Supporting Information

Enhancement of CO\textsubscript{2}/N\textsubscript{2} mixture separation using the thermodynamic stepped behavior of adsorption in metal-organic frameworks

Qingyuan Yang,* Linlin Ma, Chongli Zhong, Xiaohui An, Dahuan Liu

Laboratory of Computational Chemistry, Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, China

E-mail: qyyang@mail.buct.edu.cn

The difference of the isosteric heats of adsorption at 195 K

![Graphs showing the difference of the isosteric heats of adsorption between CO\textsubscript{2} and N\textsubscript{2} in IRMOFs at 195 K as a function of pressure.]

Figure S1. The difference of the isosteric heats of adsorption between CO\textsubscript{2} and N\textsubscript{2} in IRMOFs at 195 K as a function of pressure.
**Individual contribution for the isosteric heats of adsorption of CO$_2$ at 195 K**

![Graphs showing isosteric heats of adsorption](image)

**Figure S2.** Isosteric heats of adsorption contributed individually from the CO$_2$-CO$_2$ and CO$_2$-MOF interactions as a function of pressure.

**Contour plots of the center of mass probability in IRMOF-10 at 195 K**

![Contour plots](image)

(a) P=0.5 MPa  (b) P=0.7 MPa

**Figure S3.** Contour plots of the center of mass (COM) probability densities of CO$_2$ in the CO$_2$/N$_2$ mixture adsorbed in IRMOF-10 at 195 K (Zn, blue; O, red; C, gray and H, white).