

머신러닝 기법과 분자모델링의 융합 연구를 통한
나노 다공성 물질 개발
Development of Nanoporous Materials Using Computational Modeling
combined with Machine Learning

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Nanoporous materials are of great interest in applications ranging from gas separation and storage, to catalysis. The chemistry of these materials allows us to obtain an essentially unlimited number of new materials by combining different molecular building blocks, which exceeds the growth of synthesized nanoporous materials published in the recent experimental works. This sheer abundance of structures requires novel computational techniques to shed light on the existing or even unexplored libraries, as well as to facilitate the search for materials with optimal properties. In this talk, I will discuss our recent efforts into the discovery and design of novel nanoporous materials using computational modeling combined with machine learning techniques.