

Supporting Information for

Sulfur-Doped Crown Ether Graphane for Enhanced Helium Separation

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Table S1 The kinetic diameter (D) of gas molecules and the energy barrier (E_{barrier}) (eV) when passing through CG-S6 and CG-6 membranes, and the adsorption height (H) of gas molecules when stably adsorbed on CG-S6. The D values are obtained from reference¹.

	$D(\text{\AA})$	E_{barrier}		$H(\text{\AA})$
		CG-S6	CG-6	CG-S6
He	2.60	0.20	0.01	2.83
Ne	2.82	0.50	0.05	3.22
Ar	3.54	1.97	0.42	3.28
CH ₄	3.80	3.12	0.80	3.71
N ₂	3.64	1.52	0.16	3.01

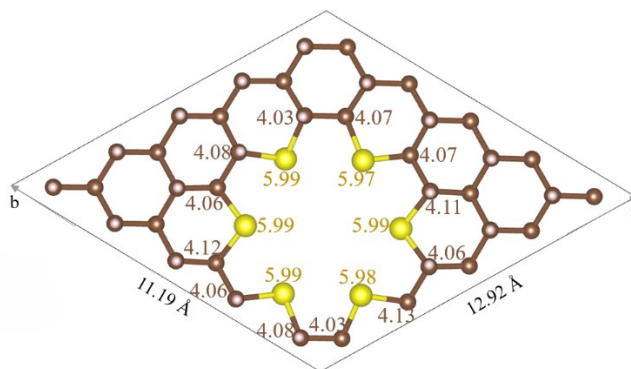


Fig. S1 Bader charge analysis of sulfur atoms and the adjacent carbon atoms in CG-S6.

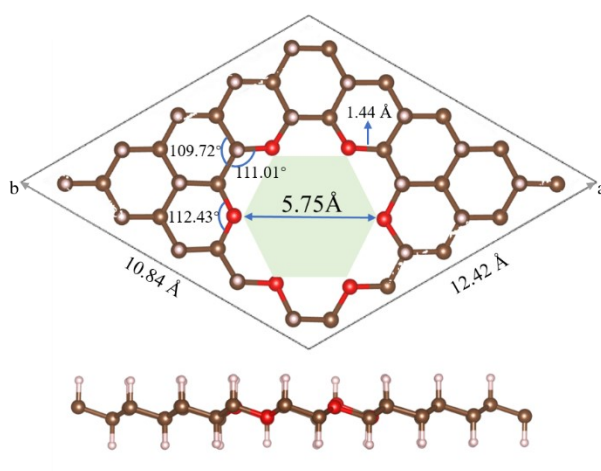


Fig. S2 Optimized structure and pore size of CG-6, with brown, red, and white spheres representing carbon, oxygen, and hydrogen atoms, respectively. The key bond lengths and bond angles are labeled for reference.

References

- 1 J.-R. Li, R. J. Kuppler and H.-C. Zhou, Selective gas adsorption and separation in metal–organic frameworks, *Chem. Soc. Rev.*, 2009, **38**, 1477.