

## Supporting Information

### Monodispersed Ultramicroporous Semi-Cycloaliphatic Polyimides for Highly Efficient Adsorption of CO<sub>2</sub>, H<sub>2</sub> and Organic Vapors

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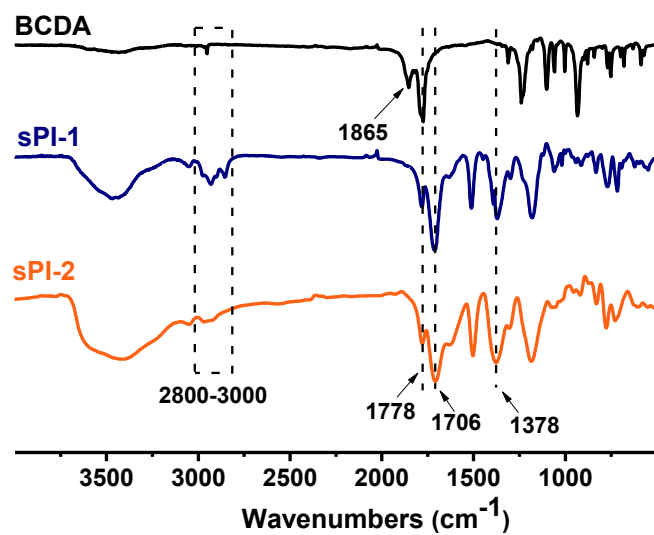
Email: zgwang@dlut.edu.cn

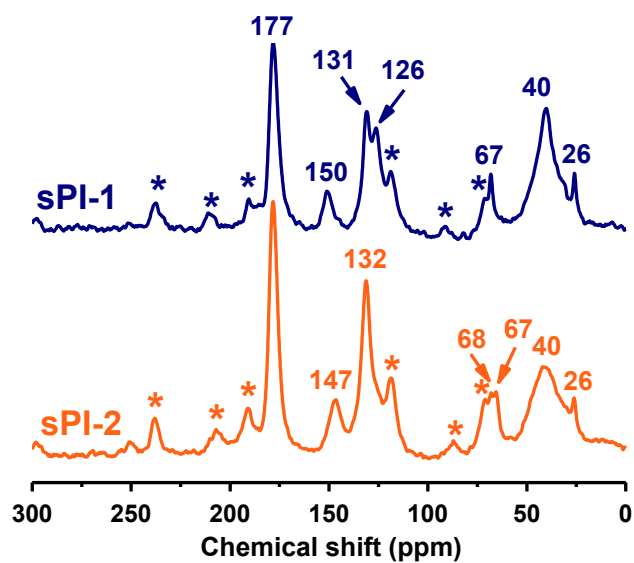
**Table S1.**  $K_H$ ,  $A_0$ , and  $Q_0$  Values for CO<sub>2</sub> Adsorption in Cycloaliphatic sPIs

| Sample | T/K | $K_H/\text{mol g}^{-1} \text{Pa}^{-1}$ | $A_0/\ln(\text{mol g}^{-1} \text{Pa}^{-1})$ | $Q_0/\text{kJ/mol}$ |
|--------|-----|--|---|---------------------|
| sPI-1  | 273 | $2.105 \times 10^{-7}$                 | -15.376                                     | 31.3                |
|        | 298 | $6.591 \times 10^{-8}$                 | -16.535                                     |                     |
| sPI-2  | 273 | $2.841 \times 10^{-7}$                 | -15.074                                     | 31.4                |
|        | 298 | $8.897 \times 10^{-8}$                 | -16.235                                     |                     |

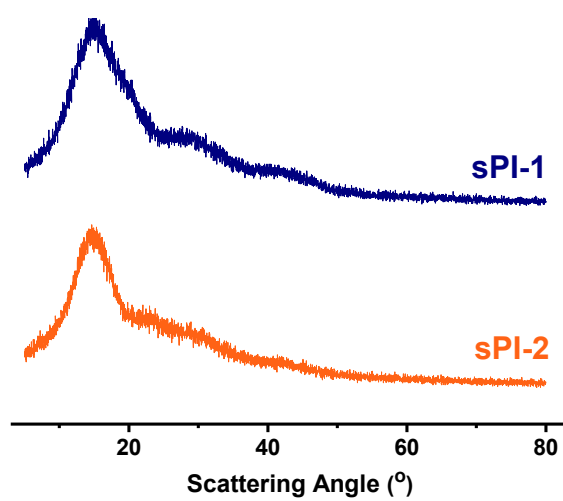
**Table S2.**  $K_H$ ,  $A_0$ , and  $Q_0$  Values for  $H_2$  Adsorption in Cycloaliphatic sPIs

