Computational Exploration of functionalized Zirconium Metal-Organic Polyhedra (MOP)

윤성현, 정용철†, 김주용
부산대학교
(greg@pusan.ac.kr†)

Metal-Organic Polyhedra (MOP) are an emerging class of discrete molecules with predesigned porosity. Depending on the pore size, the window size, and the type of ligand, MOP can be used for gas storage, separation, and catalysis applications. One of the less understood, but important physical properties of MOP is the positions of ligands that form the windows. In this work, we have used molecular modeling to analyze the window size distributions and the relative energetic stability of MOP structures as a function of the ligand orientations.