Estimation of Na ion and water structure in cages of hydrated zeolite NaY by Molecular Dynamics study

김진철, 허윤영, 곽상규*
울산과학기술대학교
(skkwak@unist.ac.kr*)

In the synthesis of NaY(Si/Al = 2.69) zeolite, sodium ion and water are trapped in Faujasite zeolite, which is a microporous crystal aluminosilicate with three structurized cages. Molecular dynamics (MD) simulations were performed to capture 'molecular 'framework of Na ion and water in the hydrated zeolite NaY, which ware categorized with adsorbed and evaporated states. Computational analyses such as radial distribution function, bond order parameter, and structure factor revealed that six water molecules form a crown-like ring structure, where a sodium ion resides in the center of water-cage, in the 12 ring openings of the supercage. Additionally, the tetrahedral shapes of water molecules and Na ions in the sodalite cage have been observed. We also report molecular behavior of those structures with respect to the temperature variation from 298K to 353K.