

## *Supporting Information*

# **Ultradeep Removal of Moisture in Gases to Parts-per-Billion Levels: The Exploration of Adsorbents**

Lin Zhang,<sup>†,#</sup> Zheng-Zhong Kang,<sup>‡,§,#</sup> Shi-Chao Qi,<sup>†</sup> Xiao-Qin Liu,<sup>\*,†</sup> Zhi-Min Wang,<sup>†</sup> and Lin-Bing Sun<sup>\*,†</sup>

<sup>†</sup>Jiangsu National Synergetic Innovation Center for Advanced Materials (SICAM), State Key Laboratory of Materials-Oriented Chemical Engineering, College of Chemical Engineering, Nanjing Tech University, Nanjing 210009, China

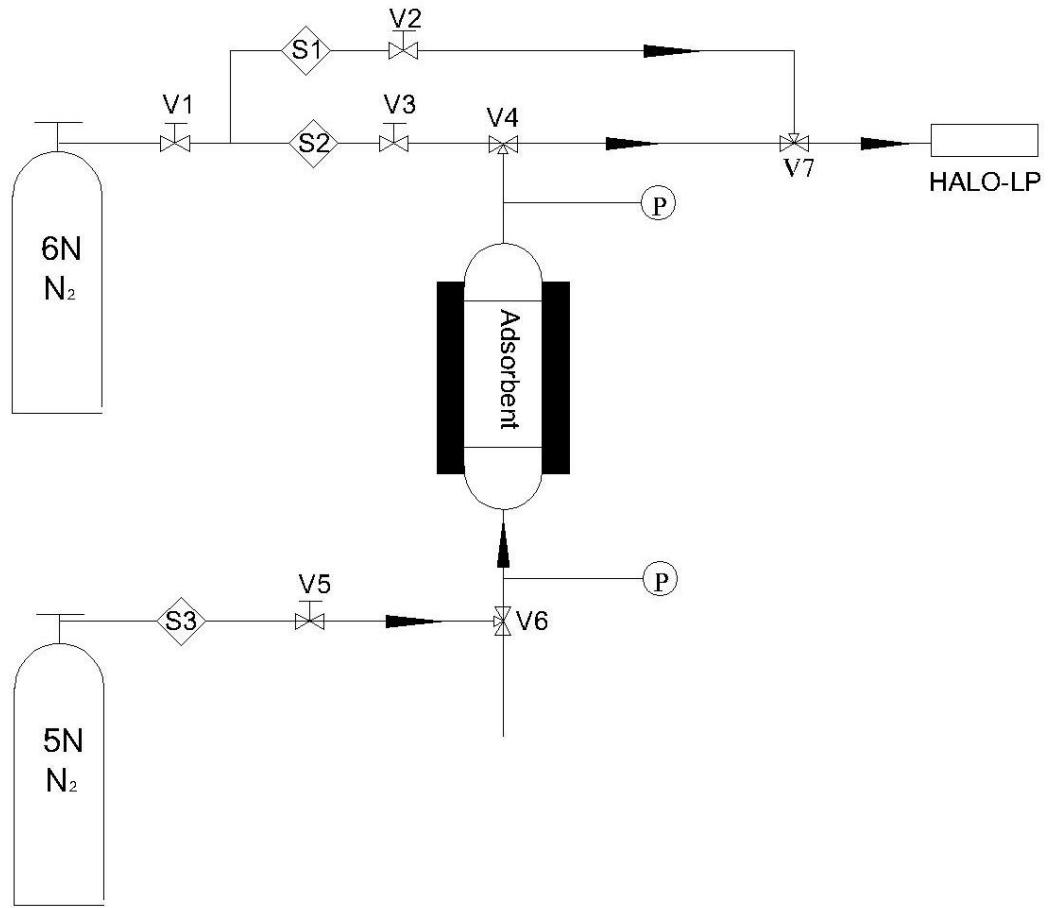
<sup>‡</sup>Department of Chemistry, Zhejiang University, Zheda Road 38, Hangzhou, 310027, China

