

Supplementary Information:

Exploration of functionalized graphene membranes for selective separating CO₂/N₂: a multi-scale computational study

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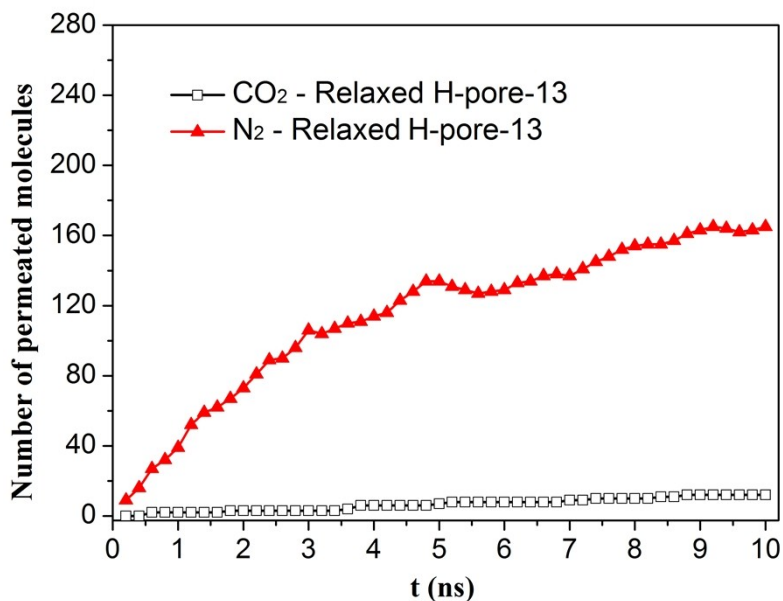


Fig. S1 The number profiles of permeated molecules for equimolar N₂/CO₂ mixture through the relaxed H-pore-13 graphene membranes at 298K, as a function of simulation time.

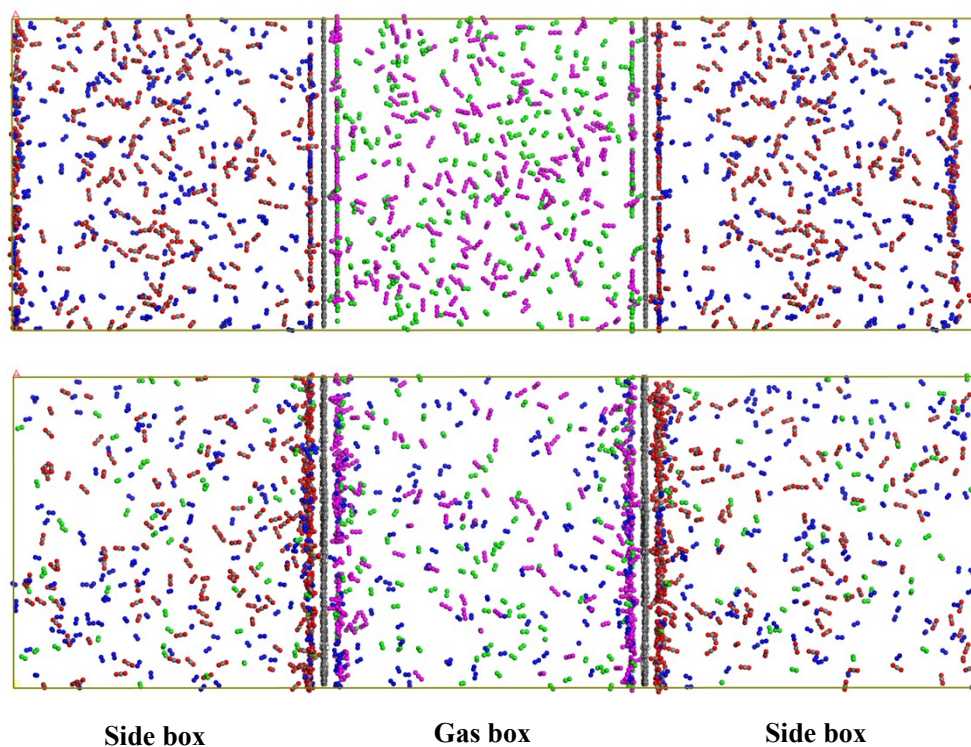


Fig. S2 Snapshots of the equimolar N₂/CO₂ mixture permeating through the relaxed H-pore-13 graphene membranes (a) before and (b) after a MD simulations time of 10 ns (C, gray or pink; N, blue or green; O, red or pink; H, white).

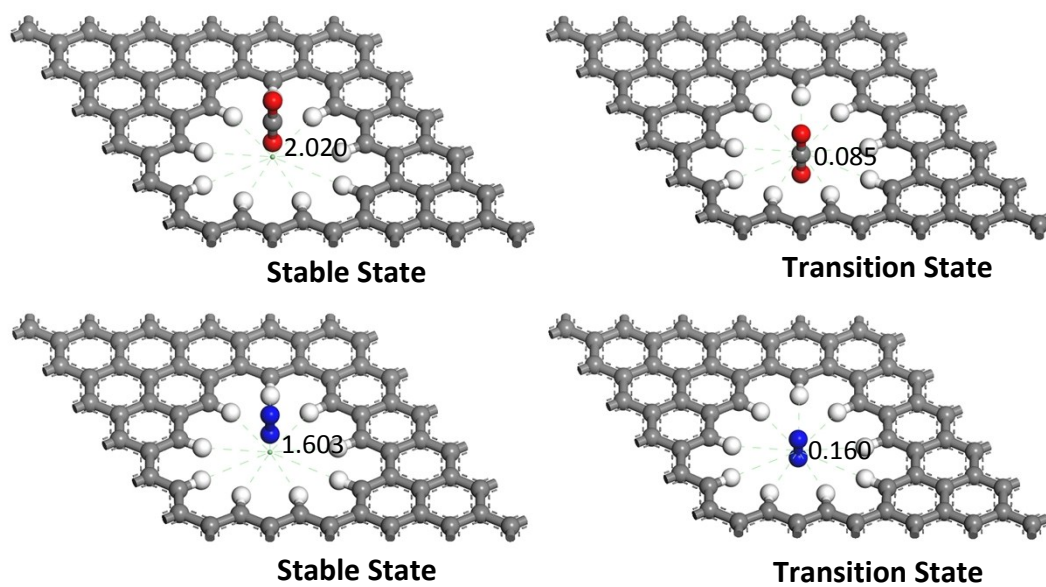


Fig. S3 The stable state and transition state for the CO₂ and N₂ gases passing through H-pore-13. (C, gray; N, blue, O, red; H, white).