Supplementary Information:

A Molecular Dynamics Study of Enhanced CO_2 Separation via Boron Nitride Nanotubes Embedded in a Silicon Nitride Membrane

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Figure S1A and B display the simulation system of (18, 18) and (20, 20) BNNTs embedded in a silicon nitride (Si_3N_4) membrane, respectively. Dimension of the Si_3N_4 membrane is 3.80 x 3.95 nm^2 and the diameters of (18, 18) and (20, 20) BNNTs are 2.5 nm and 2.8 nm, respectively.

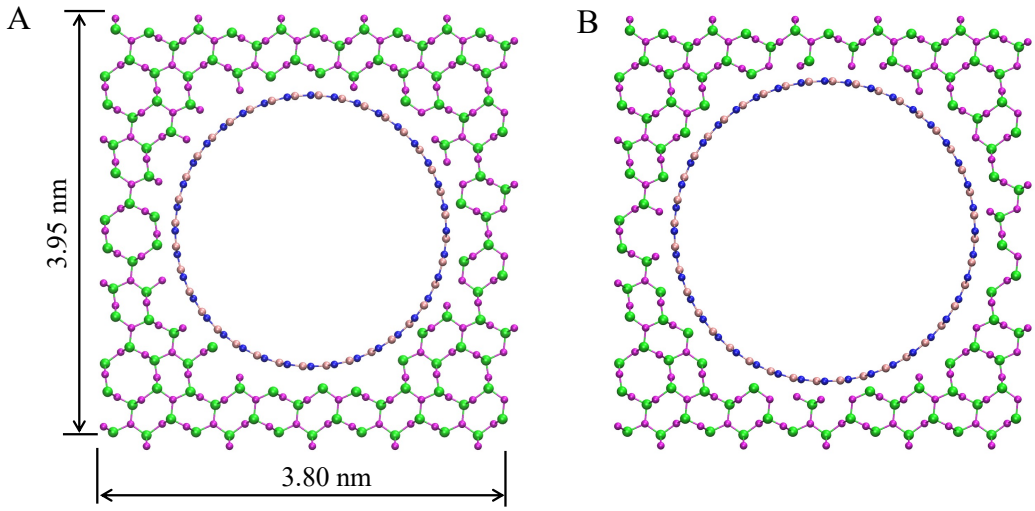

Figure S1 Simulation systems of: (A) (18, 18) BNNT-Si_3N_4 and (B) (20, 20) BNNT-Si_3N_4

Figure S2A and B show distribution of the non-uniform electric fields inside the (18, 18) and (20, 20) BNNTs. The electric fields are generated by the positive charges of silicon atoms and the negative charges of nitrogen atoms in the Si_3N_4 membrane.

