Supplementary Information for

Molecular Dynamics Exploration of the Barrier Properties of Small Gas Molecules in the Semicrystalline Parylene C

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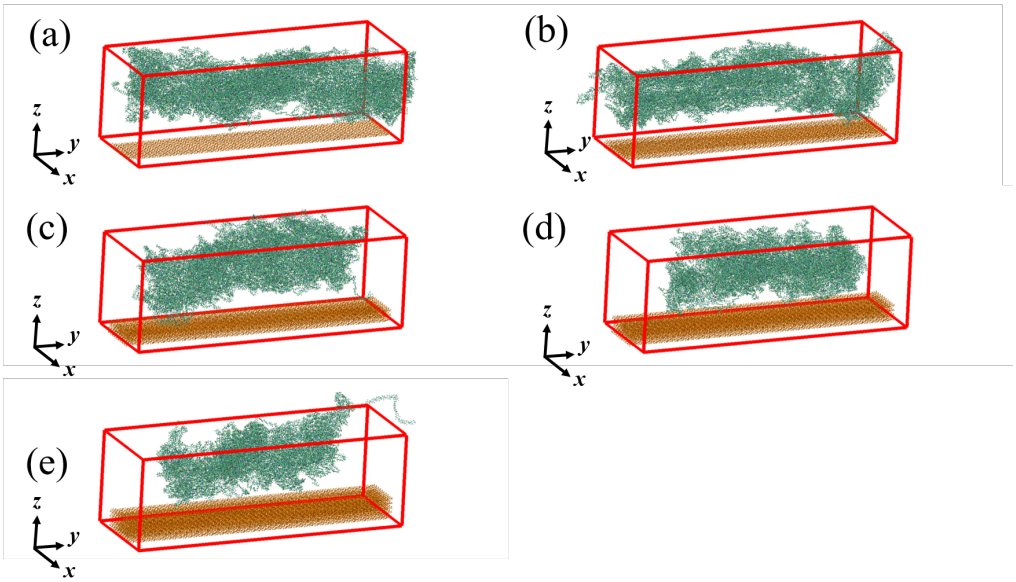

Fig. S1 Initial structures of parylene C models which contain 10%-50% aligned chains. (a) 10%; (b) 20%; (c) 30%; (d) 40%; (e) 50%.

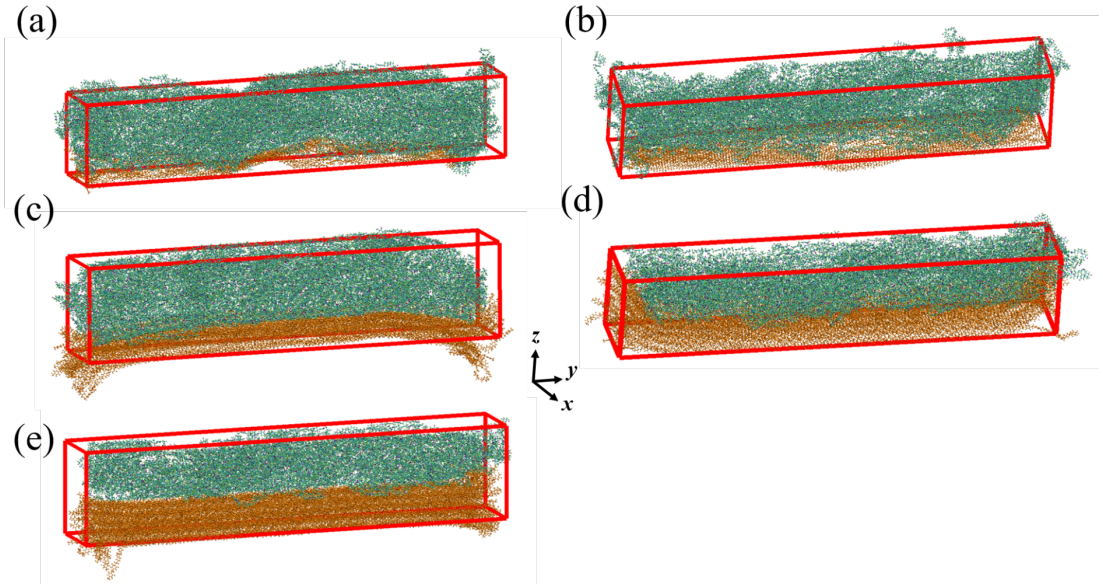

Fig. S2 Final structures of parylene C models with 17%-44% crystallinity. (a) 17%; (b) 24%; (c) 30%; (d) 34%; (e) 44%.

