# Modeling gas adsorption properties in triangular metal-organic frameworks with defects

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Defects in metal-organic frameworks (MOFs) have been received tremendous attention during the past few years because the introduction of defects in MOFs could introduce new active sites for gas separation. One type of defects is linker defects, in which the linkers connecting the inorganic nodes is removed during the activation process. Depending on the solvents used during the synthesis, the solvent molecules occupy the open metal sites created from linker defects and provide additional interaction sites for gas adsorption.
In this work, we used a combination of molecular modeling techniques and macroscopic breakthrough simulations to model the adsorption characteristics of triangular MOF, which has been received attention for its separation capability of hexane isomers. We have created different degree of defect models for triangular MOFs, on the basis of solvents that has been used in the experiments. Configurational-biased grand canonical Monte Carlo (CB-GCMC) simulations are carried out to test hexane isomer selectivity and precombustion $CO_2/H_2$ separation capability. Breakthrough simulations are carried out to elucidate the impact of defects on gas separation applications.