Supporting Information

Solvent-Free Molten Co-Assembly to Ordered Mesoporous Carbon for Efficiently Supported Adsorption and Separation of SO_2

Xun Kan, Feiyu Song, Fangyao Li, Shuying Xiao, Fujian Liu*, Lilong Jiang

National Engineering Research Center for Chemical Fertilizer Catalyst (NERC-CFC), School of Chemical Engineering, Fuzhou University, Fuzhou, 350116, China.

E-mail: fjliu@fzu.edu.cn

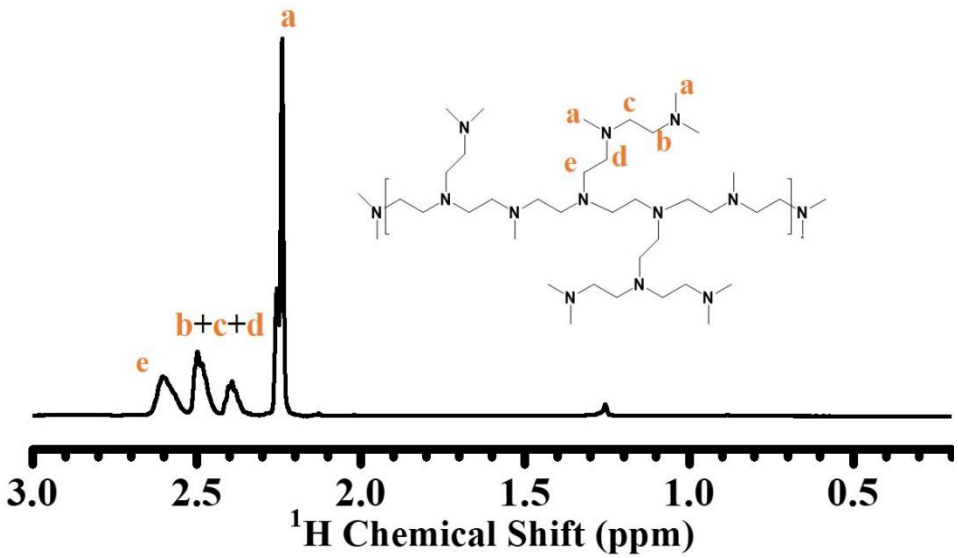


Figure S1 ^{1}H NMR spectra of mPEI.

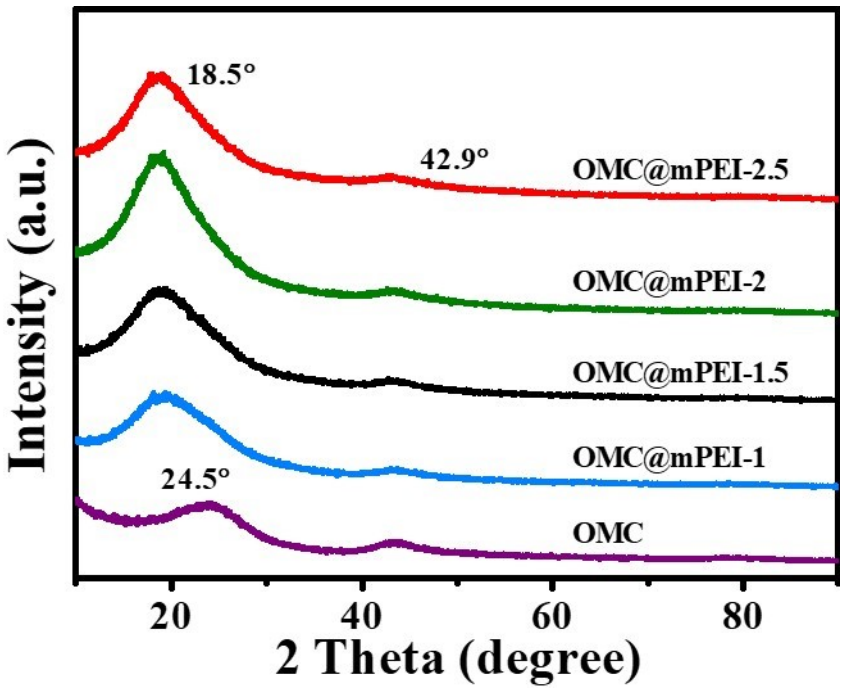


Figure S2 Wide-angle XRD patterns of OMC and various OMC@mPEI-x.

