Intrinsic thermal management capability of elastic layer-structured metal-organic framework-11 exhibiting multi-gate adsorption for CO_2

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We show that flexible metal-organic frameworks (MOFs) exhibiting 'multi-gate openings/closings' for CO_2 can intrinsically suppress the exothermic heat released by adsorption and the endothermic heat gained by desorption, both of which result in the reduction of the working capacity of CO_2 in a separation process.[1] We use the elastic layer-structured metal-organic framework-11 (ELM-11) [Cu(4,4'-bipyridine)$_2$(BF$_4$)$_2$],[2-6] which exhibits a two-step gate adsorp-tion isotherm, as a model system for flexible MOFs, and perform free energy analyses with the aid of grand canonical Monte Carlo simulations for ELM-11 structures that were determined by the Rietveld method using in-situ synchrotron X-ray powder diffraction data. We demonstrate that the thermal management capabilities of ELM-11 for gate-closings at lower and higher pressure during the desorption process are nearly identical and quite effective (38% and 35%, re-spectively). Moreover, we also show that the intrinsic thermal management of the adsorption process can work as well as it does for the desorption process, which suggests that flexible MOFs exhibiting multi-gate openings/closings are promising materials for further development into systems with intrinsic thermal management mechanisms for carbon capture and storage applications.

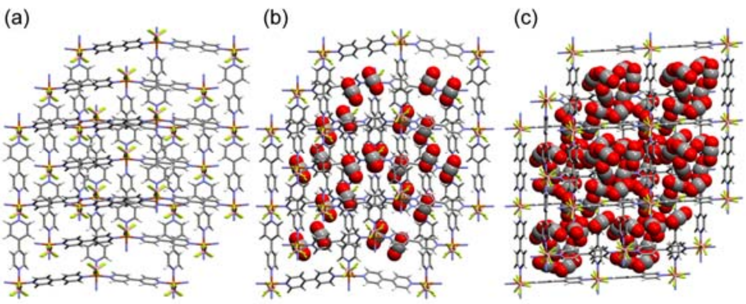

Fig. 1 Crystal structures of ELM-11 with different CO_2 loadings at 195 K: (a) after evacuation, (b) after 1st gate adsorption encapsulating 2CO_2, (c) after 2nd gate adsorption encapsulating 6CO_2.

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