

Supplementary Information:

High Selectivity of CO₂ Capture with Single- and Double-Walled Carbon Nanotubes

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Figure S1 shows the MD simulation result for a system consisting of (8, 8) SWCNT and a mixture of N₂ – O₂ in the reservoir. The mole fraction of the mixture is 0.5. As presented in Figure S1, the number of O₂ molecule in the CNT is higher than that of N₂ molecule. The result indicates that the CNT preferentially adsorbs O₂ instead of N₂. Using the data after 2 ns, the average mole fraction of O₂ in the CNT is 0.69. This means that the selectivity of S_{O_2/N_2} is 2.2.

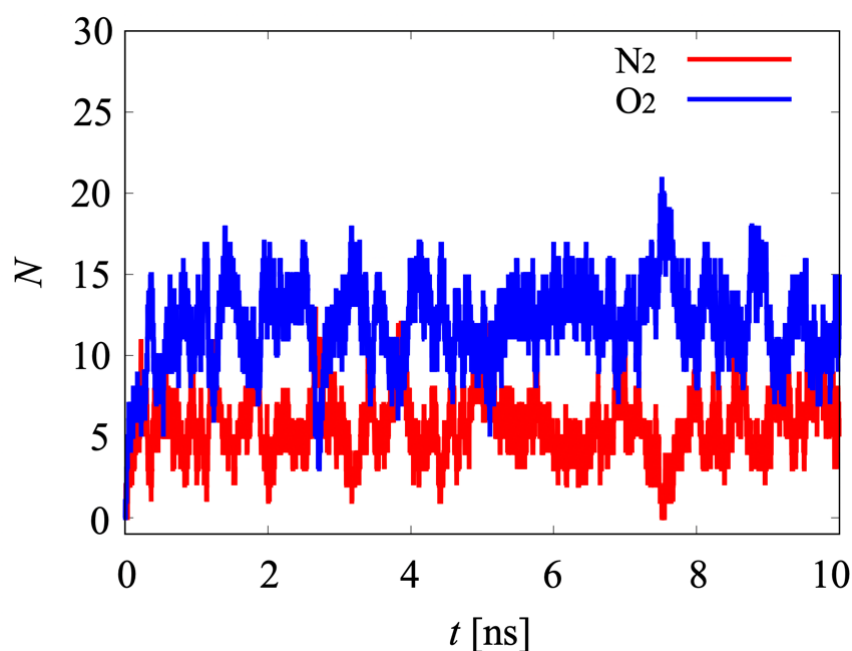


Figure S1 MD simulation with (8, 8) SWCNT and a N₂ – O₂ binary mixture in the reservoir. The vertical axis represents the number of molecules (N) inside the SWCNT.

Figure S2 shows snapshot of MD simulation for CO₂ – graphene sheets system without CNT with NVT constant at 300 K. The reservoir was filled with CO₂ gas molecules at 90 bar or at the density of 0.17 gram/cm³. The CO₂ molecules form solid ice structure at the

graphene sheets as shown in Figure S2-B.

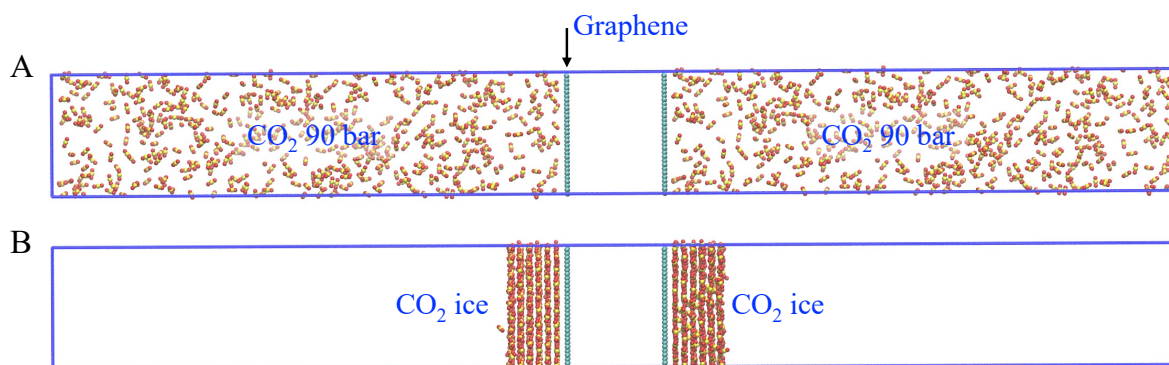


Figure S2 MD simulation of CO₂ – graphene system: (A) Initial condition, the pressure of CO₂ gas in the reservoir is 90 bar, (B) The CO₂ forms solid ice at the graphene sheets.