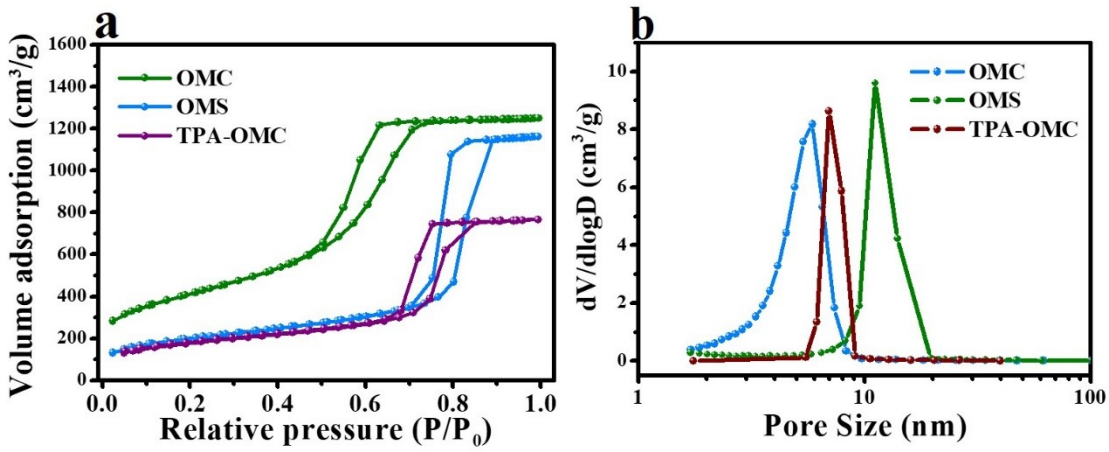


Figure S3 (a) N_2 adsorption-desorption isotherms at −196 °C and (b) pore size distributionsof OMC, OMS and TPA-OMC.

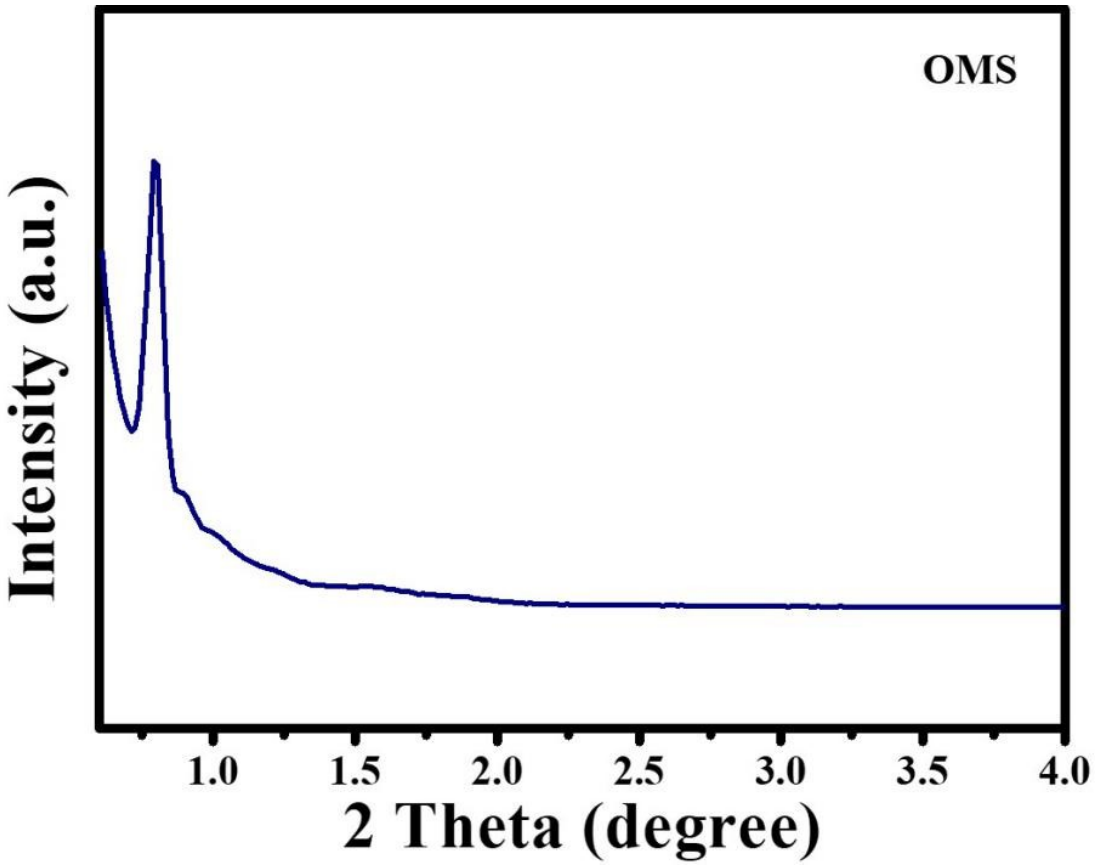


Figure S4 Low-angle XRD pattern of OMS.