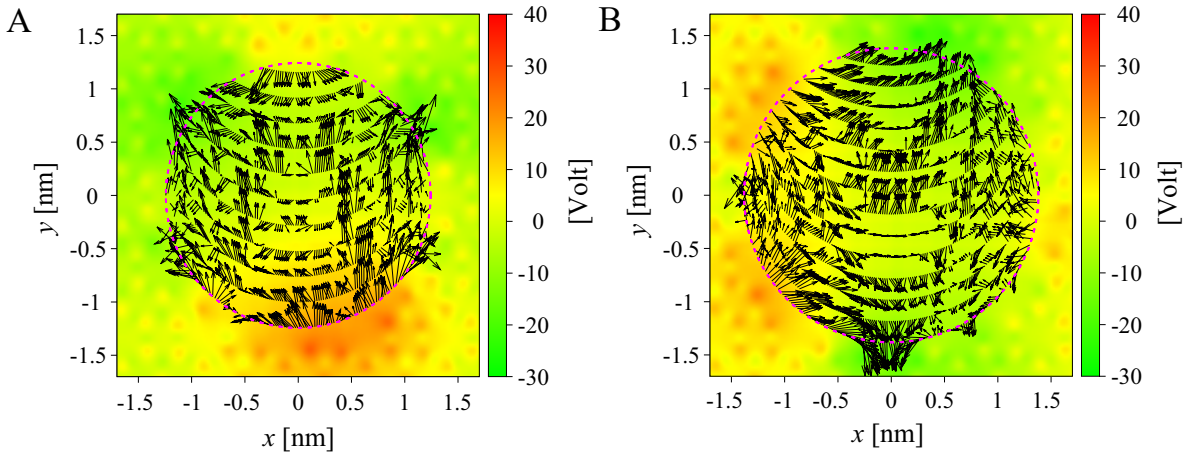

Figure S2 Distribution of electric field in the systems of: (A) (18, 18) BNNT-Si_3N_4 and (B) (20, 20) BNNT-Si_3N_4

Figure S3A represents the structure of CO_2 molecules in the (18, 18) BNNT system while Figure S3B and C are snapshots of the CO_2 structures in (18, 18) BNNT-Si_3N_4 systems. The structure in Figure S3B was obtained from simulation with normal condition where there are positive and negative charges on the silicon and nitrogen atoms of the Si_3N_4 membrane, respectively. Meanwhile, the structure in Figure 3C was obtained from simulation without charges on the Si_3N_4 membrane. The charges in the membrane were removed to clarify the effect of the electric fields induced by the charges on the CO_2 structure. Structures in Figure S3A and B are obviously different. This means that the Si_3N_4 membrane affects the CO_2 structure. The CO_2 structure in Figure S3C differs from that in Figure S3B. However, the structure of Figure S3C is similar to that in Figure S3A. The results suggest that the charges of the Si_3N_4 membrane play an important role on the changing of the CO_2 structure. As explained before, the charges induce non-uniform electric fields and subsequently influences the CO_2 structure.

