

Supplementary Information

Highly selective separation of C₂H₂/CO₂ and C₂H₂/C₂H₄ in an N-rich cage-based microporous metal-organic framework

Lingzhi Yang^{1,2}, Wenpeng Xie³, Qiuju Fu³, Liting Yan¹, Shuo Zhang^{1,3}, Huimin Jiang^{1,3}, Liangjun Li³, Xin Gu³, Dandan Liu³, Pengcheng Dai³, Qingbin Zheng², Xuebo Zhao¹

¹School of Materials Science and Engineering, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250353, China

²School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen 518172, China

³Institute of New Energy, College of New Energy, State Key Laboratory of Heavy Oil Processing, China University of Petroleum (East China), Qingdao 266580, China

Correspondence should be addressed to Xuebo Zhao: zhaoxuebo@upc.edu.cn and Qingbin Zheng: zhengqingbin@cuhk.edu.cn

Figure S1 to S13:

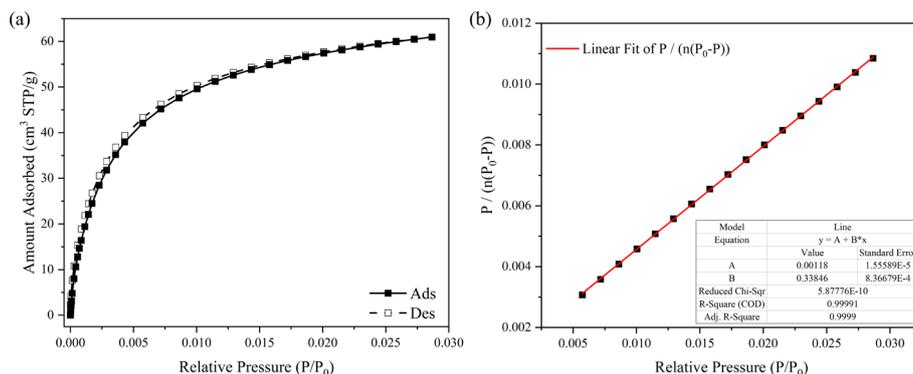


Figure S1. (a) CO₂ sorption isotherms for Cd-TZ at 273 K. (b) BET plot for CO₂ adsorption on Cd-TZ at 273 K.

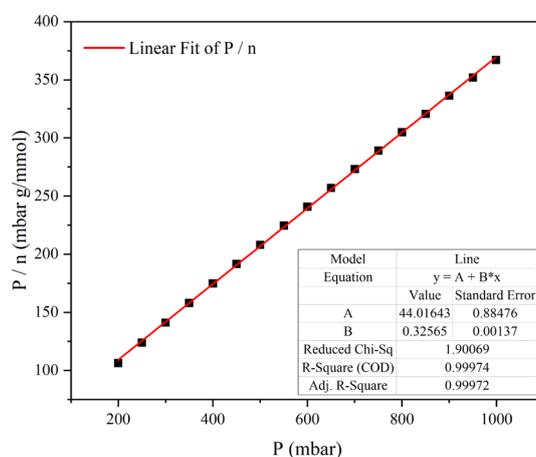


Figure S2. Langmuir plot for CO₂ adsorption on Cd-TZ at 273 K.

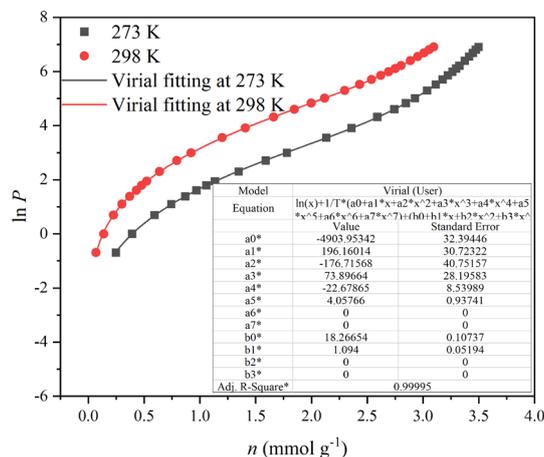


Figure S3. C₂H₂ isotherms for Cd-TZ global fitting using Virial method.