Figure S3 shows simulation of bulk system of CO₂ gas molecules at 6 bar or at the density of 0.009 gram/cm³. The simulation was performed with *NVT* constant at 300 K. The result indicates that the CO₂ molecules form solid ice structure as shown in Figure S3-B. The decrease of potential energy shown in Figure S4 confirms the phase transition of the CO₂ molecules.

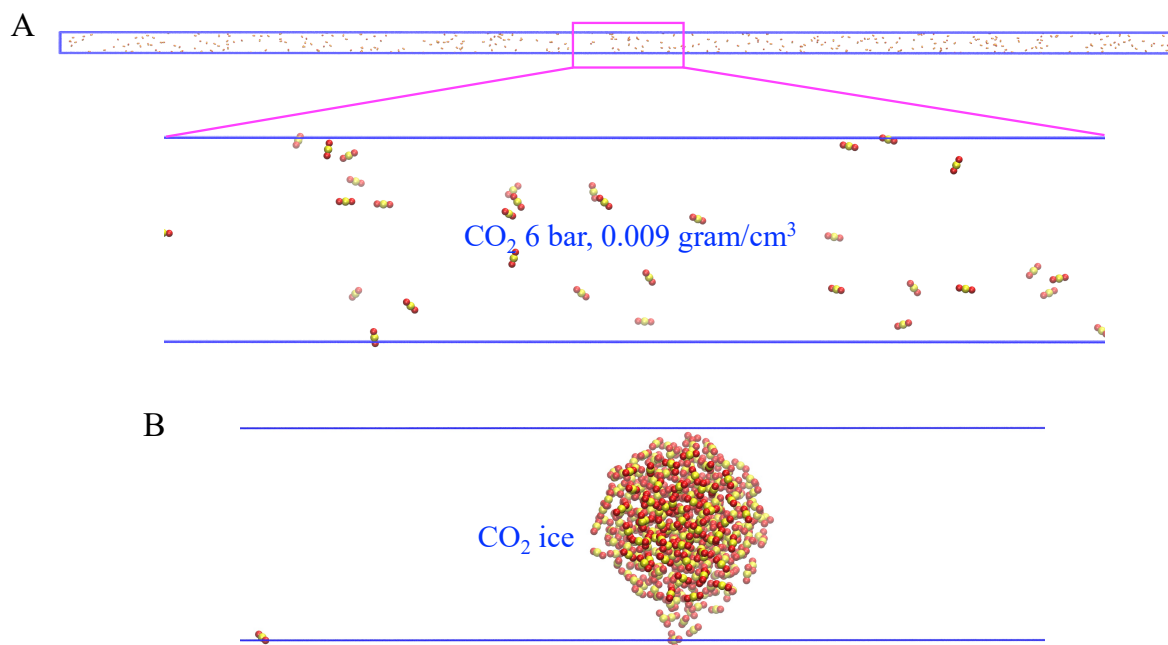


Figure S3 Simulation of CO₂ bulk system: (A) Initial condition, CO₂ gas is at 6 bar, 0.009 gram/cm³, (B) The CO₂ forms solid ice structure.

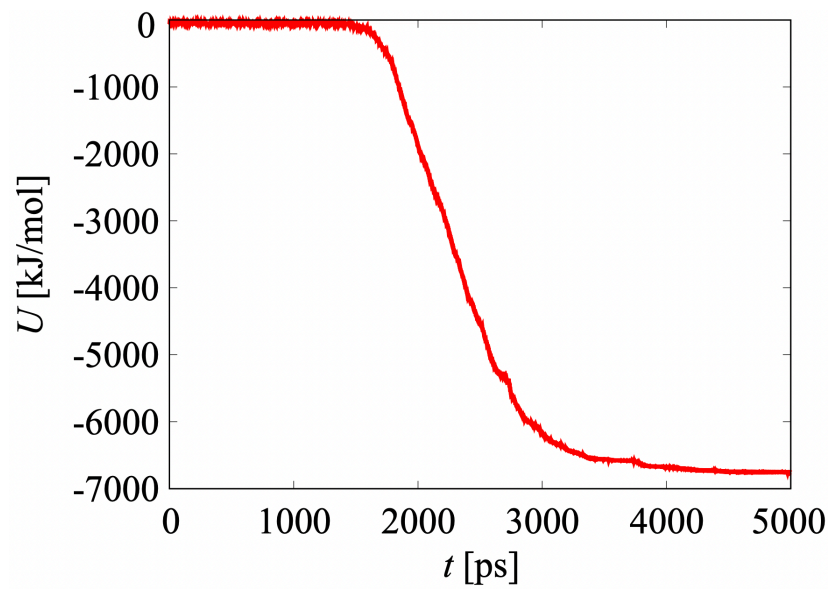


Figure S4 Potential energy of the CO₂ bulk system. The energy decreases when the CO₂ gas forms solid ice structure.