<sup>§</sup>Division of Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden

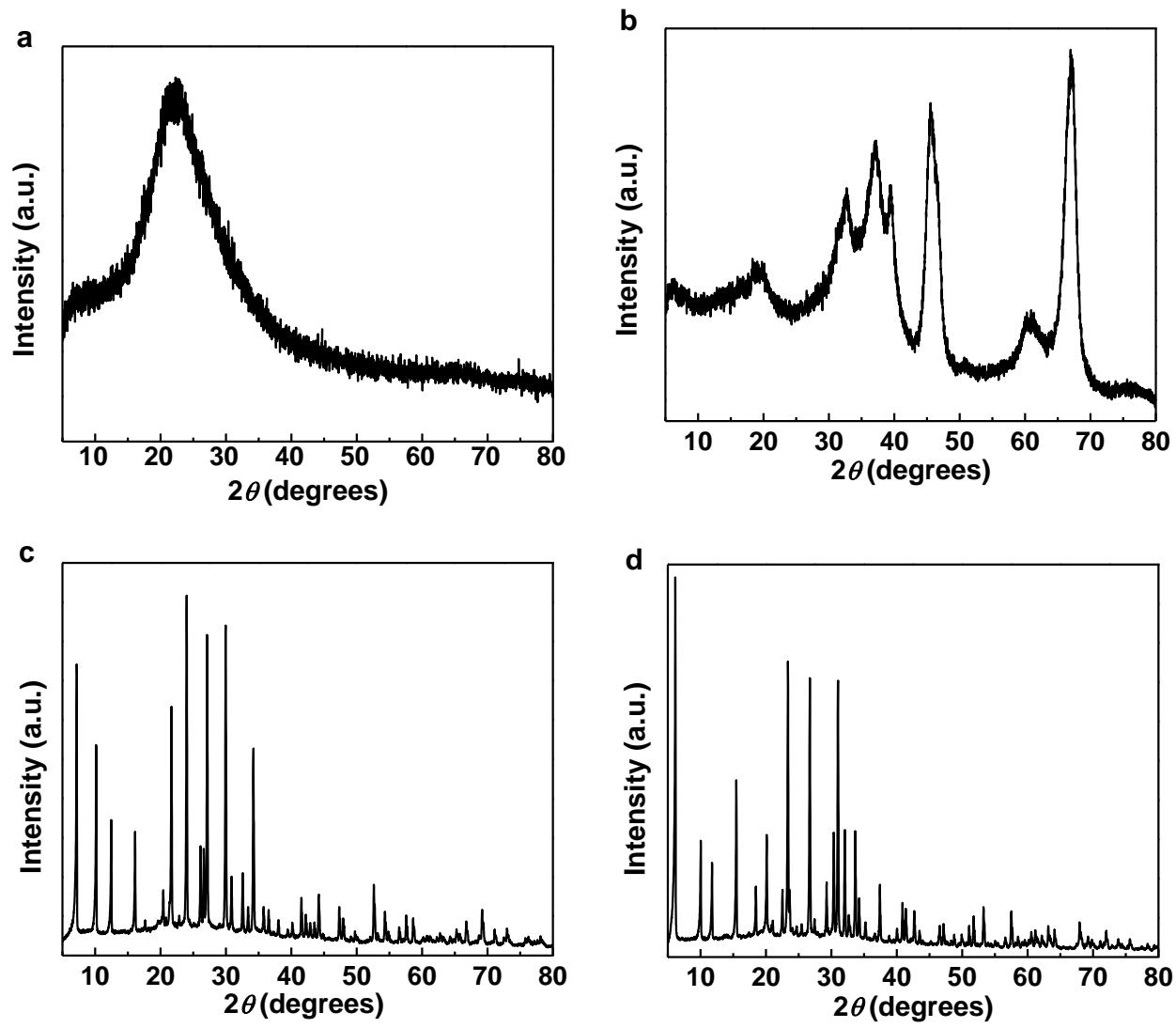
<sup>#</sup>L.Zhang and Z.-Z.Kang contributed equally to this work.

\*E-mail: [liuxq@njtech.edu.cn](mailto:liuxq@njtech.edu.cn) (X.-Q.Liu).