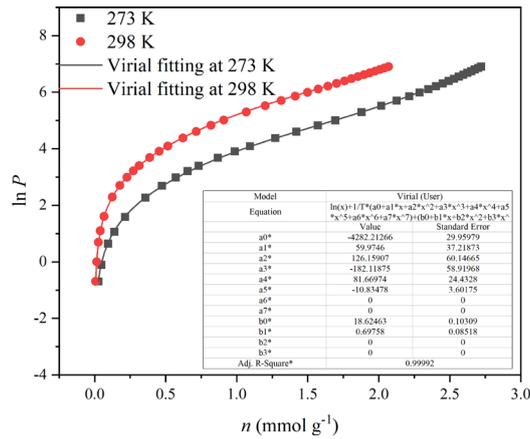


Figure S4. CO₂ isotherms for Cd-TZ global fitting using Virial method.

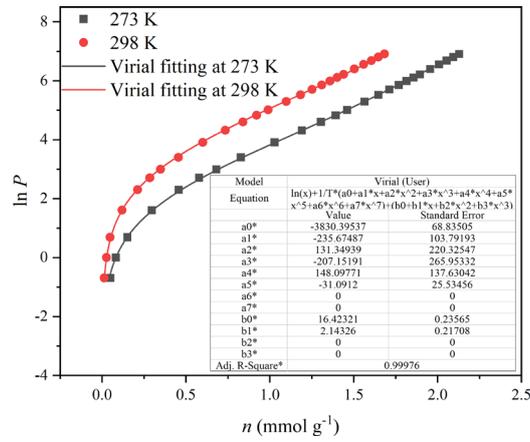


Figure S5. C₂H₄ isotherms for Cd-TZ global fitting using Virial method.

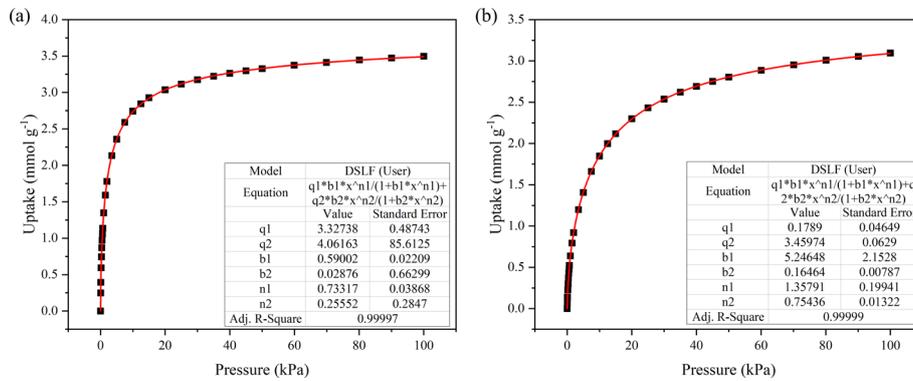


Figure S6. DSLF fitting of the C₂H₂ sorption data at 273 K (a) and 298 K (b) for Cd-TZ.

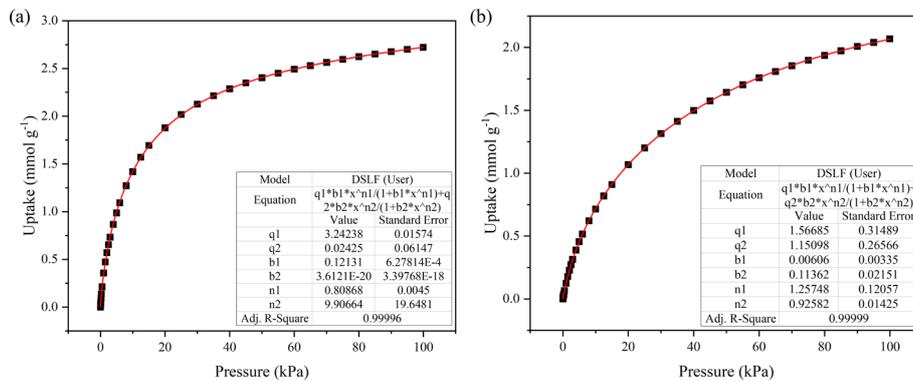


Figure S7. DSLF fitting of the CO₂ sorption data at 273 K (a) and 298 K (b) for Cd-TZ.