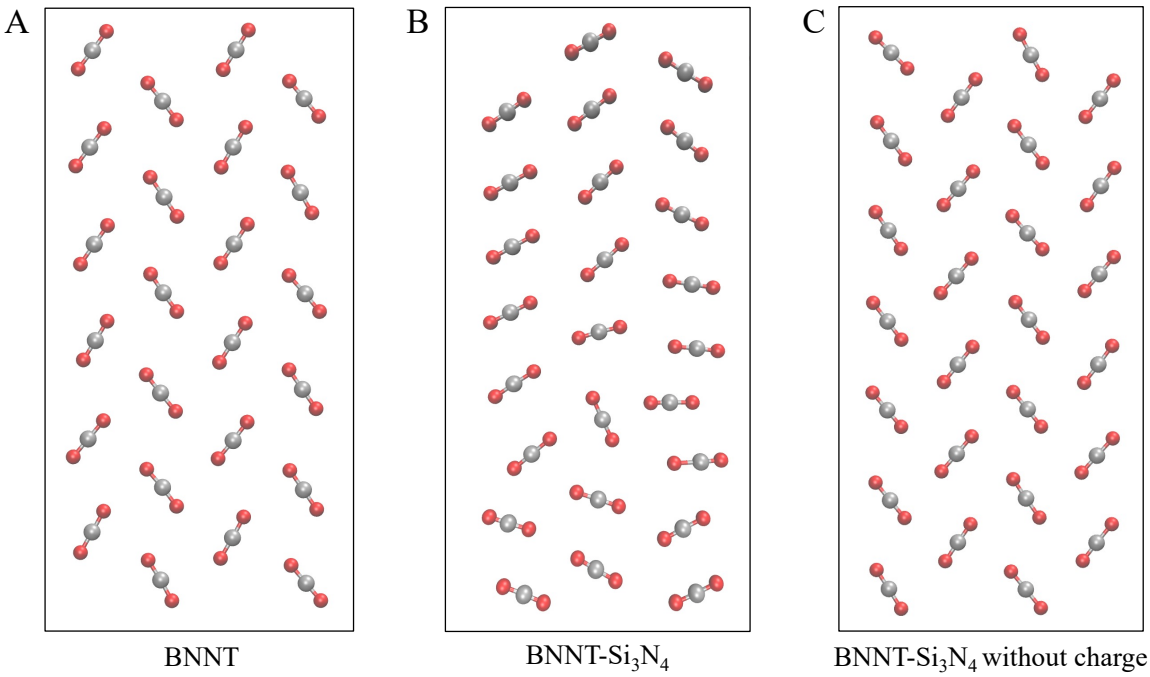

Figure S3 Structures of CO_2 molecules in the system of: (A) (18, 18) BNNT, (B) (18, 18) BNNT-Si_3N_4 , and (C) (18, 18) BNNT-Si_3N_4 without charges.

Figure S4 shows distribution of the Lennard-Jones (LJ) potential energy of CO_2 molecule inside the BNNT system and inside the BNNT-Si_3N_4 system. The LJ potential energy comes from the interaction between CO_2 with BNNT wall for the BNNT system or between CO_2 with BNNT and Si3N4 wall for the BNNT-Si_3N_4 system.