| Sample | T/K | $K_H/\text{mol g}^{-1} \text{Pa}^{-1}$ | $A_0/\ln(\text{mol g}^{-1} \text{Pa}^{-1})$ | $Q_0/\text{kJ/mol}$ |
|--------|-----|--|---|---------------------|
| sPI-1  | 77  | $1.316 \times 10^{-6}$                 | -13.541                                     | 7.21                |
|        | 87  | $3.601 \times 10^{-7}$                 | -14.837                                     |                     |
| sPI-2  | 77  | $1.724 \times 10^{-6}$                 | -13.271                                     | 7.64                |
|        | 87  | $4.402 \times 10^{-7}$                 | -14.636                                     |                     |

**Figure S1.** FT-IR spectra of dianhydride monomer BCDA and two polyimides sPIs.



**Figure S2.** Solid-state  $^{13}\text{C}$  CP/MAS NMR spectra of sPI-1 and sPI-2. Asterisks (\*) indicate peaks arising from spinning side bands.



**Figure S3.** Wide angle X-ray diffractions of sPI-1 and sPI-2

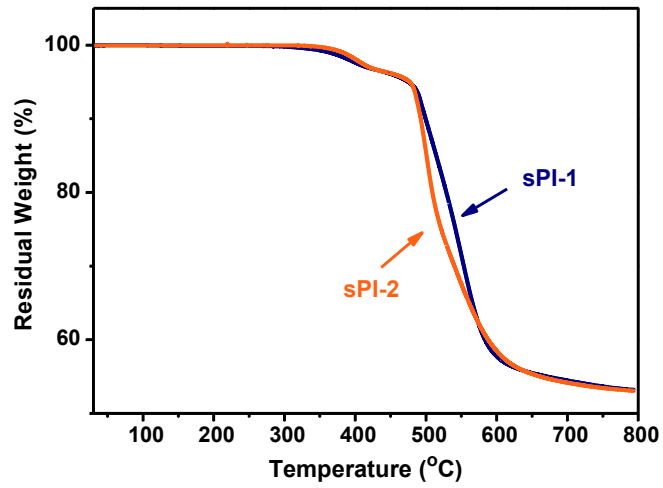


Figure S4. TGA curves of sPI-1 and sPI-2.