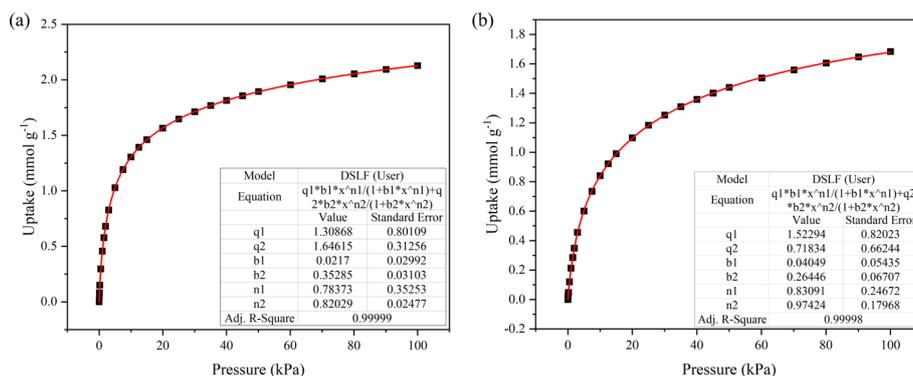


Figure S8. DSLF fitting of the C_2H_4 sorption data at 273 K (a) and 298 K (b) for Cd-TZ.

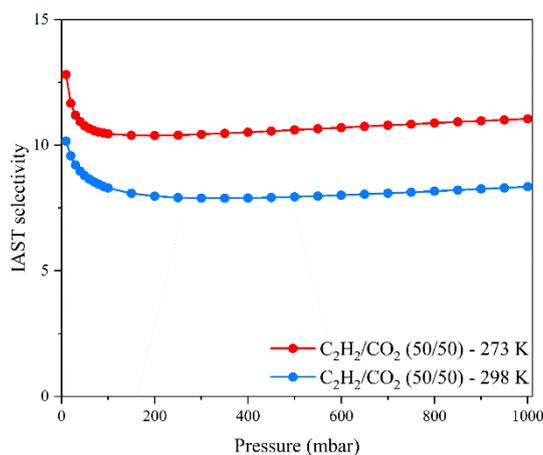


Figure S9. IAST selectivities for C_2H_2/CO_2 with compositions of 50/50 at 298 K and 273 K.

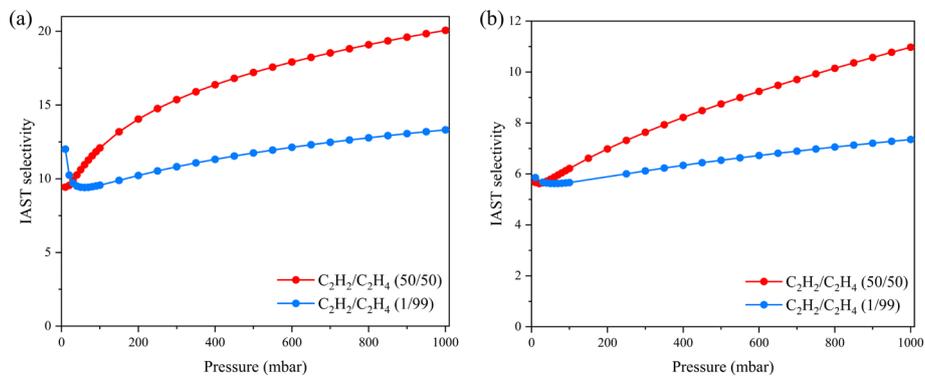


Figure S10. IAST selectivities for C_2H_2/C_2H_4 with compositions of 50/50 and 1/99 at (a) 273 K and (b) 298 K