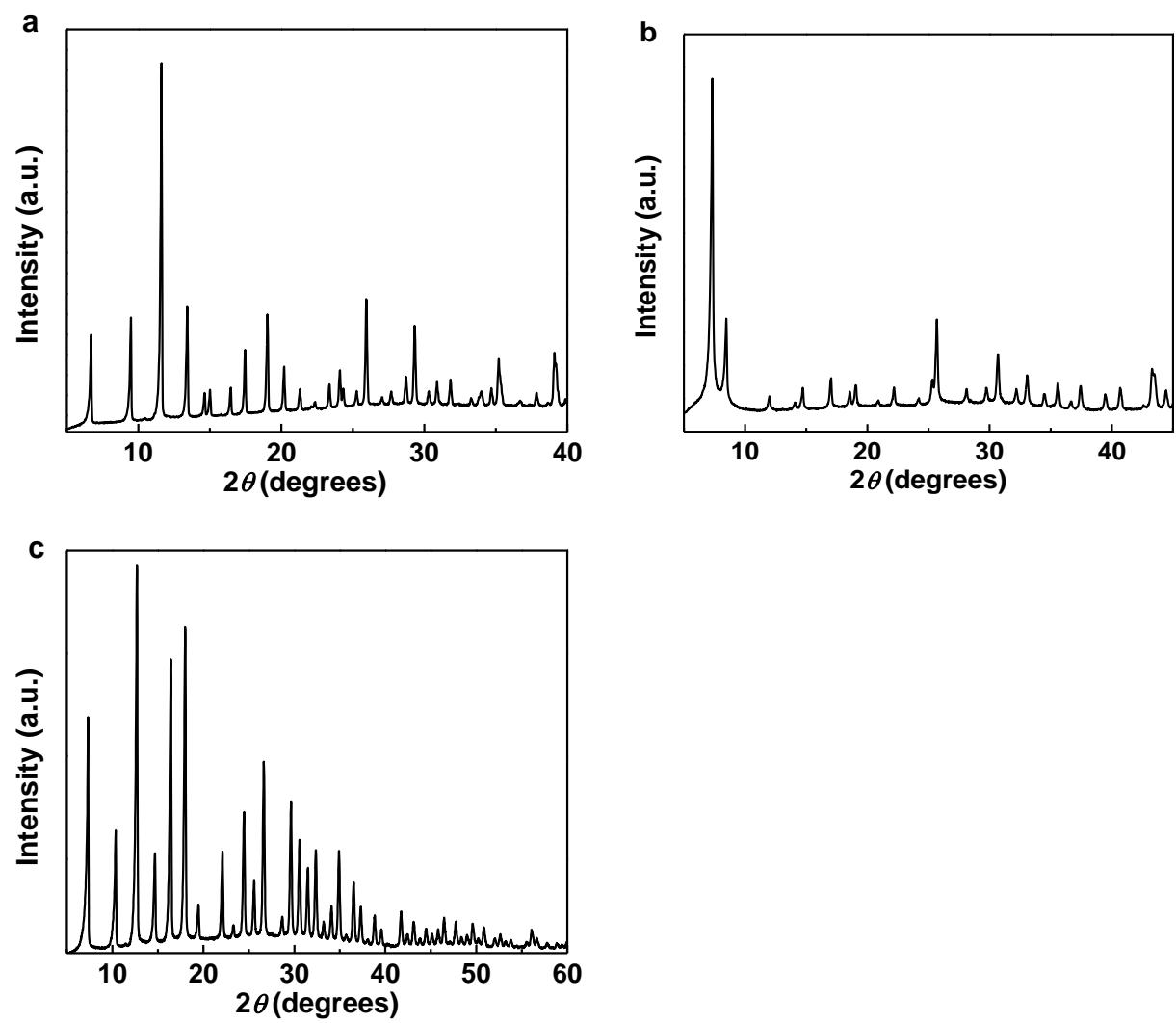
\*E-mail: [lbsun@njtech.edu.cn](mailto:lbsun@njtech.edu.cn) (L.-B.Sun).



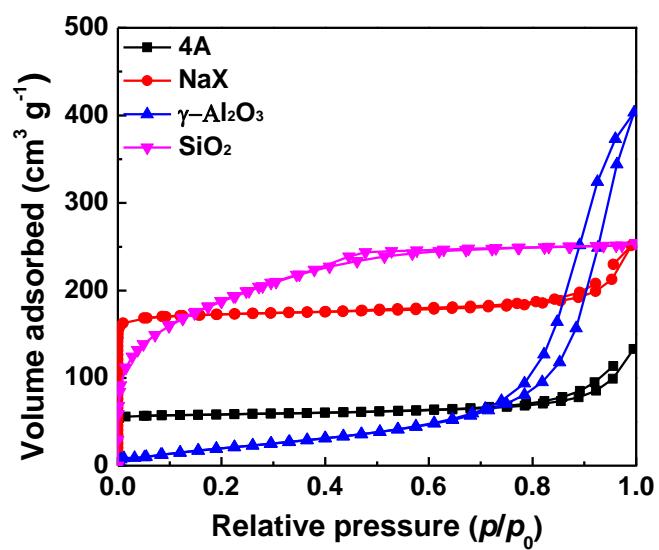
**Figure S1.** The device of testing the ability of ultra-deep dewatering of adsorbents.