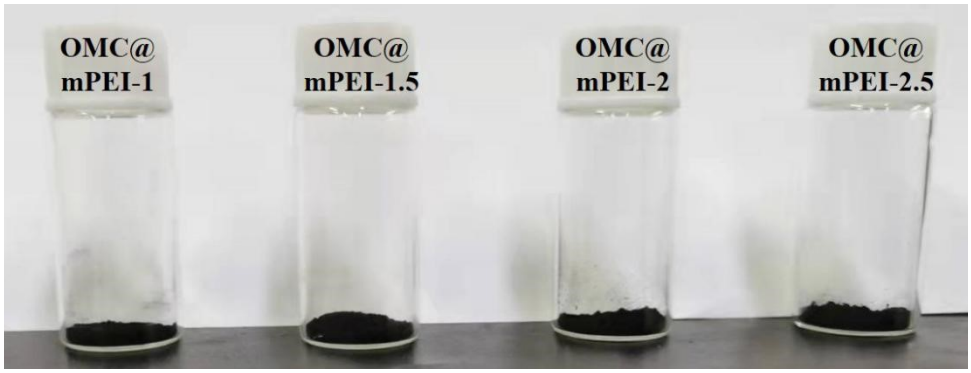


Figure S5 Photographs of OMC and various OMC@mPEI-x.

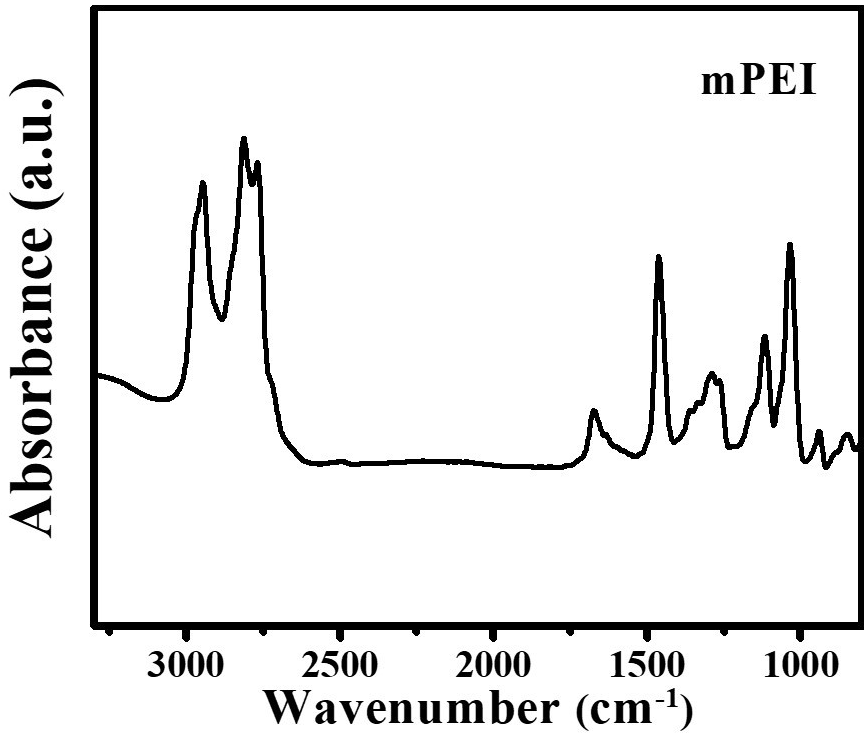


Figure S6 FT-IR spectra of mPEI.

