Grand canonical Monte Carlo simulation 기반 분자레벨 최대흡착능 targe t의 MOF 구조 설계

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Sulfur dioxide (SO2) generated by anthropogenic activities, which cause serious environmental problems and pose substantial health effects. In this study, we have constructed a database of metal-organic frameworks (MOFs) structures for SO2 adsorption, which are derived from experiment but are immediately suitable for molecular simulations. For this, grand canonical Monte Carlo simulations (GCMC) is performed for screening of top performing structures for SO2 adsorption. We investigated the structural, chemical and physical properties of the MOF and experimental database. This study provides the insight knowledge at a molecular level of SO2 adsorption capacities in MOF materials that can inspire the experimental development and further design of new MOFs for SO2 adsorption. Acknowledgments: This work was supported by the National Research Foundation (NRF) grant funded by the Korean government (MSIT) (No. NRF-2017R1E1A1A03070713), and Korea Ministry of Environment (MOE) as Graduate School specialized in Climate Change.