

补充材料

冠醚石墨烷对氦气分离性能的理论研究*

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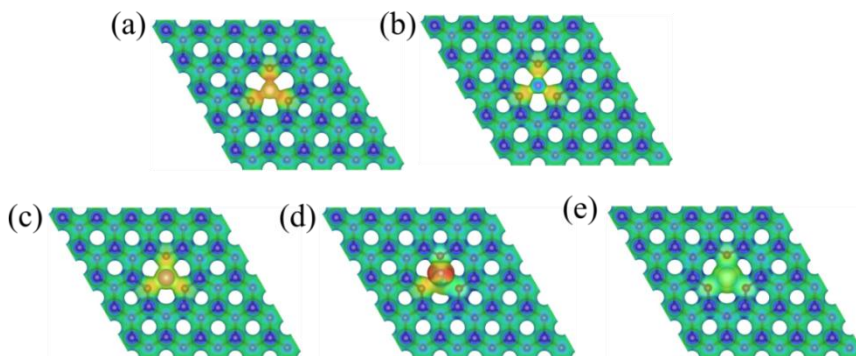


图 S1 气体通过 CG-3 的静电势等值面图 (a) He; (b) H₂; (c) Ne; (d) N₂; (e) Ar

Fig. S1. Electrostatic potential isosurfaces of (a) He, (b) H₂, (c) Ne, (d) N₂ and Ar molecules passing through CG-3 membrane.

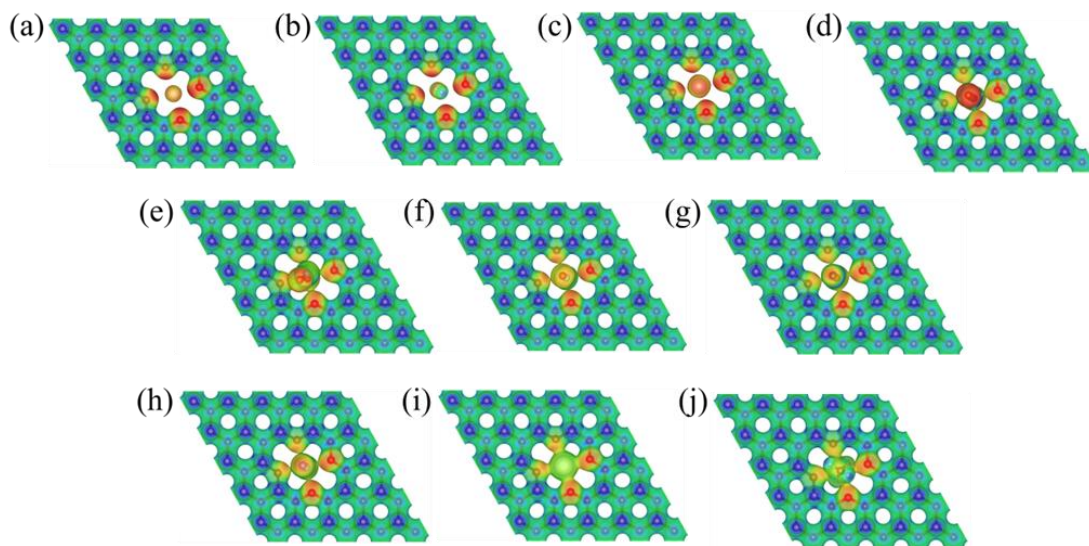


图 S2 气体通过 CG-4 的静电势等值面图 (a) He; (b) H₂; (c) Ne; (d) CO₂; (e) NO₂; (f) NO; (g) CO; (h) N₂; (i) Ar; (j) CH₄

Fig. S2. Electrostatic potential isosurfaces of (a) He, (b) H₂, (c) Ne, (d) CO₂, (e) NO₂, (f) NO, (g) CO, (h) N₂, (i) Ar and (j) CH₄ molecules passing through CG-4 membrane.