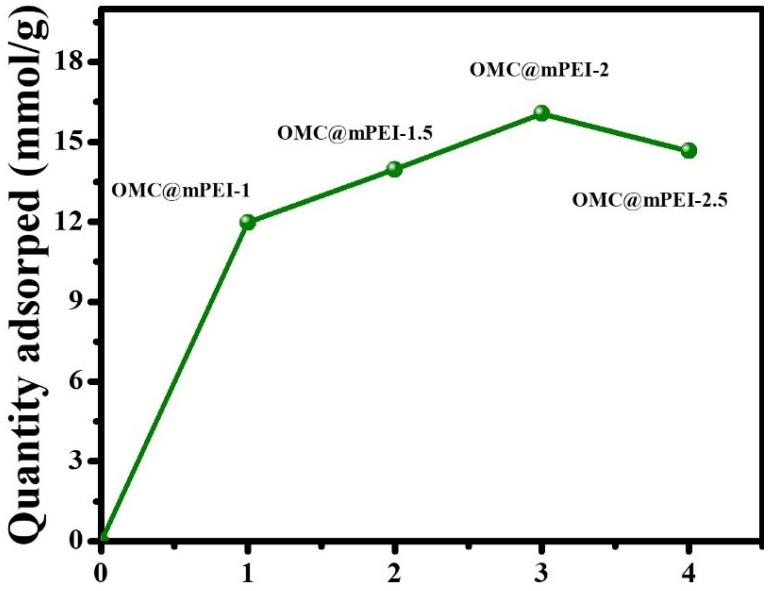


Figure S7 SO_2 adsorption capacities of OMC@mPEI-x samples at 25 ℃ and 1 bar.

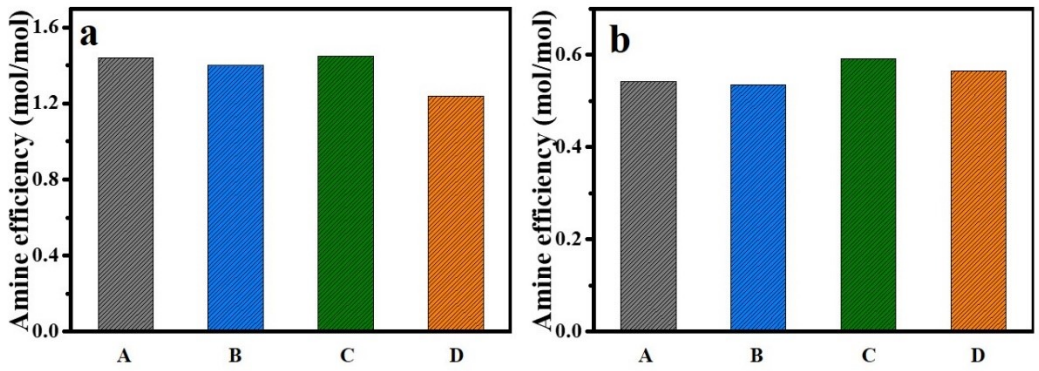


Figure S8 mPEI efficiencies of (A) OMC@mPEI-1, (B) OMC@mPEI-1.5, (C) OMC@mPEI-2 and (D) OMC@mPEI-2.5 for SO_2 adsorption at 25 ℃ and different pressures: (a) 1 bar and (b) 0.002 bar.

Note: the mPEI utilization efficiency of OMC@mPEI-*x* was calculated from the following equations of S1 and S2:

$$M = \frac{x}{1+x} Mi \tag{S1}$$

$$n = \frac{m}{M} \tag{S2}$$

where M is the molar of tertiary amine group per g catalyst; *x* represents the mass ratio of mPEI to OMC; n is the utilization efficiency of mPEI; m is the adsorption capacity of SO_2 (mmol/g); ($Mi =$ 16.6 mmol/g for the molar of tertiary amine group per g PEI).

