Machine Learning-Driven Discovery of Metal-Organic Frameworks for Efficient CO2 Capture in Humid Condition

유현석, 이용진†
인하대학교
(yongjin.lee@inha.ac.kr†)

This poster presents a computational study to design tailor-made metal-organic frameworks (MOFs) for efficient CO_2 capture in humid conditions.

Target-specific MOFs were generated in our computational platform incorporating the Monte Carlo tree search and recurrent neural networks according to the objective function values that combine three requirements of high adsorption performance, experimental accessibility of designed materials, and good hydrophobicity to be applied in humid conditions. With a given input of 27 different combinations of metal node and topology net information from experimental MOFs, our approach successfully designed promising and novel metal-organic frameworks for CO_2 capture, satisfying the three requirements.

Furthermore, the detailed analysis of the structure-property relationship identified that moderate D_i (the diameter of the largest included sphere) of 14.18 Å and accessible surface area (ASA) of 1750 m^2/g values are desirable for high-performing MOFs for CO_2 capture, which is attributed to the trade-off relationship between good adsorption selectivity and high adsorption capacity.