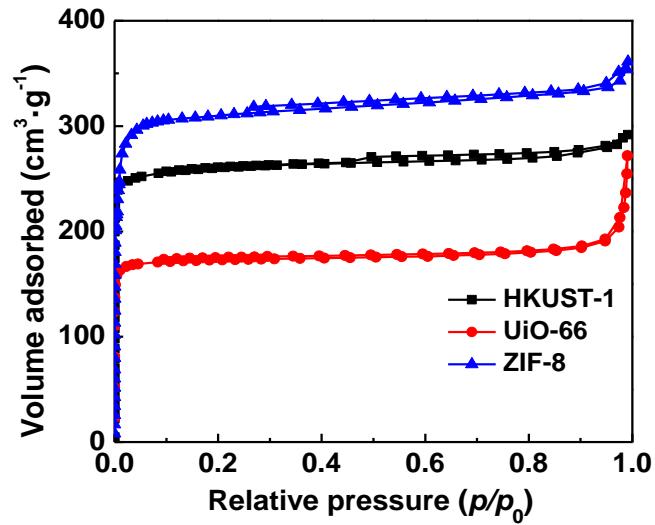
**Figure S2.** XRD patterns of (a)  $\text{SiO}_2$ , (b)  $\gamma\text{-Al}_2\text{O}_3$ , (c) 4A zeolite, and (d) NaX zeolite.



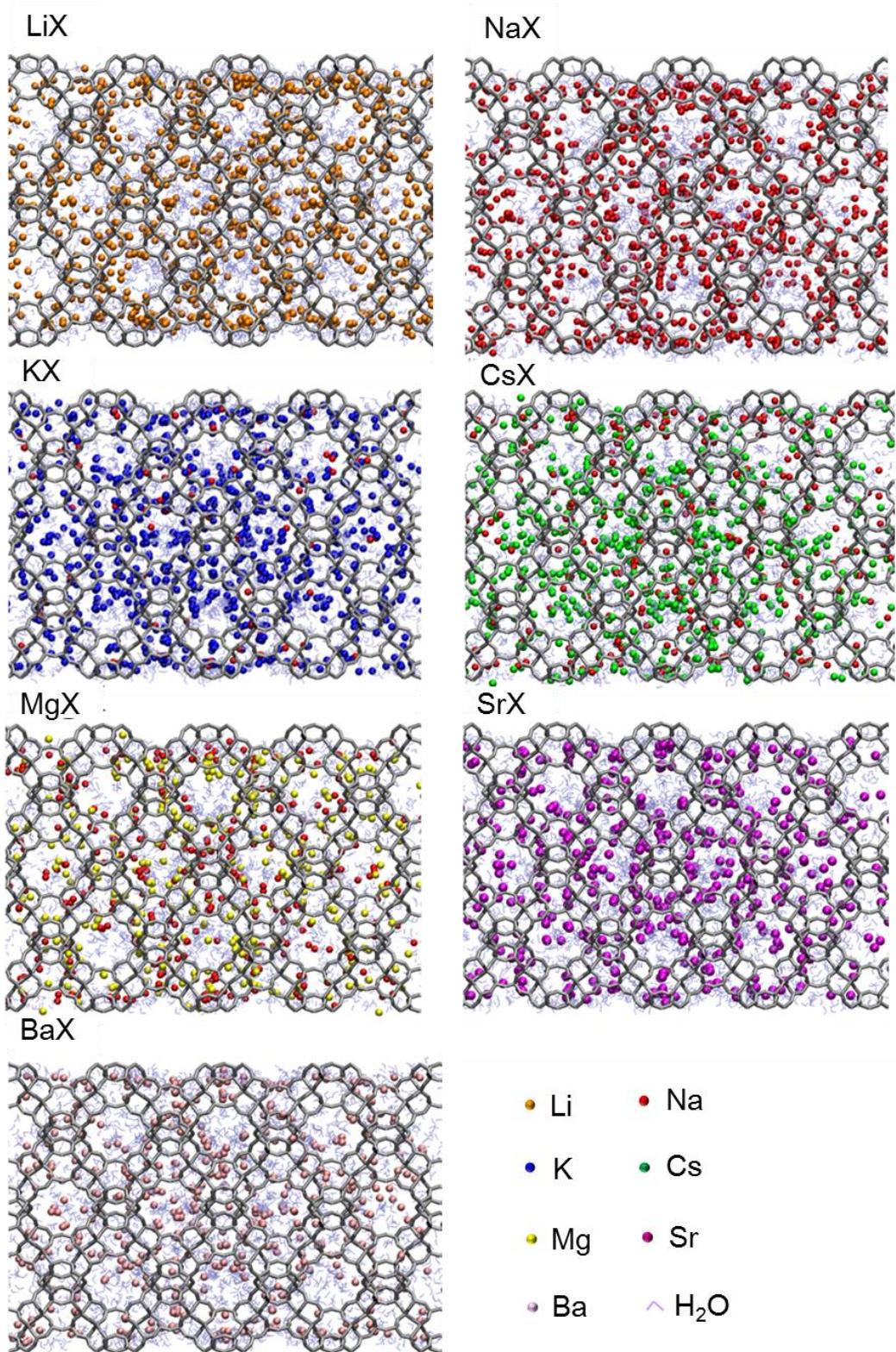
**Figure S3.** XRD patterns of (a) HKUST-1, (b) UiO-66, and (c) ZIF-8.