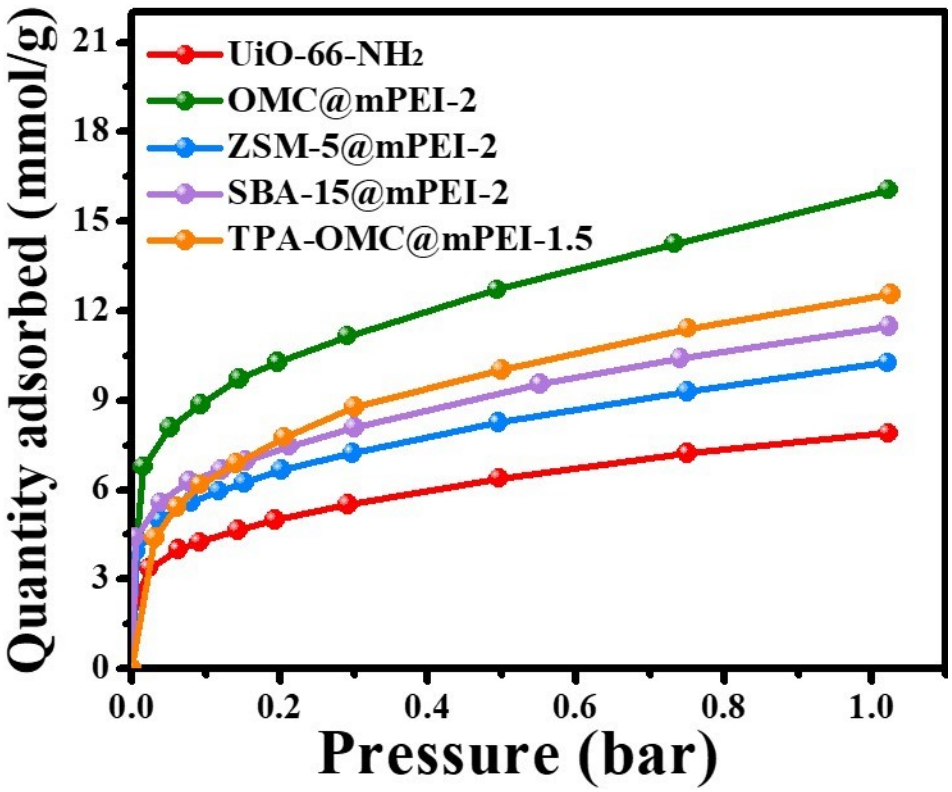


Figure S9 SO_2 adsorption isotherm of UiO-66-NH_2, OMC@mPEI-2, ZSM-5@mPEI-2, SBA-15@mPEI-2, and TPA-OMC@mPEI-1.5 at 25 ℃ and 1 bar.

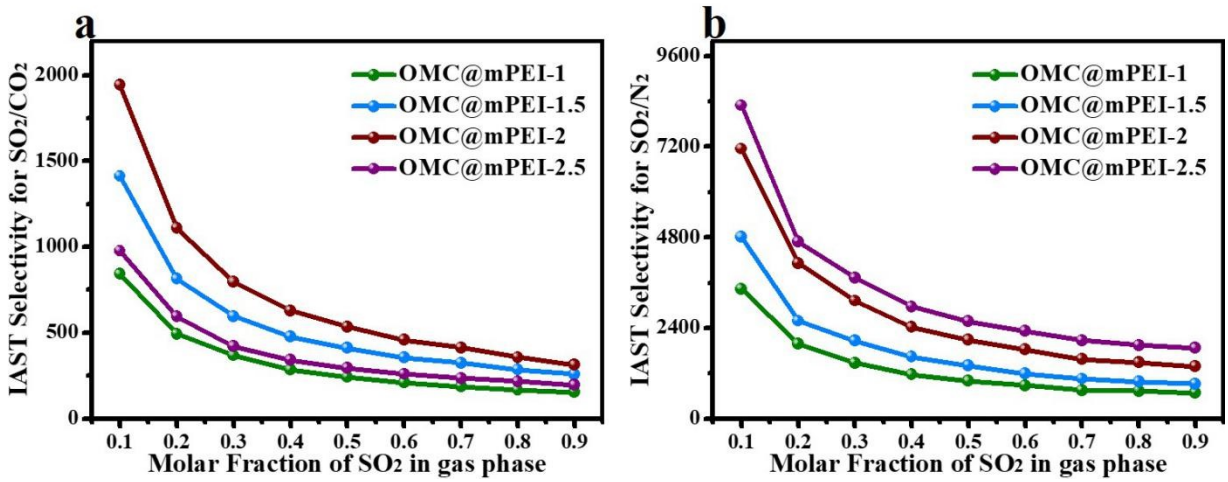


Figure S10 IAST selectivities of OMC@mPEI-x for (a) SO_2/CO_2 and (b) SO_2/N_2 at 50 °C.

