# Identification on Effect of Linker Vacancy Defects in Metal-organic Framework Membranes

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The intra-crystalline defects in Metal-organic frameworks (MOF) have been considered to have a crucial role in their material properties. In this work, we focused on the linker vacancy defects in MOF membranes and investigated their influence on the H2/CH4 seperation using atomically-detailed simulations. Defective structures were modeled for the 236 numbers of candidate MOFs and their separation performances were compared with non-defective structures. Our results show the existence of linker vacancy defects can arise the significant performance change in MOF membranes and the best material might not be the best once the defect is taken into account. This suggests the necessity of the defect consideration in predicting the membrane performance, and choosing the defect-insensive MOFs not to face the unpredicted degradation of membranes.