Diffusion and adsorption behaviors of guest molecules in different zeolite structures

김기웅, 이수호, 이광순, 이원보*
서강대학교
(wonbo.lee@gmail.com*)

A study of molecular simulation was conducted to investigate the adsorption phenomena of guest molecules consist of CO2 and N2 in different zeolites. After we assumed that the diffusion characteristics and adsorption behavior are correlated, we have studies both of dynamic and equilibrium system. First, the molecular dynamic study was carried out to find out the diffusion characteristics of guest molecules into zeolite structures. It showed distinct diffusion behavior as the pore length and size are varied. The self-diffusion constants were calculated using kinetic theory with obtained MSD (Mean Square Displacement). Second, the GCMC (Grand Canonical Monte Carlo) simulation was consecutively conducted to look for the isotherm of guest molecules. From the results, the qualitative correlations between bulk diffusion and adsorption behavior were established.