다공성 고체물질을 이용한 이산화탄소 포집 및 기체분리의 원자레벨 설계 (Carbon dioxide capture and gas separations using porous solids : A computational design)

정유성*
KAIST EEWS 대학원
(ysjn@kaist.ac.kr*)

Metal-organic frameworks (MOFs) have been studied as a promising class of solid adsorbents for diverse gas capture and separations, such as selective separations and storage of CO2, H2, O2, and small hydrocarbon molecules. In such selective gas adsorptions, largely two types of mechanisms have been used: (1) size/shape exclusions and (2) different host-guest interactions. For the first strategy, the target molecule should have a distinctive kinetic diameter or shape from the other mixtures in reference to the pore of adsorbents. For the second strategy, differences in various physicochemical properties can be utilized for separation. In this talk, I will talk about our recent progress on understanding the underlying mechanisms of some of these separations that involve CO2 or hydrocarbons (alkane/alkane separation and alkene/alkene isomers separation) as well as suggesting a new design strategy to improve the uptakes and selectivities using first-principles calculations.