Epoxide cycloaddition to CO_2 in MOF-508: A Computational Investigation

남수명, Robin Babu[1], 정용철[1,†]
부산대학교; [1]부산대학교 화공생명공학부
(greg.chung@pusan.ac.kr[†])

Cycloaddition reaction can be used to combine CO2 with epoxides to produce useful chemicals, such as cyclic carbonates. Generally, these type of reactions are carried out at an elevated temperature and pressure, which requires a lot of energy, and have low conversion rates. Metal-organic frameworks (MOFs) are a porous materials that can be used as a catalyst for such reaction. In this work, we used grand canonical Monte Carlo (GCMC) simulations to characterize active sites in MOF-508. Density Functional Theory (DFT) calculations are subsequently carried out to elucidate the reaction pathway for the cycloaddition reaction.