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Supplementary File

Impact of impurity gas on CO_2 capture from flue gas using carbon nanotubes: A molecular simulation study

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1. Effect of single impurity on the adsorption of CO_2/N_2 mixtures in lager CNTs

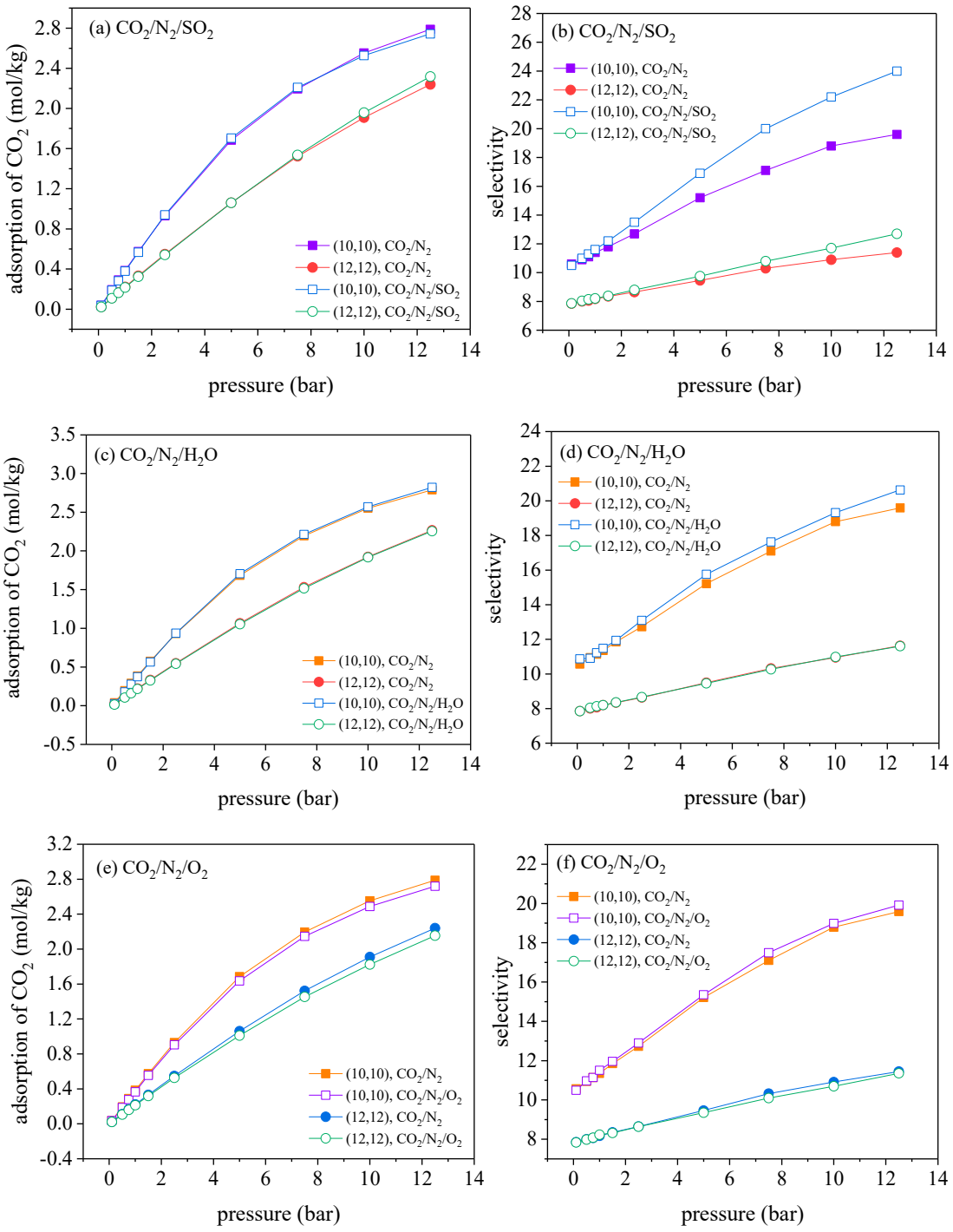


Figure S1. Adsorption isotherms for CO_2 in the presence of impurities, (a) SO_2, (c) H_2O, and (e) O_2, and the corresponding CO_2/N_2 selectivity (b, d and f), in the (10, 10) and (12, 12) CNTs.