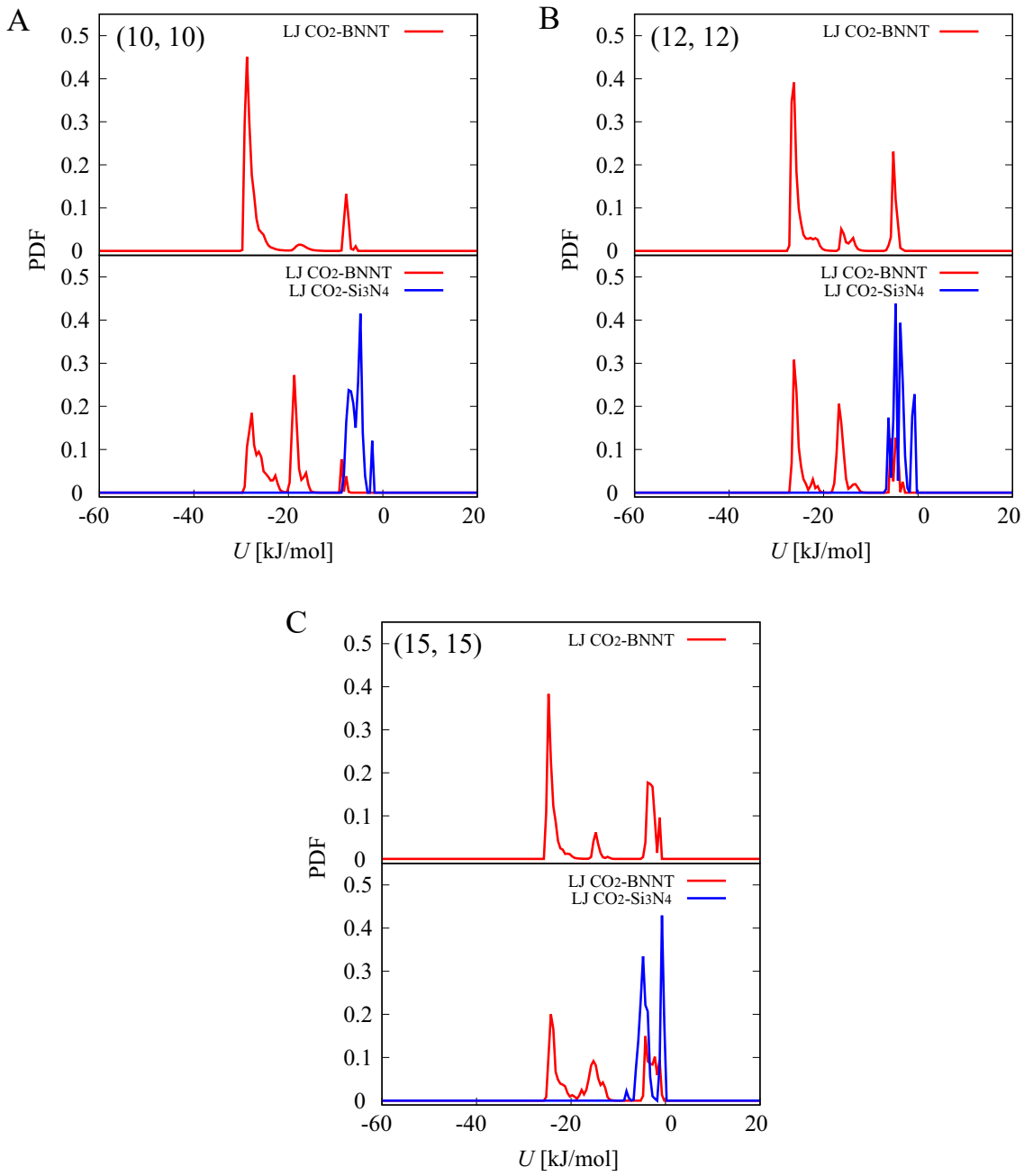

Figure S4 Distribution of the Lennard-Jones (LJ) potential energy of CO_2 in the BNNT system (upper) and in the BNNT-Si_3N_4 system (lower) using: (A) (10, 10), (B) (12, 12), and (C) (15, 15) BNNTs. PDF on the vertical axis means the probability distribution function.

Distributions of the Coulomb potential energy of the CO_2 molecule inside the (10, 10), (12, 12), and (15, 15) BNNT-Si_3N_4 systems are displayed in Figure S5. The potential energy is from the electrostatic interaction between the CO_2 with the Si_3N_4 membrane.

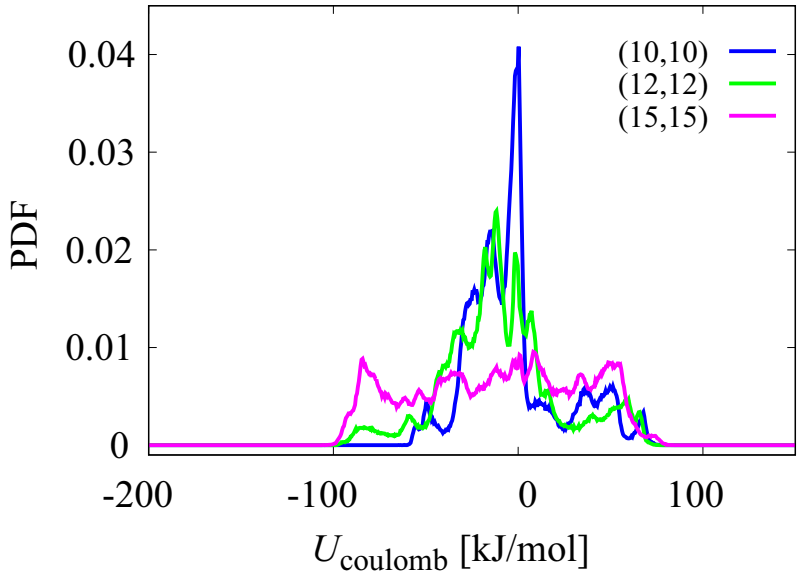

Figure S5 The Coulomb potential energy of the interaction between CO_2 molecules inside the (10, 10), (12, 12), and (15, 15) BNNTs with the Si_3N_4 membrane.

Potential energies within the CO_2 structure inside the (10, 10), (12, 12), and (15, 15) BNNTs of the BNNT system and BNNT-Si3N4 system are shown in Figure S6. The potential energy consists of the van der Waals (or the Lennard-Jones) interactions and the electrostatic interactions within the CO_2 structure.

