Theoretical Study on the Effect of Nested Defects for Water Adsorption in Zeolite

박세영, 신선우, 김유진, 이지은, 이정현, 김진철, 곽상규†
울산과학기술원

Zeolites are useful for CO_2 gas separation from post-combustion gases. Also, from previous studies, it has been suggested that the separation performance of CO_2 would be affected by water molecules, which always exist in post-combustion gases. Unrealistically, so far, the zeolite structure has been considered as perfect, ignoring the presence of naturally formed defects (i.e. nested silanol defects), which can easily interact with water molecules. Thus, we theoretically investigated both issues by grand canonical Monte Carlo (GCMC) and molecular dynamics (MD) simulations in this study. To accurately describe the interaction between water and zeolite, we optimized the intermolecular potential energy parameters for reproducing the experimental water adsorption amounts in three kinds of zeolites (i.e. DDR, MFI, and CHA). We found that the number of adsorbed water molecules were found similar regardless of the defect density. Interestingly, it was noticeable that the water molecules were aggregated near the defects from our MD simulation. It implies that the permeability of CO_2 can be significantly affected by water around the defective sites.