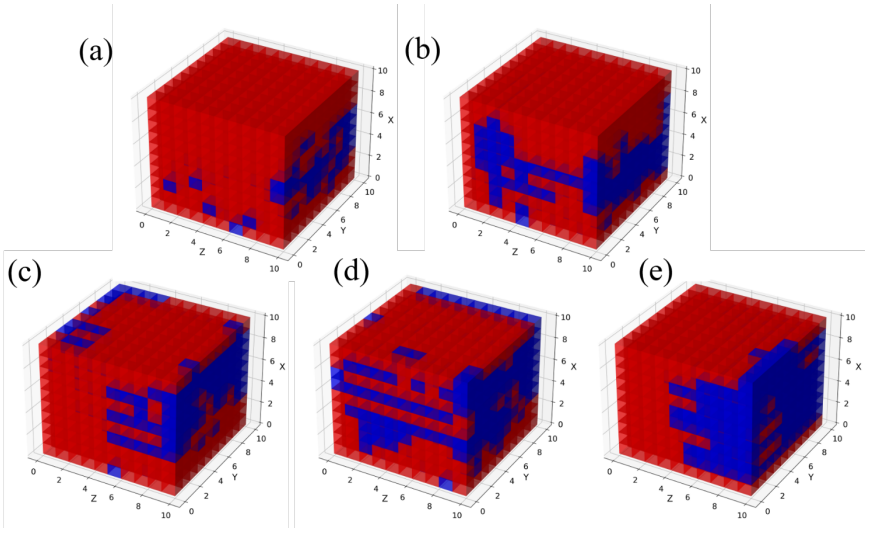

Fig. S3 The crystalline region (blue) and the amorphous region (red) in semi-crystalline parylene C with 50% transparency. The X-, Y- and Z-axis are defined as the number of bins. (a) 17% crystallinity; (b) 24% crystallinity; (c) 30% crystallinity; (d) 34% crystallinity; (e) 44% crystallinity.

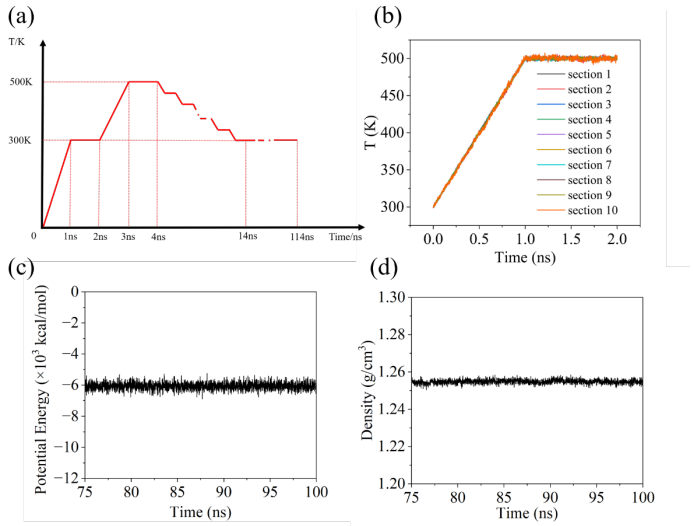

Fig. S4 (a) Schematic diagram of the whole simulated annealing and final 100 MD simulation. (b) Temperature change in the process of heating up and high temperature equilibrium using the 17% crystallinity parylene C as an example. (c) Potential energy evolution along the time course using the 17% crystallinity parylene C as an example. (d) Density evolution along the time course using the 17% crystallinity parylene C as an example.

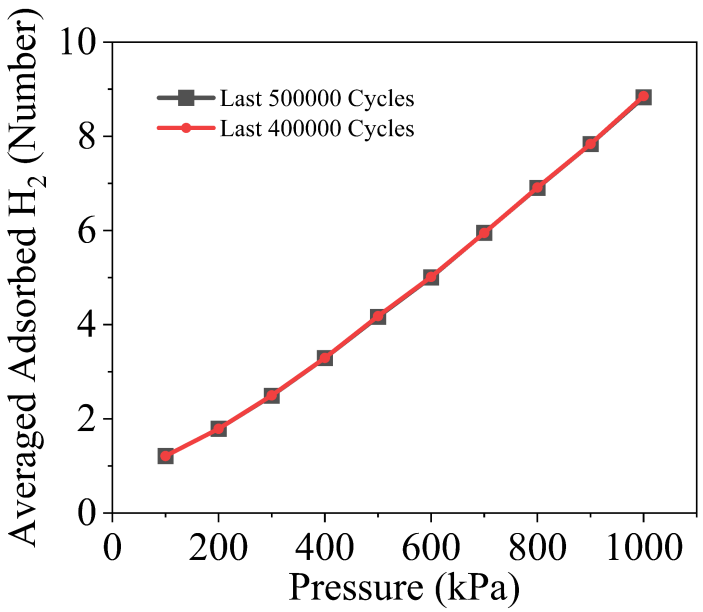

Fig. S5 The averaged adsorption of H_2 in 30% crystallinity parylene C.