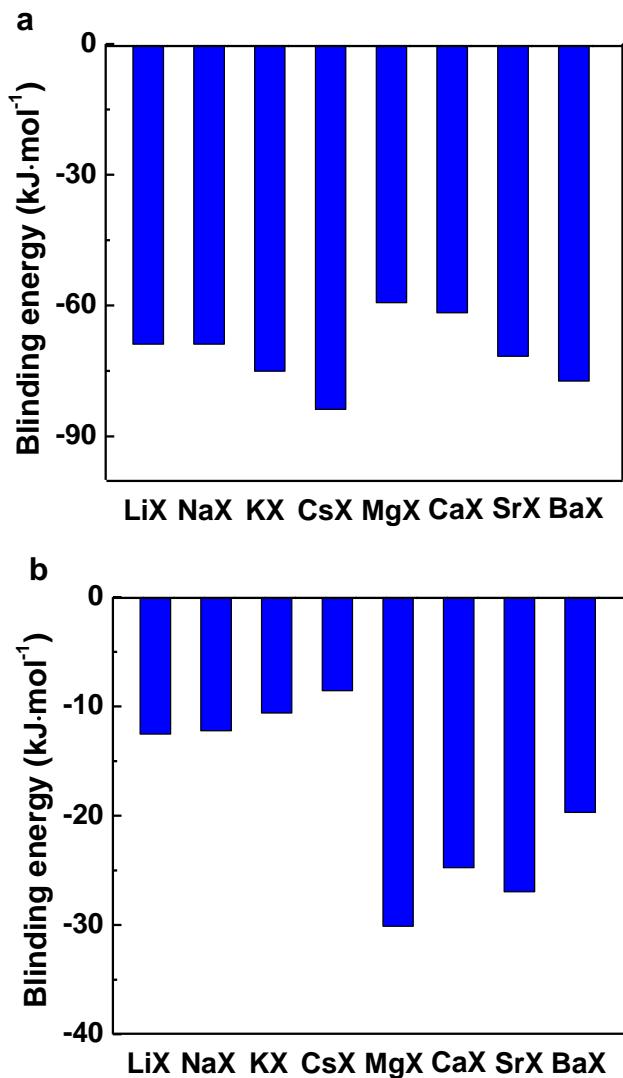
**Figure S4.** N<sub>2</sub> adsorption-desorption isotherms of 4A, NaX,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, and SiO<sub>2</sub>.



**Figure S5.** N<sub>2</sub> adsorption-desorption isotherms of HKUST-1, UIO-66, and ZIF-8.



**Figure S6.** Snapshot of the distribution of water molecules and extra-framework cations within X zeolites, as inferred from MD simulations.



**Figure S7.** Average binding energy per  $\text{H}_2\text{O}$  molecular (a) with framework and (b) with different ions in X zeolites calculated from MD simulations.