# Electronic Supplementary Information

## Mechanistic insight into highly efficient gas permeation and separation in a shape-persistent ladder polymer membrane

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**Table S1.** A 21-step MD compression and relaxation scheme.[1,2]

| Step | Slow Decompression Conditions | Duration (ps) |
|---|---|---|
| 1 | NVT, $T_{max}$ | 50 |
| 2 | NVT, $T_{final}$ | 100 |
| 3 | NPT, $0.02P_{max}$, $T_{final}$ | 50 |
| 4, 5 | NVT, $T_{max}$; NVT, $T_{final}$ | 50, 100 |
| 6 | NPT, $0.6P_{max}$, $T_{final}$ | 50 |
| 7, 8 | NVT, $T_{max}$; NVT, $T_{final}$ | 50, 100 |
| 9 | NPT, $P_{max}$, $T_{final}$ | 50 |
| 10, 11 | NVT, $T_{max}$; NVT, $T_{final}$ | 50, 100 |
| 12 | NPT, $0.5P_{max}$, $T_{final}$ | 5 |
| 13, 14 | NVT, $T_{max}$; NVT, $T_{final}$ | 5, 10 |
| 15 | NPT, $0.1P_{max}$, $T_{final}$ | 5 |
| 16, 17 | NVT, $T_{max}$; NVT, $T_{final}$ | 5, 10 |
| 18 | NPT, $0.01P_{max}$, $T_{final}$ | 5 |
| 19, 20 | NVT, $T_{max}$; NVT, $T_{final}$ | 5, 10 |
| 21 | NPT, $P_{final}$, $T_{final}$ | 800 |

**Table S2.** Atomic charges and bond lengths of $CO_2$, $CH_4$, $N_2$, $O_2$ and $H_2$.

| Molecule | Atom | Charge ($e$) | Bond length (Å) |
|---|---|---|---|
| $CO_2$[3] | C | 0.576 | 1.180 |
| | O | –0.288 | |
| $CH_4$[4] | C | –0.660 | 1.090 |
| | H | 0.165 | |
| $N_2$[5] | N | 0 | 1.102 |
| $O_2$[6] | O | 0 | 1.208 |
| $H_2$[7] | H | 0 | 0.740 |

