An improved CO_2 adsorption efficiency for the zeolites impregnated with the amino group

김기웅, 이수호, 이광순, 이원보*
서강대학교
(wblee92@sogang.ac.kr*)

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. 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 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. As well as the adsorption isotherm, CO_2/N_2 adsorption selectivity was also calculated, and it suggested that although the modified TON has a low adsorption capacity of CO_2, it has a high adsorption selectivity of CO_2 over N_2 comparable with other sorbents. In the diffusion behaviors, the mixture in the modified TON has a lower diffusivity than the mixture in the normal TON, which is interpreted via single file mobility.