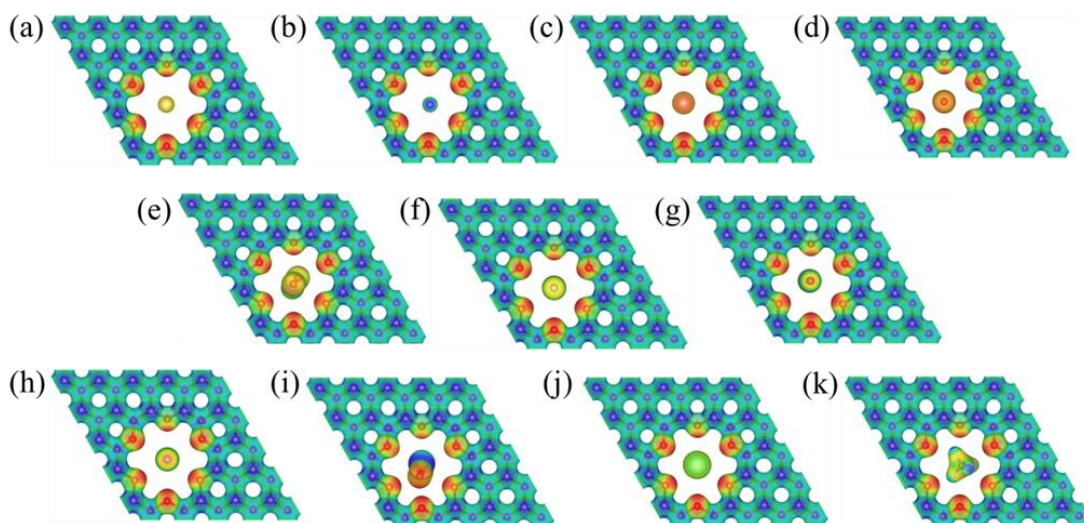


图 S3 气体通过 CG-6 的静电势等值面图 (a) He; (b) H₂; (c) Ne; (d) CO₂; (e) NO₂; (f) NO; (g) CO; (h) N₂; (i) Ar; (j) CH₄

Fig. S3. Electrostatic potential isosurfaces of (a) He, (b) H₂, (c) Ne, (d) CO₂, (e) NO₂, (f) NO, (g) CO, (h) N₂, (i) SO₂, (j) Ar, and (k) CH₄ molecules passing through CG-6 membrane.

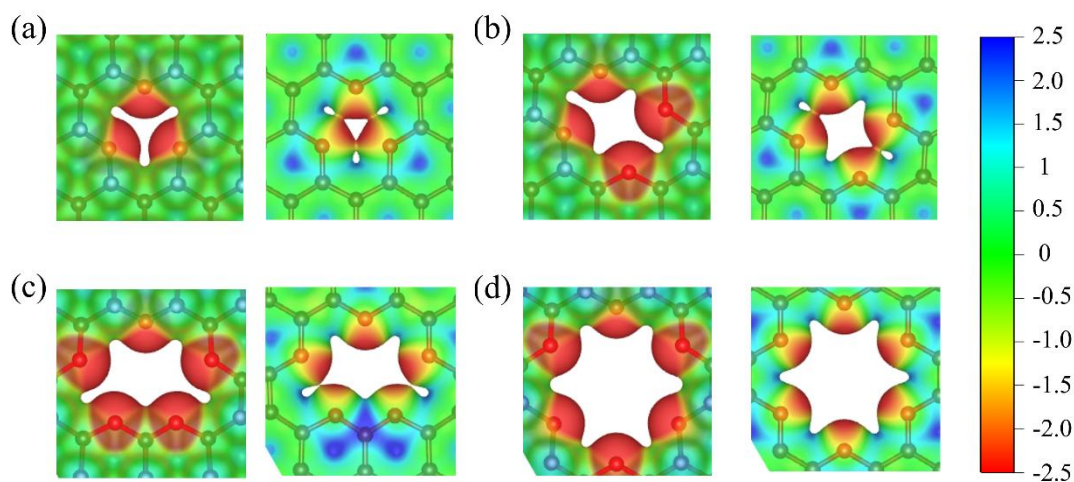


图 S4 冠醚石墨烷和含有同样大小冠醚孔的石墨烯结构的静电势等值面图 (a) CG-3; (b) CG-4; (c) CG-5; (d) CG-6

Fig. S4. Electrostatic potential isosurfaces of crown ether graphanes and graphenes containing the same crown ether nanopores (a) CG-3, (b) CG-4, (c) CG-5, (d) CG-6.