2. Isotherm curves of single impurity in ternary mixtures

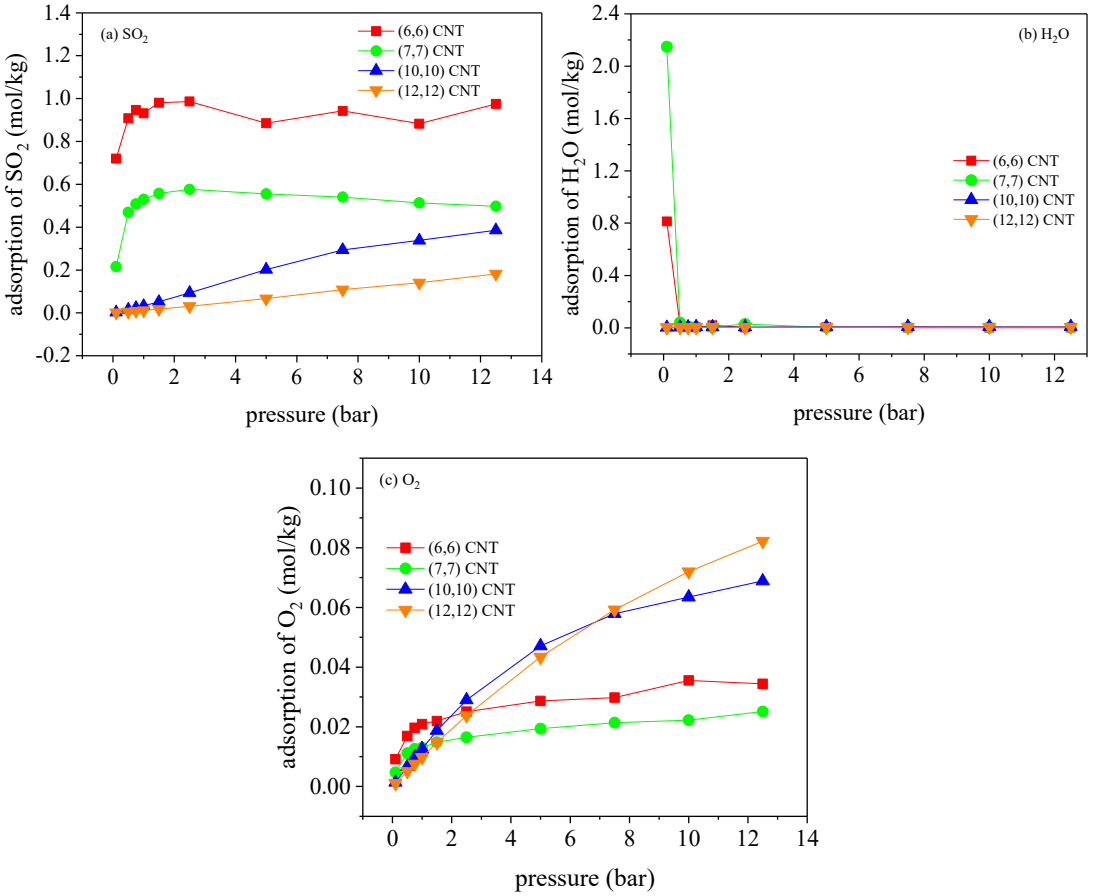
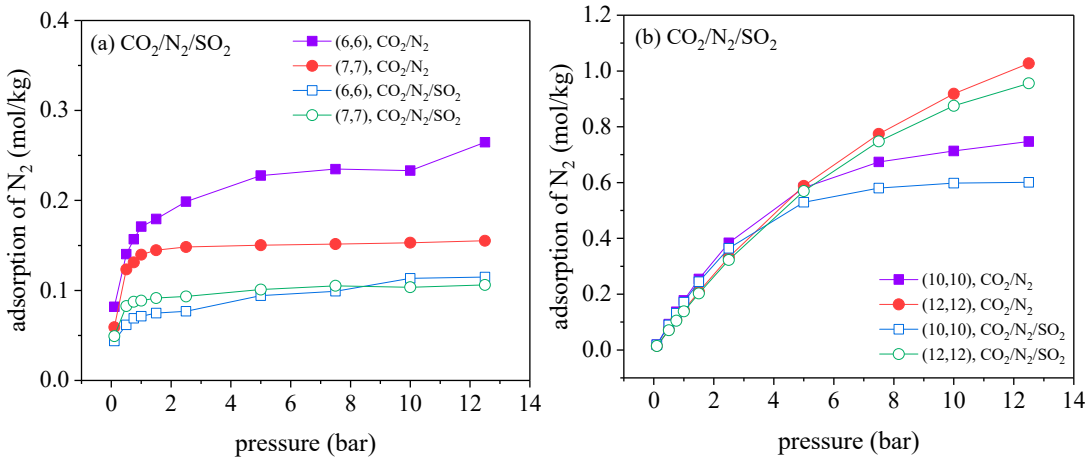


Figure S2. Isotherm curves with pressure for (a) SO_2 in $CO_2/N_2/SO_2$, (b) H_2O in $CO_2/N_2/H_2O$, and (c) O_2 in $CO_2/N_2/O_2$, in (6, 6), (7, 7), (10, 10) and (12, 12) CNTs at temperature of 300 K.



