

Supporting Information

Heptazine-based graphitic carbon nitride as an efficient hydrogen purification membrane

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We test the influence of the periodicity of the adsorbates on the energy barrier. The permeation barrier of H₂ through 1×1 g-C₃N₄ is 0.55 eV and it through 2×2 g-C₃N₄ is 0.48 eV. The permeation barriers of gas molecules permeating 2x2 supercells are 0.1~0.2 eV lower than that in the 1x1 unit cell, indicating that the periodicity of adsorbates plays a role in the energy barriers. However, every pore of g-C₃N₄ is a possible pathway to diffuse when the surrounding is filled with massive gas molecules. Thus the structure of unit cell is adopted in our paper.

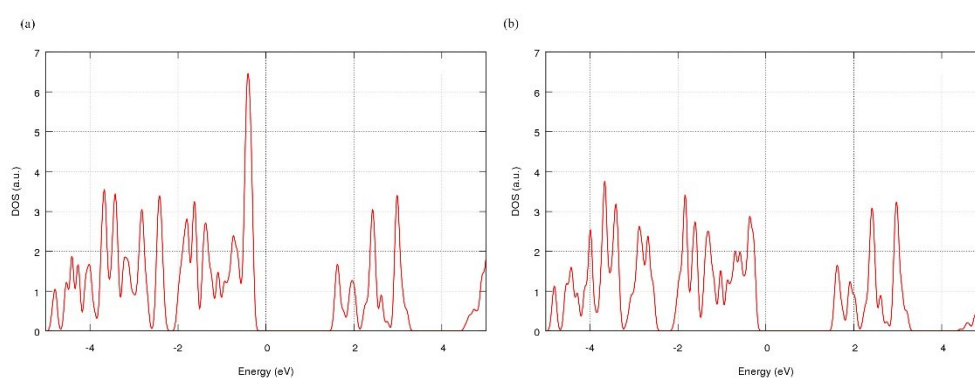


Figure S1. DOS of (a) H₂O adsorbed on g-C₃N₄ and (b) pure buckled g-C₃N₄.

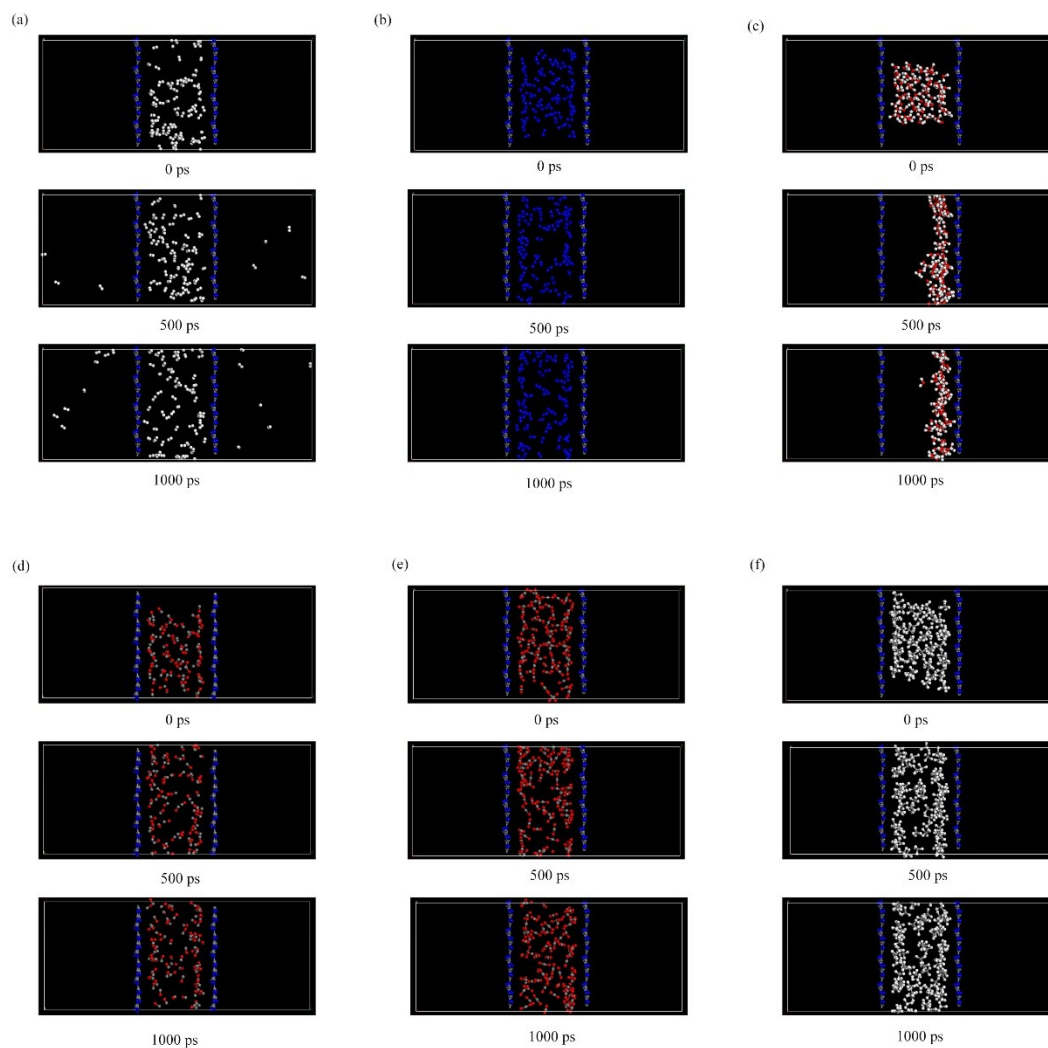


Figure S2. Snapshots of (a) H_2 , (b) N_2 , (c) H_2O , (d) CO , (e) CO_2 and (f) CH_4 permeating through $\text{g-C}_3\text{N}_4$ nanosheet in the 0~1000ps MD simulation at 300K. The blue, grey, white and red beads represent the nitrogen, carbon, hydrogen, and oxygen atoms respectively.