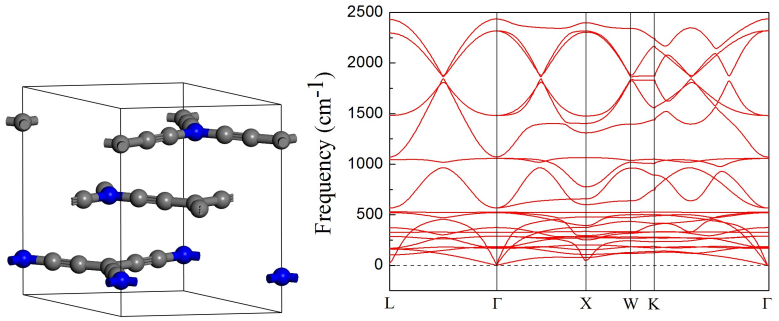


Figure ESI-2 Sketches for the B doping in T-carbon system with different dopant concentrations (left), and their phonon dispersion maps (right).

3 N doping in T-carbon



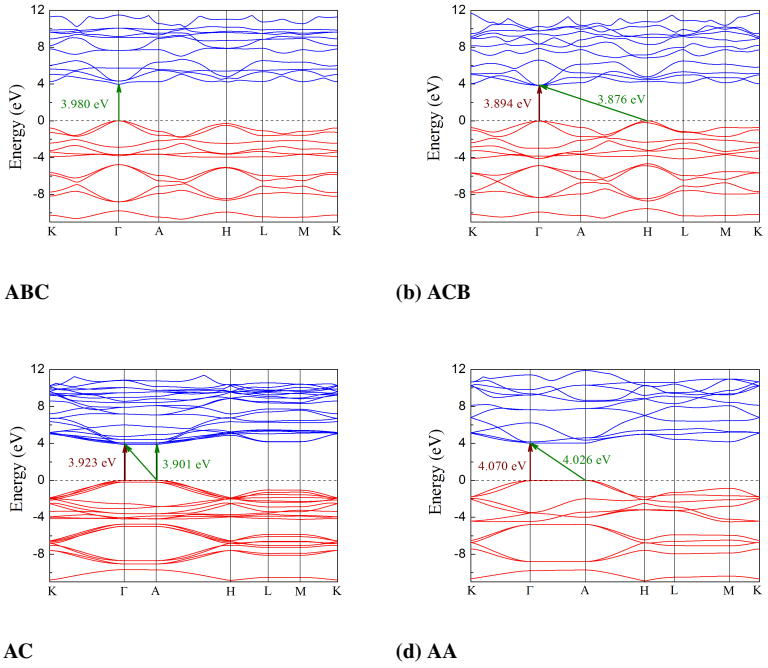
(a) T-C_{31}N



(b) C_7N ⇒ N doped α-graphyne

Figure ESI-3 Sketches for the N doping in T-carbon system with different dopant concentrations (left), and their phonon dispersion maps (right).

4 T-C_3N



(a) ABC **(b) ACB**

(c) AC **(d) AA**

Figure ESI-4 The electronic energy band structures for bulk T-C_3N with four different stacking forms. The sketches for the corresponding atomic configurations can be found in the main text.

5 PMF free energy for α-graphyne

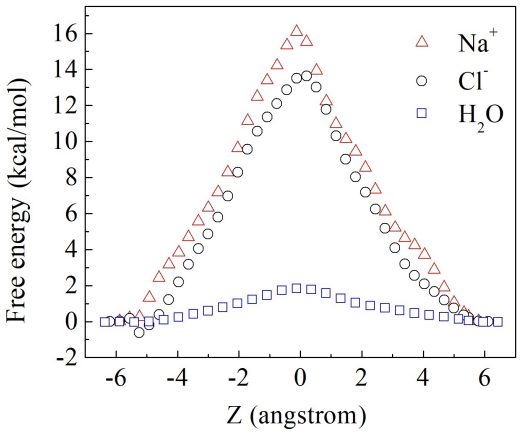


Figure ESI-5 PMF free energies for Na^+, Cl^-, and water across the α-graphyne monolayer obtained by using ASMD simulations which were also employed in the research discussed in main text for T-C_3N. The kinetic energy barriers for the permeation processes through α-graphyne monolayer obtained from our ASMD simulations are consistent very well with the literature report[9].

References

[1] X.-L. Sheng, Q.-B. Yan, F. Ye, Q.-R. Zheng, G. Su, T-carbon: A novel carbon allotrope, *Phys. Rev. Lett.* **106**, 155703 (2011).

[2] H. Ren, H. Chu, Z. Li, T. Yue, Z. Hu, Efficient energy gap tuning for T-carbon via single atomic doping, *Chem. Phys.* **518**, 69-73 (2019).

[3] J. Zhang, R. Wang, X. Zhu, A. Pan, C. Han, X. Li, D. Zhao, C. Ma, W. Wang, H. Su, C. Niu, Pseudo-topotactic conversion of carbon nanotubes to T-carbon nanowires under picosecond laser irradiation in methanol, *Nat. Commun.* **8**, 683 (2017).

[4] H. Dong, A. R. Oganov, Q. Zhu, G.-R. Qian, The phase diagram and hardness of carbon nitrides, *Sci. Rep.* **5**, 9870 (2015).

[5] C. Kittel, Introduction to Solid State Physics, *John Wiley & Sons, New York,* (1996).

[6] R. A. Andrievski, Superhard materials based on nanostructured high-melting point compounds: achievements and perspectives, *Int. J. Refract. Met. Hard Mater.* **19**, 447 (2001).

[7] Ph. Niedermann, W. Hänni, N. Blanc, R. Christoph, J. Burger, Chemical vapor deposition diamond for tips in nanoprobe experiments, *J. Vac. Sci. Technol. A* **14**, 1233 (1996).

[8] H. J. McSkimin, P. Andreatch, Jr., Elastic Mouli of Diamond as a Function of Pressure and Temperatur, *J. Appl. Phys.* **43**, 2944-2948 (1972).

[9] M. Xue, H. Qiu, W. Guo, Exceptionally fast water desalination at complete salt rejection by pristine graphyne monolayers, *Nanotechnology* **24**, 505720 (2013).