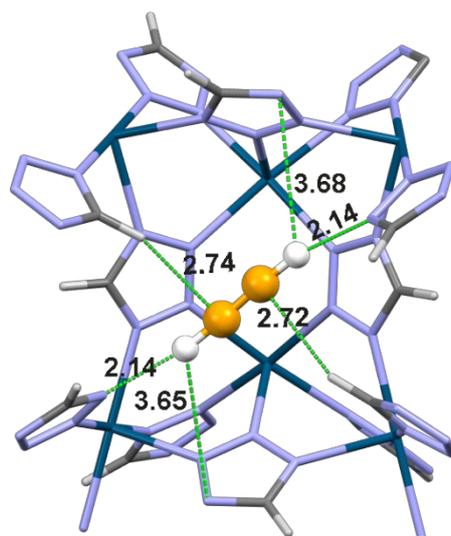


Figure S11. The interaction between Cd-TZ and C_2H_2 in the preferential adsorption sites. Cd, C, N and H in Cd-TZ are represented by dark blue, bright grey, lavender and white, respectively; C and H in C_2H_2 is represented by bright yellow and white, respectively. The labeled distance is measured in Å.

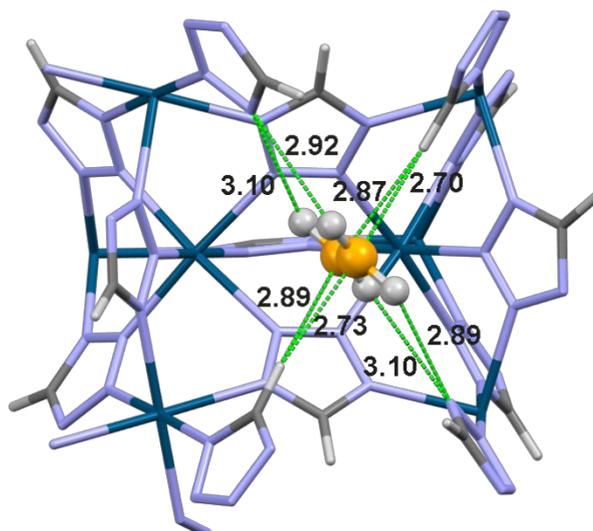


Figure S12. The interaction between Cd-TZ and C_2H_4 in the preferential adsorption sites. Cd, C, N and H in Cd-TZ are represented by dark blue, bright grey, lavender and white, respectively; C and H in C_2H_4 is represented by bright yellow and white, respectively. The labeled distance is measured in Å.

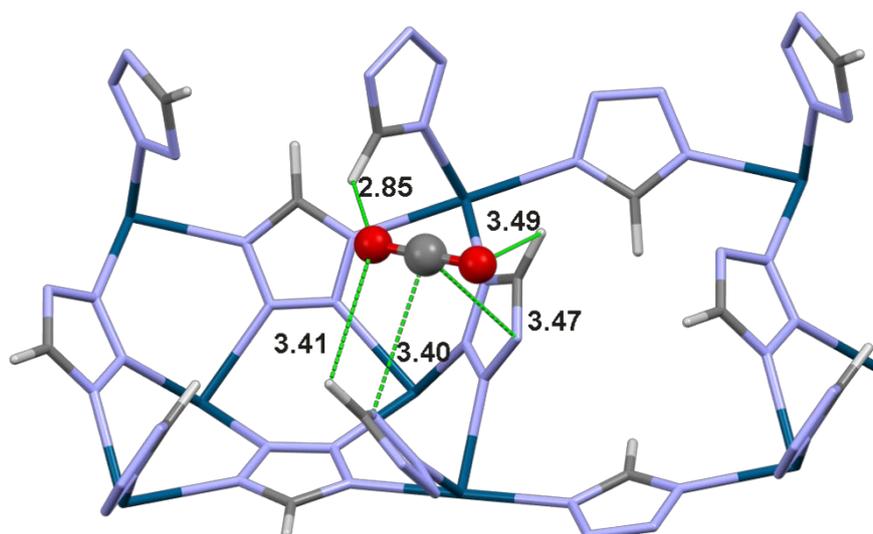


Figure S13. The interaction between Cd-TZ and CO₂ in the preferential adsorption sites. Cd, C, N, O, H in Cd-TZ and CO₂ are represented by dark blue, bright grey, lavender, red and white, respectively. The labeled distance is measured in Å.