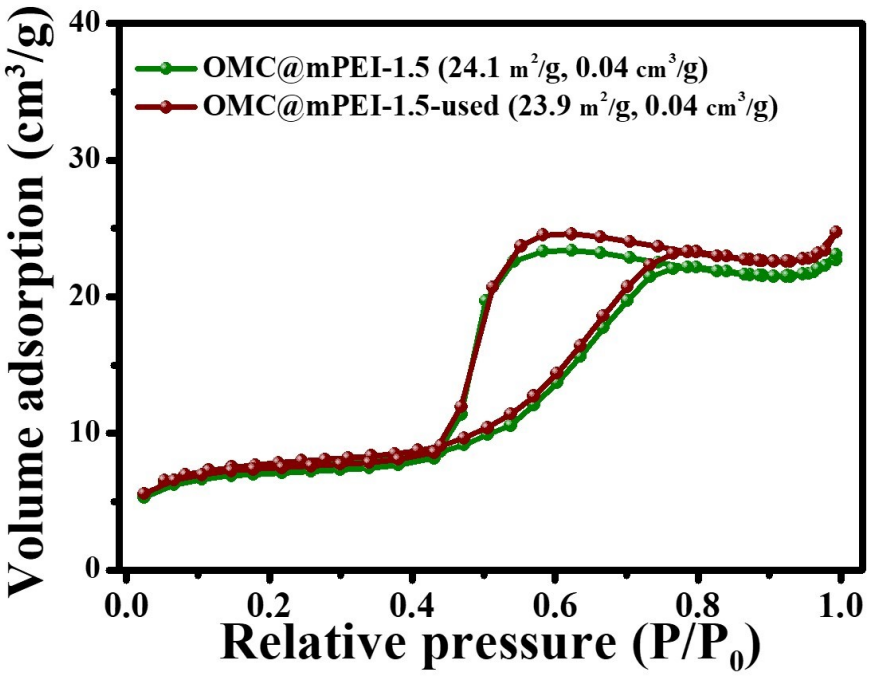


Figure S11 N_2 adsorption-desorption isotherms at −196 °C of fresh OMC@mPEI-1.5 and used OMC@mPEI-1.5 in SO_2 adsorption.

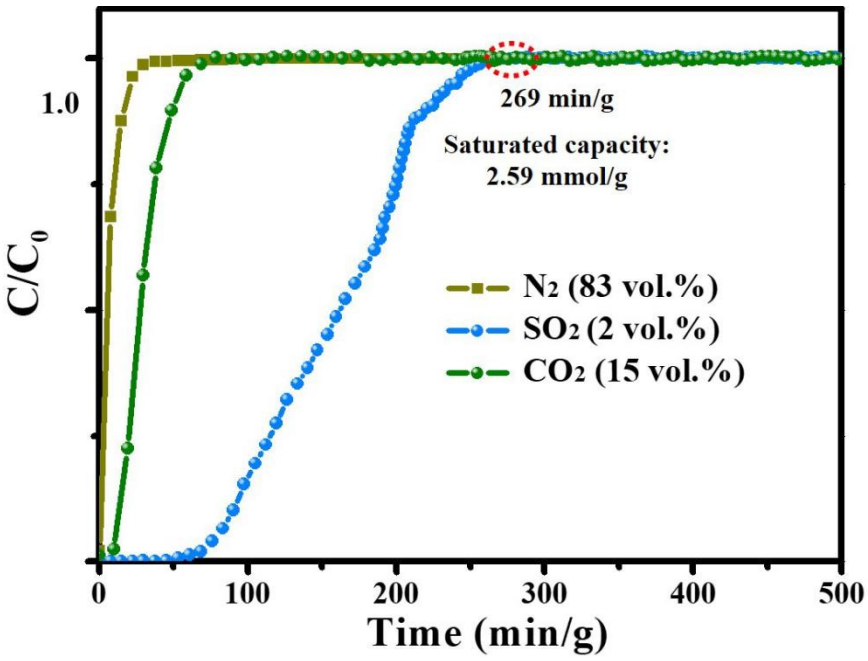


Figure S12 Breakthrough curves of SBA-15@mPEI-2 for $SO_2/CO_2/N_2$ gas mixture (20 mL/min) at 25 °C

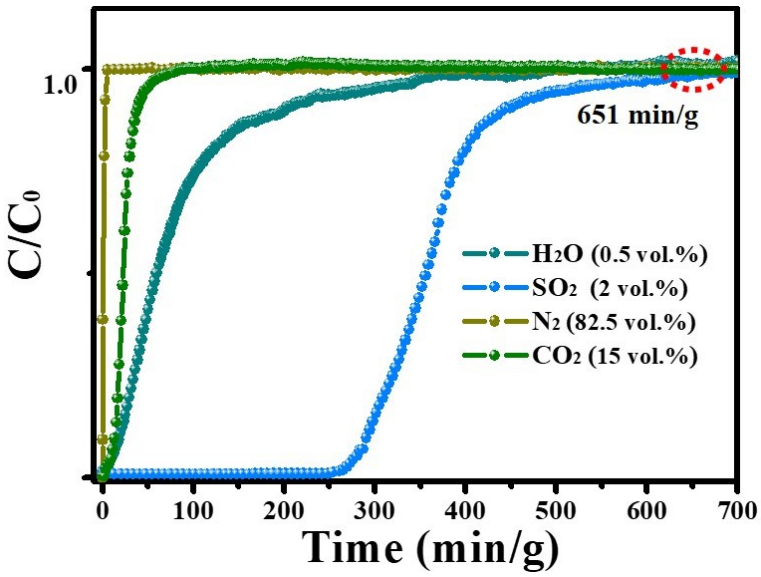


Figure S13 Breakthrough curves of OMC@mPEI-2 for $SO_2/CO_2/N_2/H_2O$ gas mixture (20 mL/min) at 25 °C

Table S1 SO_2 capacities of different porous solid adsorbents.