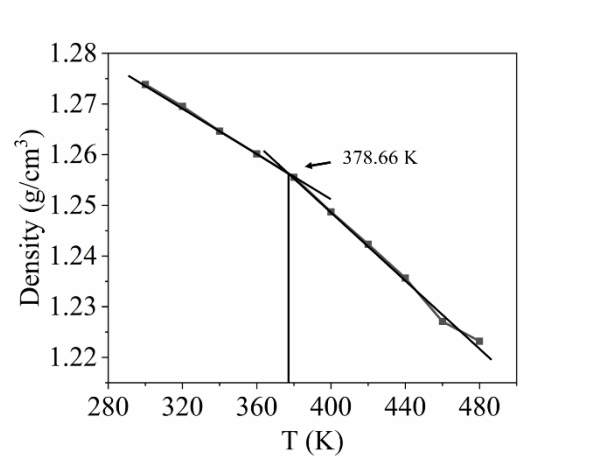

Fig. S6 The temperature dependence of density for the 44% crystallinity parylene C.

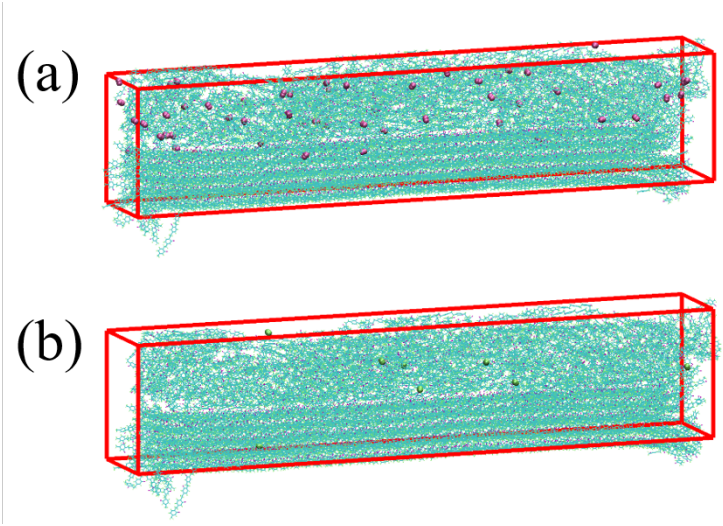

Fig. S7 The snapshots of (a) O_2 and (b) H_2 adsorbed in parylene C.

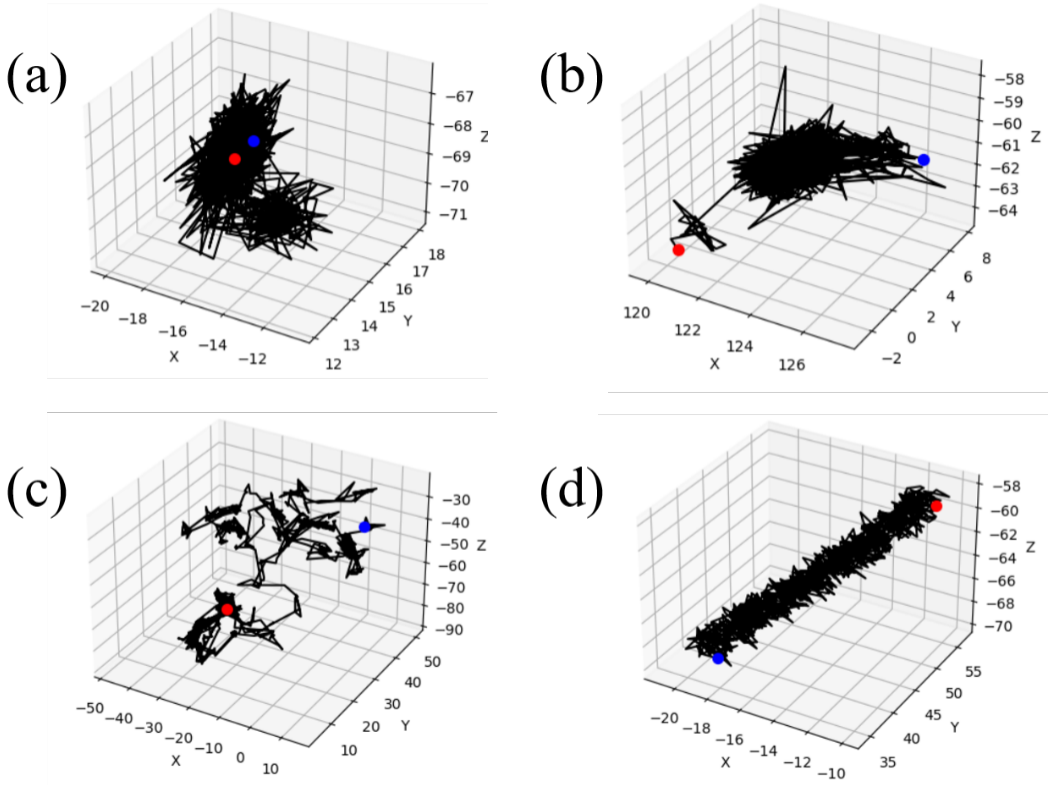

Fig. S8 One molecule diffusion trajectory of (a)N_2; (b)H_2O; (c)H_2; (d)O_2; The blue and red dots represent the position of the small molecule gas in the first and last frames, respectively.