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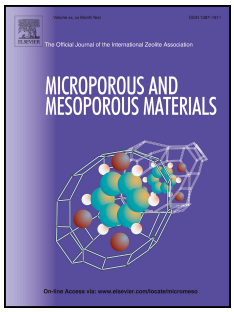

Molecular dynamics simulation of acetylene diffusion in MOF-508a and MOF-508b

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Graphical Abstract

The self-diffusion of acetylene molecules in MOF-508a and MOF-508b was calculated in the temperature range of 300-900 K by the molecular simulation. It was shown that the self-diffusion in MOF-508a is much higher than MOF-508b and increases with increasing the temperature and loading.

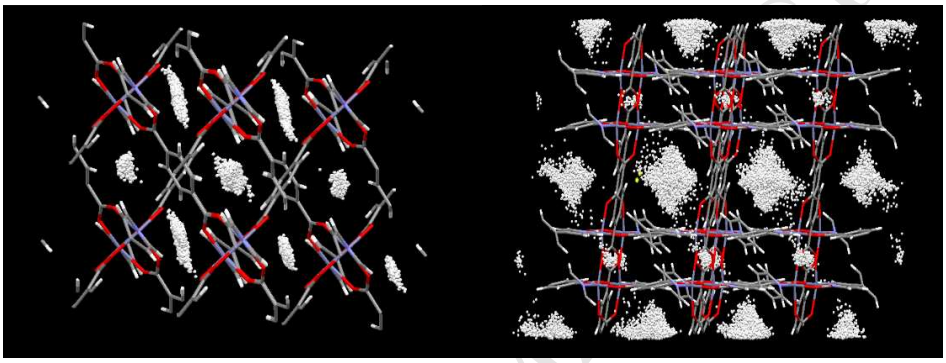

Fig. 1. Trajectory of 6 acetylene molecules in 800 K in MOF-508b (left) and MOF-508a (write).