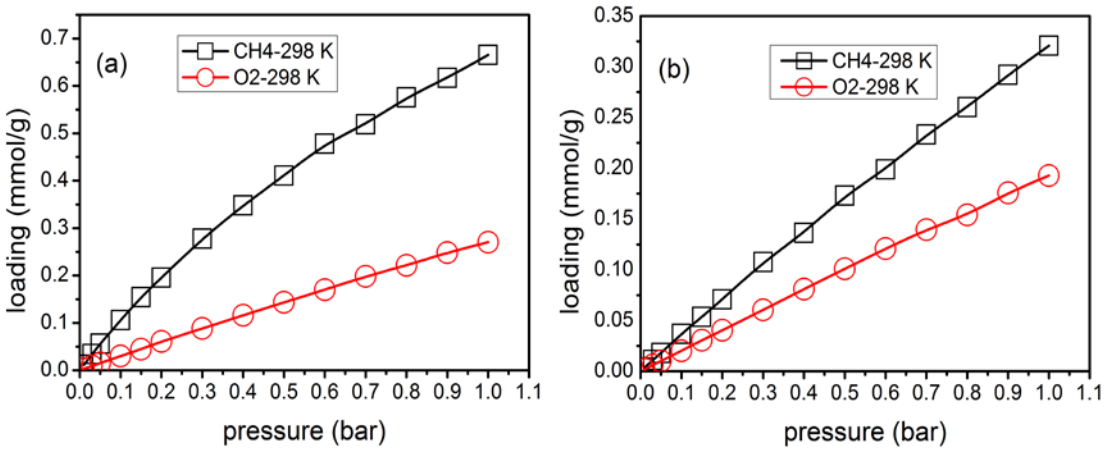


**Fig. S1** Simulated sorption isotherms of $CH_4$ and $O_2$ in (a) PIM-EA-TB and (b) PIM-SBI-TB.

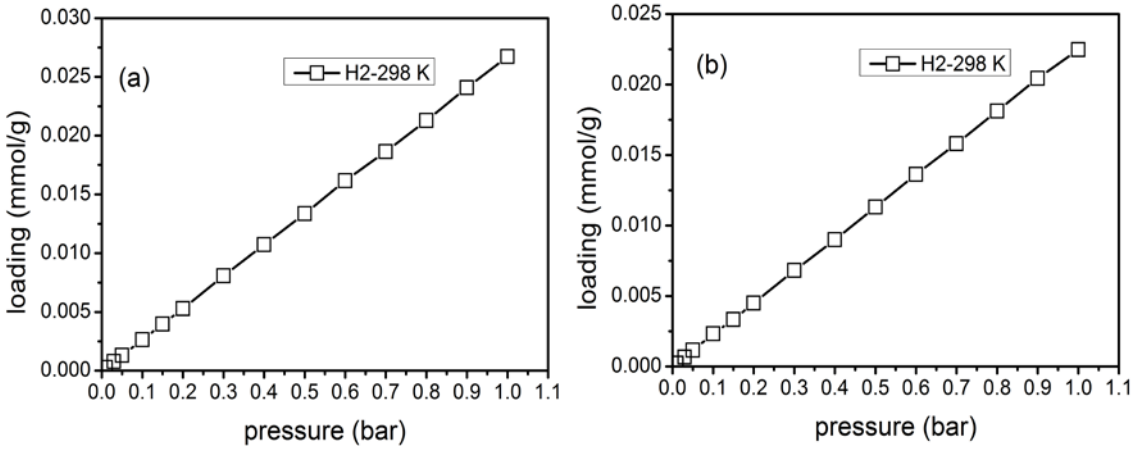


**Fig. S2** Simulated sorption isotherms of $H_2$ in (a) PIM-EA-TB and (b) PIM-SBI-TB.

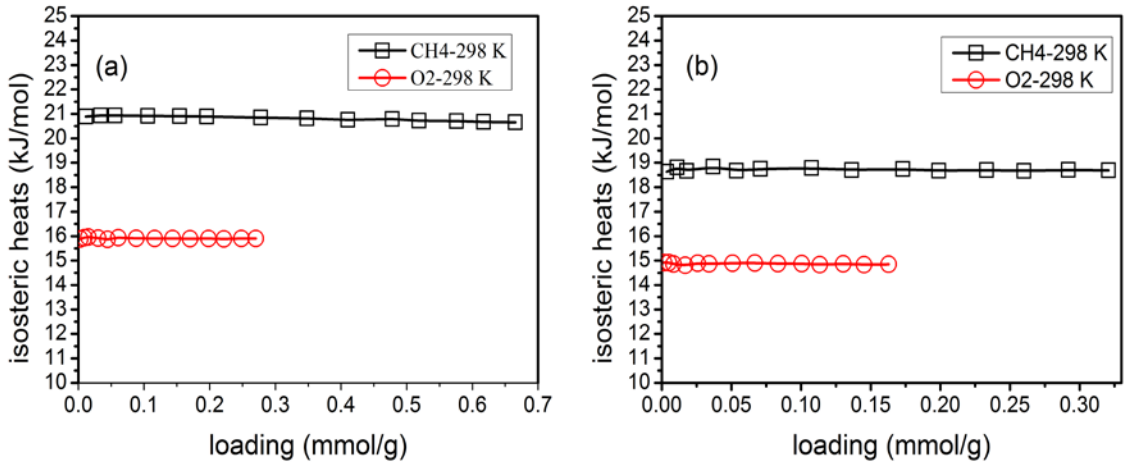


**Fig. S3** Simulated isosteric heats of $CH_4$ and $O_2$ sorption in (a) PIM-EA-TB and (b) PIM-SBI-TB.