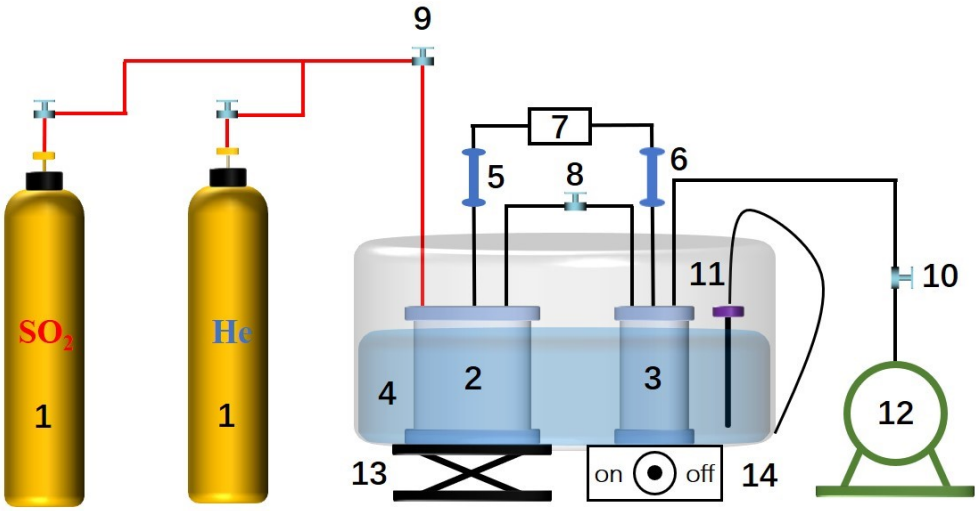
Samples	Condition	SO_2 capacities (mmol/g)	Ref.
OMC@mPEI-2	25 °C, 1.0 bar	16.1	This work
OMC@mPEI-2	25 °C, 0.002 bar	3.9	This work
UiO-66-NH_2	25 °C, 1.0 bar	7.9	This work
ZSM-5@mPEI-2	25 °C, 1.0 bar	10.1	This work
SBA-15@mPEI-2	25 °C, 1.0 bar	11.5	This work
TPA-OMC@mPEI-1.5	25 °C, 1.0 bar	12.5	This work
P(Ph-4MVIm-Br)	25 °C, 0.002 bar	1.6	(S1)
SIFSIX-2-Cu-i	25 °C, 0.002 bar	2.3	(S2)
DT-NPC-3	25 °C, 0.1 bar	5.2	(S3)
ACT	25 °C, 1.0 bar	7.9	(S4)
CFT-CSU38	25 °C, 0.1 bar	7.9	(S5)
MIL-160	25 °C, 0.97 bar	7.3	(S6)
Mg-MOF-74	25 °C, 1.0 bar	8.6	(S7)
MFM-600	25 °C, 1.0 bar	5.0	(S8)
MFM-300(In)	25 °C, 1.0 bar	8.3	(S9)
MFM-300(Al)	25 °C, 1.0 bar	7.1	(S10)
MFM-202a	25 °C, 1.0 bar	10.2	(S11)
GU-1	25 °C, 1.0 bar	7.6	(S12)
HNIP-TBMB-1	25 °C, 1.0 bar	7.2	(S13)

Table S2 IAST selectivities of different porous solid adsorbents.

Samples	Condition	Temperature	IAST selectivity	Ref.
OMC@mPEI-2	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	1789	This work
SIFSIX-2-Cu-i	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	87.1	(S2)
ELM-12	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	30	(S2)
MIL-160	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	124	(S6)
MFM-601	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	67.5	(S8)
MFM-300(In)	SO_2/CO_2	25 °C	33.6	(S9)

	(0.1:0.9 v/v, 1 bar)			
Mg-gallate	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	321	(S14)
Co-gallate	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	143	(S14)
MFM-170	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	32	(S15)
NKU-100	SO_2/CO_2 (0.5:0.5 v/v, 100000 Pa)	25 °C	940	(S16)
DMOF-TM	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	169	(S17)
ECUT-111	SO_2/CO_2 (1:99 v/v, 1 bar)	25 °C	25.2	(S18)
HBU-20	SO_2/CO_2	25 °C	44.3	(S19)

	(0.1:0.9 v/v, 1 bar)			
2.0mPEI@g-C3N4	SO_2/CO_2 (0.1:0.9 v/v, 1 bar)	25 °C	630	(S20)



Scheme S1 Diagram for dual-chamber equipment used for measurements of SO_2 adsorption isotherms (1: gas cylinder; 2: storage chamber; 3: adsorption chamber; 4: water bath; 5~6: pressure transducers; 7: digital displayer; 8~10: needle valve; 11: temperature probe; 12: vacuum pump; 13: elevator platform; 14: magnetic stirrer).

