Accelerating Materials Discovery via High-Throughput Molecular Simulation

정용철†
부산대학교
(chungre83@gmail.com†)

Discovery and development of new materials often take several decades which is a serious bottleneck for the deployment of such materials to the market. In this aspect, high-throughput molecular simulation is a powerful method to predict the performance of large-number of materials prior to experimental synthesis and testing. By doing so, experimentalists can focus on those materials with promising performance which can cut-down on the cost and time associated with the development of new materials, such as metal-organic frameworks (MOFs). In this talk, I will provide examples on how high-throughput molecular simulations can help to find optimal MOFs from a large number of MOF structures for the application in pre-combustion CO2 capture and hexane isomer separation.