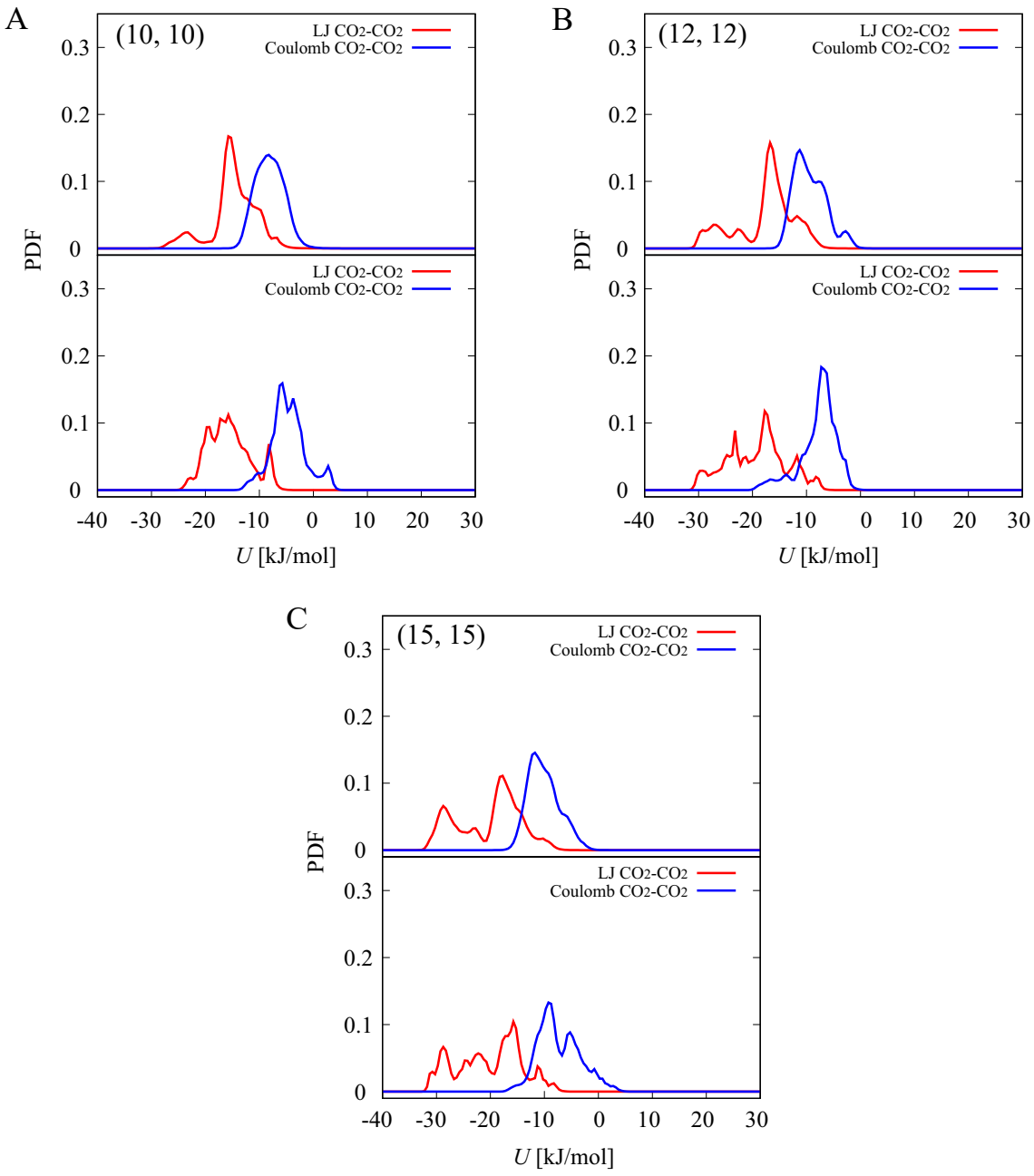

Figure S6 Potential energy within the CO_2 structure inside the BNNT system (upper) and inside the BNNT-Si_3N_4 system (lower) using: (A) (10, 10), (B) (12, 12), and (C) (15, 15) BNNTs.