Theoretical study on enantioselective separation of 2-Methyl-1-butanol by MOF-74

임형용, 이정현, 김진철, 곽상규†
울산과학기술원
(skkwak@unist.ac.kr†)

Even though MOFs are known for good separators for gas mixtures, a few members of MOFs have been studied for enantioselective separations. Therefore, we aim to study the enantioselective separation of 2-methyl-1-buanol by Fe-MOF-74 by using molecular modeling and simulation methods, which are density functional theory (DFT) calculation and grand canonical Monte Carlo (GCMC) simulation. A force field for Fe-MOF-74 was derived by optimizing the parameters (e.g. bond stretch, angle bend, torsion...) and it was utilized in the calculation of adsorption isotherms of 2-methyl-1-butanol in Fe-MOF-74. To verify the derived force field working of Fe-MOF-74, we calculated and compared the mechanical properties with the results of the DFT calculation. With that MOF, GCMC simulation was performed by using the derived force field in order to capture the difference in adsorption of the 2-methyl-1-butanol. The loading of *(R)* and *(S)*-enantiomers in Fe-MOF-74 showed remarkable difference of separation factor ($S_{B/A}$) compared to the one from [{Cu(sala)}$_n$], which is a single-handed helical framework material, indicating that Fe-MOF-74 is a highly promising separator.