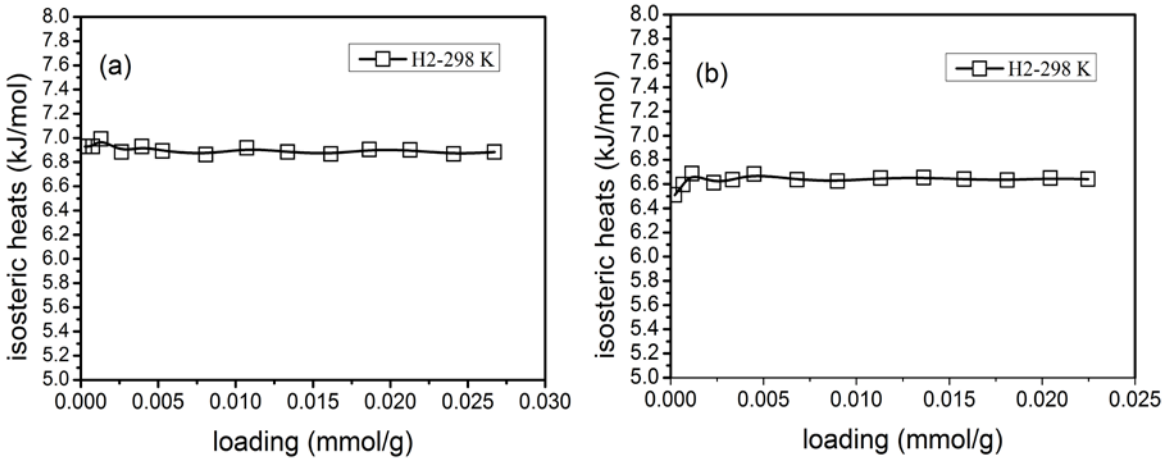


**Fig. S4** Simulated isosteric heats of $H_2$ sorption in (a) PIM-EA-TB and (b) PIM-SBI-TB.

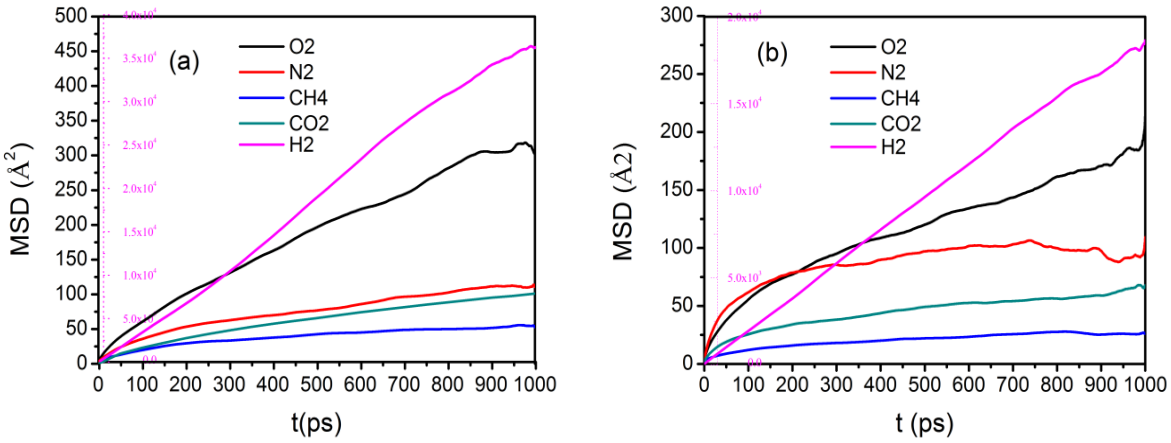


**Fig. S5** MSDs of $O_2$, $N_2$, $CH_4$, $CO_2$ and $H_2$ in (a) PIM-EA-TB and (b) PIM-SBI-TB.

## References


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