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The computational study of amino group impregnation on the zeolite surface toward the behaviors of adsorption and diffusion KIWOONG KIM, SOOHO LEE, KWANG SOON LEE, WON BO LEE, Sogang University — The molecular dynamic and Grand Canonical Monte Carlo simulation study were conducted to investigate the adsorption and diffusion behaviors of mixture of CO_2 and N_2. Pure silicalite structures of zeolites TON, AFI, and LTL were selected as the host materials to be evaluated in this study. The effect of surface modification of TON, realized by impregnating the amino functional group on TON surface, on the adsorption and the diffusion were analyzed and compared with the normal TON structure. The results show that, in the adsorption behaviors, the modified TON adsorbs more CO_2 than the normal TON structure, however, at high pressure regions, CO_2 uptake is lower than the normal TON due to reductions of pore volume. This effect was quantitatively analyzed for the various amino functional group; methyl-, ethylamine, and ammonia. In the diffusion behaviors, the mixture in the modified TON has a lower diffusivity than the mixture in the normal TON due to additional attractive interaction between the amino group and mixture. In addition, the single file mobilities as well as the self-diffusion coefficients were employed to describe the observed diffusion behaviors.

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