MOF-5/graphene oxide의 시뮬레이션을 통한 가스 흡착 분석(Computational Analysis of Gas Adsorption in MOF-5/GO Composite Materials)

김지한†
KAIST 생명화학공학과
(jihankim@kaist.ac.kr†)

Recently, composite materials have attracted significant amount of attention from the research community due to their unique properties. From a computational point of view, it is very challenging to model these materials due to the lack of clarity in structural information. In this talk, we investigate MOF-5/graphene oxide composite material which was first synthesized by Petit et al. (2009). Unlike other metal-organic framework/GO composite materials, it has been experimentally verified that MOF-5/GO possesses significant degree of structural order, making it relatively easier to model. The self-assembly patterns of the MOF-5 and the GO layers are computationally identified using previously published experimental isotherm data as proxy. With the structural information in hand, our study focuses on gas adsorption properties at infinite dilution conditions and we evaluate synergetic gas adsorption/separation effects by comparing performances between the composite and the pure-component host material.