Electronic Supplementary Information

Amine post-functionalized POSS-based porous polymers exhibiting simultaneously enhanced porosity and carbon dioxide adsorption properties

Dengxu Wang,a,b* Wenyan Yang,b Shengyu Feng,a,b* Hongzhi Liu,b*

a National Engineering Technology Research Center for Colloidal Materials, Shandong University; b Key Laboratory of Special Functional Aggregated Materials & Key Laboratory of Colloid and Interface Chemistry (Shandong University), Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, P. R. China

*Corresponding Authors. Tel: +86 531 88364866. Fax: +86 531 88564464. E-mail: dxwang@sdu.edu.cn; fsy@sdu.edu.cn; liuhongzhi@sdu.edu.cn.
Table of contents

**Fig. S1** (a) The FT-IR spectra of HPP-1, HPP-1-EDA at 24 h and 72 h; (b) the FT-IR spectra were enlarged from 2000 cm\(^{-1}\) to 800 cm\(^{-1}\)

**Fig. S2** (a) The FT-IR spectra of HPP-1, HPP-1-HDA at 24 h and 72 h; (b) the FT-IR spectra were enlarged from 2000 cm\(^{-1}\) to 800 cm\(^{-1}\)

**Fig. S3** TGA curves of HPP-1, HPP-1-EDA and HPP-1-HDA under N\(_2\) at 10 °C min\(^{-1}\) from 30°C to 800°C

**Fig. S4** XRD patterns of HPP-1, HPP-1-EDA and HPP-1-HDA

**Fig. S5** FE-SEM images of HPP-1-EDA (left) and HPP-1-HDA (right)

**Fig. S6** HR-TEM images of HPP-1-EDA (left) and HPP-1-HDA (right)

**Fig. S7** BET plots of HPP-1 (top, \(r = 0.999970, C = 111.91\)), HPP-1-EDA (middle, \(r = 0.999910, C = 166.16\)) and HPP-1-HDA (bottom, \(r = 0.999992, C = 190.22\))

**Fig. S8** CO\(_2\) adsorption (closed symbols) and desorption (open symbols) isotherms of HPP-1-EDA and HPP-1-HDA at 273 K and 298 K

**Fig. S9** Ten cycles of CO\(_2\) uptakes of HPP-1-EDA (a) and HPP-1-HDA (b) at 273 K. After saturation, the sample was regenerated with a temperature swing to 80°C and then under vacuum.

**Fig. S10** Toth model fitting of CO\(_2\) (a) and N\(_2\) (b) adsorption isotherms of HPP-1 at 298 K

**Fig. S11** Toth model fitting of CO\(_2\) (a) and N\(_2\) (b) adsorption isotherms of HPP-1-EDA at 298 K

**Fig. S12** Toth model fitting of CO\(_2\) (a) and N\(_2\) (b) adsorption isotherms of HPP-1-HDA at 298 K
Fig. S1. (a) The FT-IR spectra of HPP-1, HPP-1-EDA at 24 h and 72 h; (b) the FT-IR spectra were enlarged from 2000 cm$^{-1}$ to 800 cm$^{-1}$

Fig. S2. (a) The FT-IR spectra of HPP-1, HPP-1-HDA at 24 h and 72 h; (b) the FT-IR spectra were enlarged from 2000 cm$^{-1}$ to 800 cm$^{-1}$
Fig. S3. TGA curves of HPP-1, HPP-1-EDA and HPP-1-HDA under N₂ at 10 °C min⁻¹ from 30°C to 800°C

Fig. S4. XRD patterns of HPP-1, HPP-1-EDA and HPP-1-HDA
Fig. S5 FE-SEM images of HPP-1-EDA (left) and HPP-1-HDA (right)

Fig. S6 HR-TEM images of HPP-1-EDA (left) and HPP-1-HDA (right)
Fig. S7 BET plots of HPP-1 (top, r = 0.999970, C = 111.91), HPP-1-EDA (middle, r = 0.999990, C = 166.16) and HPP-1-HDA (bottom, r = 0.999992, C = 190.22)
Fig. S8 CO$_2$ adsorption (closed symbols) and desorption (open symbols) isotherms of HPP-1-EDA and HPP-1-HDA at 273 K and 298 K.
Fig. S9 Ten cycles of CO$_2$ uptakes of HPP-1-EDA (a) and HPP-1-HDA (b) at 273 K.

After saturation, the sample was regenerated with a temperature swing to 80°C and then under vacuum.

**Henry’s Law selectivity of CO$_2$ over N$_2$ for HPP-1, HPP-1-EDA and HPP-1-HDA at 298 K**

A nice fitting of CO$_2$ and N$_2$ isotherms has been calculated based on Toth isotherm model.$^{[1,2]}$

\[ q = q_{\text{sat}} \frac{b^t P}{(1 + b^t)^{3/4}} \]

where $q$ is the uptake in mmol g$^{-1}$, $q_{\text{sat}}$ is the saturation uptake in mmol g$^{-1}$, $P$ is the pressure in torr, $t$ and $b$ are parameters which are specific for adsorbent pairs.
The Henry law constant $K$, quantifies the extent of the adsorption of a given adsorbate by a solid. The magnitude of $K$ depends on the properties of both adsorbate and solid. For the Toth isotherm, the Henry law constant is defined by the following equation:

$$K = \lim_{P \to 0} \left( \frac{dq}{dP} \right) = b^{1/t} q_{sat}$$

Finally, the Henry’s Law selectivity $S_{\alpha/\beta}$ of gas $\alpha$ over $\beta$ is given by the following equation:

$$S_{\alpha/\beta} = \frac{K_\alpha}{K_\beta}$$

![Graph](image1)

**Fig. S10** Toth model fitting of CO$_2$ (a) and N$_2$ (b) adsorption isotherms of HPP-1 at
Fig. S11 Toth model fitting of CO$_2$ (a) and N$_2$ (b) adsorption isotherms of HPP-1-EDA at 298 K
Fig. S12 Toth model fitting of CO$_2$ (a) and N$_2$ (b) adsorption isotherms of HPP-1-HDA at 298 K.

References