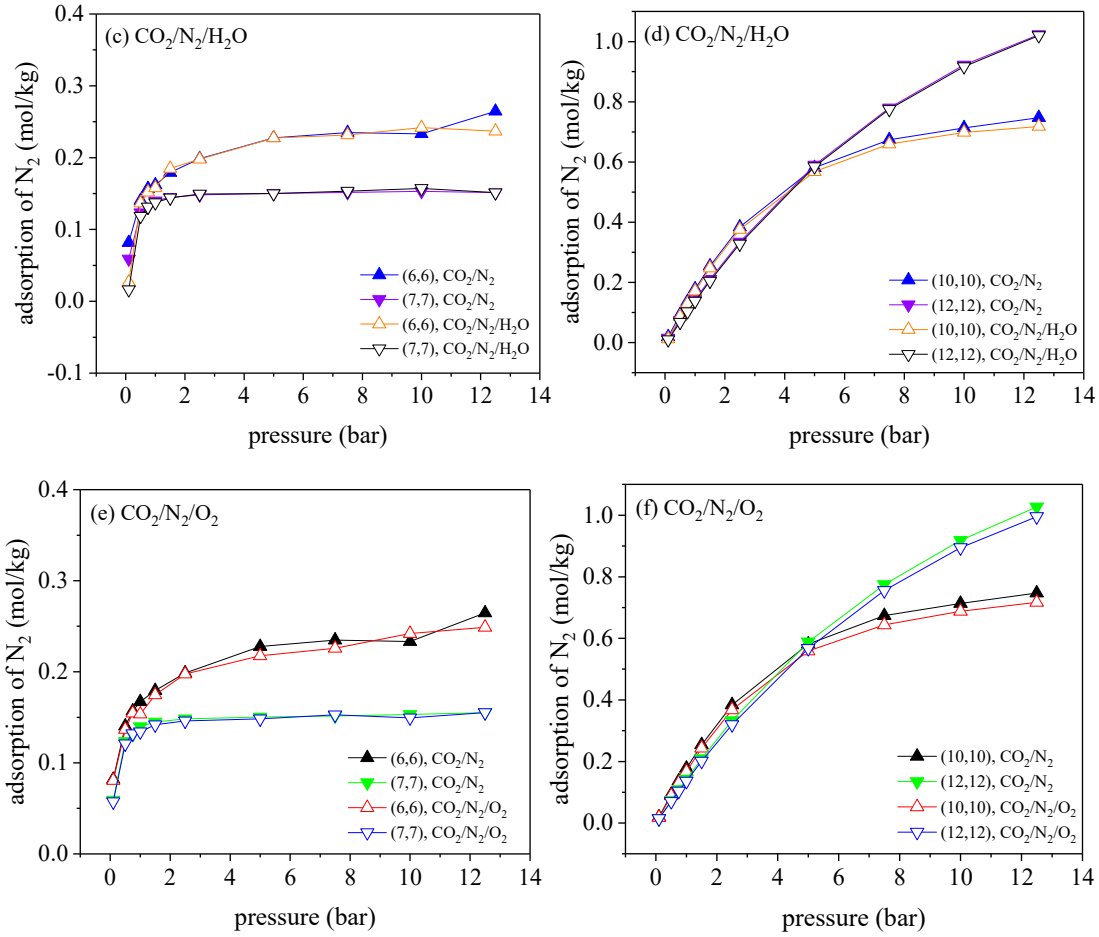


Figure S3. The adsorption of N_2 in the presence of impurities which are (a, b) SO_2, (c, d) H_2O and (e, f) O_2. The leaf side is these mixtures in the (6, 6) and (7, 7) CNTs, and the right side is that in (10, 10) and (12, 12) CNTs.

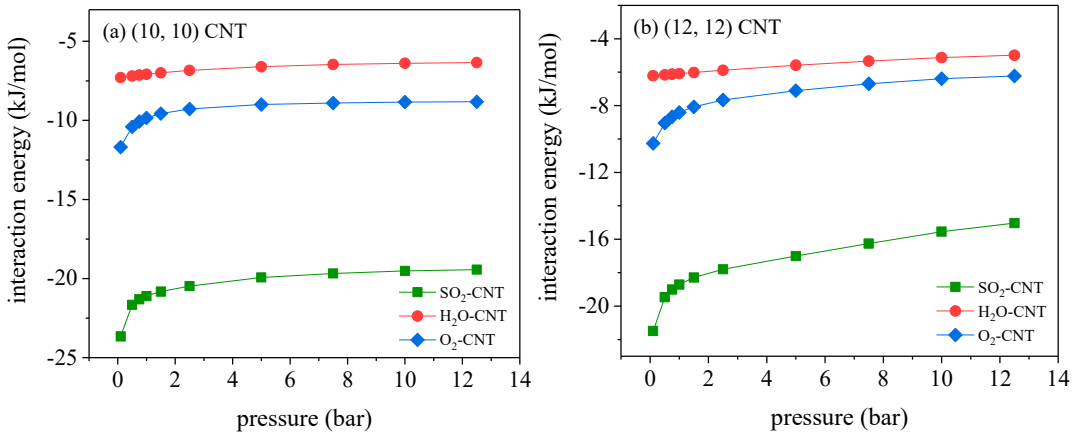


Figure S4. Variation interaction energy of X-CNT which X represents SO_2, H_2O and O_2 with pressure in the (10, 10) (a) and (12, 12) (b) CNTs.