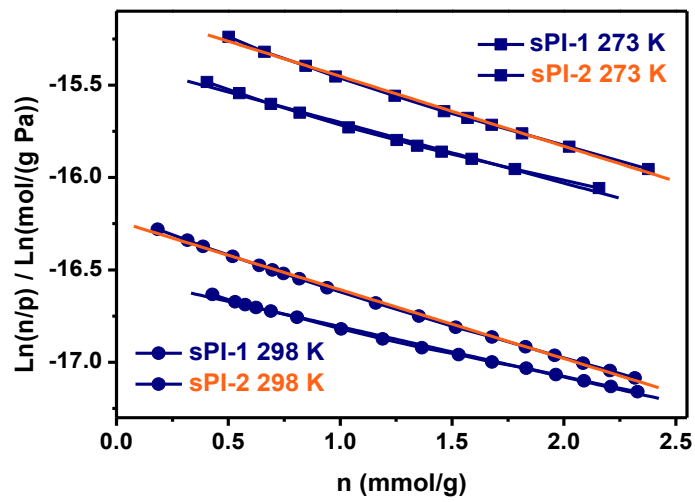
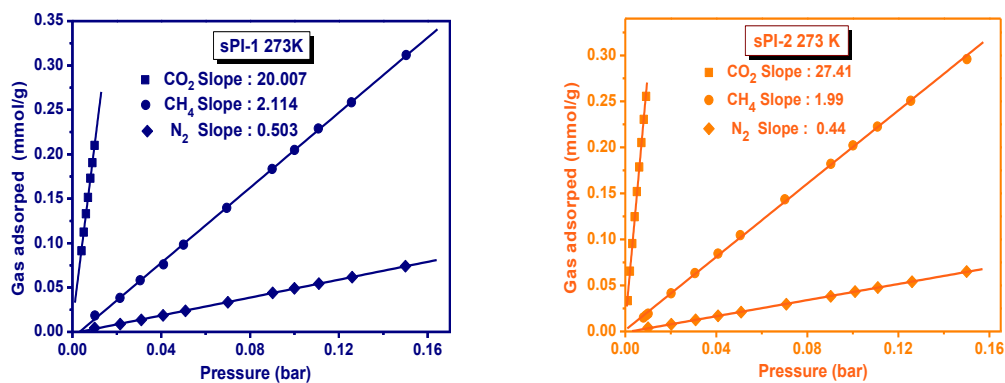
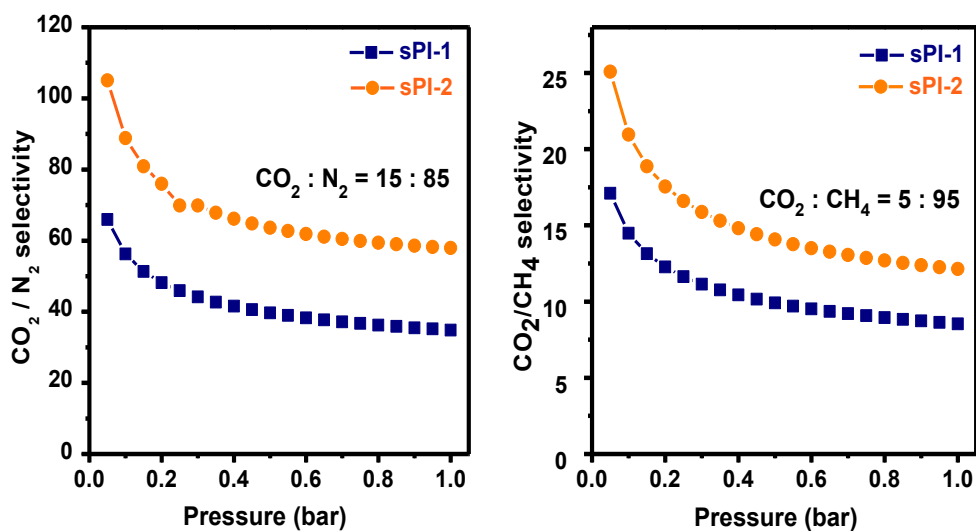


Figure S5. Virial plots of CO<sub>2</sub> for sPI-1 and sPI-2



**Figure S6.** Adsorption isotherms of CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub> at 273K for sPI-1 and sPI-2



**Figure S7.** IAST selectivities for CO<sub>2</sub>/N<sub>2</sub> and CO<sub>2</sub>/CH<sub>4</sub> mixtures for sPI-1 and sPI-2 at 273 K.

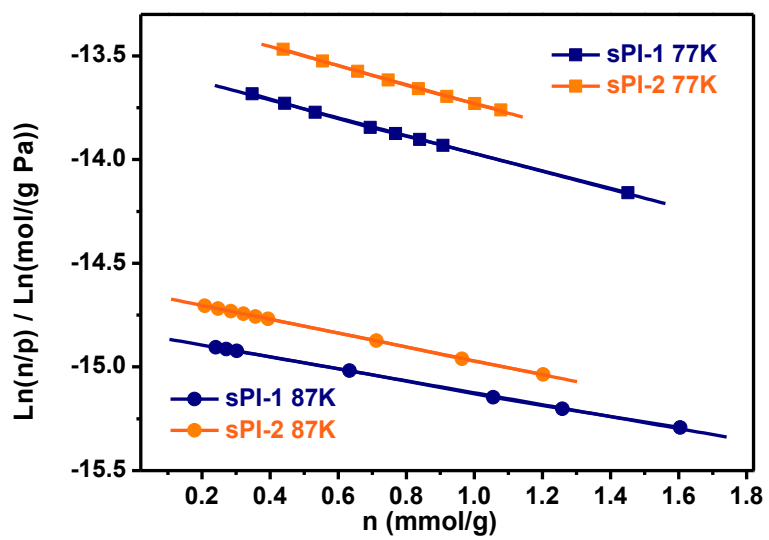


Figure S8. Virial plots of H<sub>2</sub> for sPI-1 and sPI-2