Measuring procedures:

The equipment has two chambers made of 316 L stainless steel: one is used for the storage of SO_2, and the other is used for the adsorption of SO_2. The temperature of two chambers is controlled by a water bath. The pressures in two chambers are monitored by two Wideplus-8 transducers respectively. In a typical run, a certain amount of sample was placed in the adsorption chamber; the equipment was completely evacuated by a pump, and a certain amount of SO_2 was introduced to the storage chamber from the cylinder; after stabilization, the pressure in storage chamber was recorded as P_0; then a certain amount of SO_2 was introduced to the adsorption chamber from the storage chamber; after stabilization, the pressures in storage chamber and adsorption chamber were recorded as P_1 and P_2 respectively; the amount of SO_2 adsorbed at the equilibrium pressure of P_2 was calculated using the following equation:

$$n = \rho_0 V_1 - \rho_1 V_1 - \rho_2 V_2 \qquad \text{(S3)}$$

where n is the amount of SO_2 adsorbed; ρ_i is the density of SO_2 at P_i (i=0~2); V_j is the free volume of chamber (j=1 for storage chamber and 2 for adsorption chamber). The values of ρ_i

were obtained from the NIST Chemistry WebBook.[S21] The values of V_j were measured using He as the probing gas. The amounts of SO_2 adsorbed at elevated pressures were measured by loading more SO_2 to the adsorption chamber. The amounts of SO_2 adsorbed were finally transformed to mmol of SO_2 per gram of sample.

Density functional theory (DFT) calculation

Density functional theory (DFT) calculations were conducted using Gaussian 16 program.[S21] Geometry optimizations and frequency calculations was performed with the wb97XD hybrid exchange-correlation functional with the def2-SVP basis set Single-point energies were further calculated with the wb97XD hybrid exchange-correlation functional with a larger basis set def2-TZVP basis set.[S22,S23] The energies reported here refer to the single-point energies. *N,N*-dimethylethanamine, *N*-ethyl-*N*-methylethanamine and triethylamine were used to represent the three kinds of tertiary amine species, and for each model, the adsorption energy (ΔE) was calculated according to the equation below:

$\Delta E = E(\text{amine\_ } SO_2) - E(\text{amine}) - E(SO_2)$

Where E(amine _SO_2), E(amine) and $E(SO_2)$ are the energies of optimized model of adsorbed SO_2, amine and SO_2, respectively.

Bond distances are in angstrom.

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Single-point energies (a.u.) and Cartesian coordinates

SO_2

E = -548.6516585

S	0.000000000	0.370418000	0.000000000
O	1.246194000	-0.370418000	0.000000000
O	-1.246194000	-0.370418000	0.000000000

N,N-dimethylethanamine

E = -213.8001251

N	0.456881000	-0.003335000	-0.296842000
C	0.627537000	1.377046000	0.091788000
H	1.504121000	1.803717000	-0.418623000
H	-0.244401000	1.979355000	-0.199879000
H	0.778952000	1.505021000	1.189216000
C	1.657358000	-0.772797000	-0.071292000
H	1.531870000	-1.796614000	-0.455727000
H	2.506177000	-0.316792000	-0.603618000
H	1.935711000	-0.847302000	1.005652000
C	-0.708860000	-0.632221000	0.296150000
H	-0.690476000	-1.695587000	0.006835000
H	-0.654297000	-0.616266000	1.411545000
C	-2.032036000	-0.030014000	-0.156267000
H	-2.871278000	-0.638619000	0.211171000
H	-2.179857000	0.991588000	0.224090000
H	-2.078681000	0.002767000	-1.255040000

N,N-dimethylethanamine-SO_2

E = -762.472943

N	-0.686793000	0.568604000	0.151174000
C	-1.069716000	1.341533000	-1.017454000
H	-0.234861000	2.001586000	-1.291837000
H	-1.268682000	0.678621000	-1.870117000

H	-1.969237000	1.958656000	-0.830501000
C	-0.238232000	1.411568000	1.247683000
H	0.141416000	0.774509000	2.059479000
H	0.588139000	2.047924000	0.899816000
H	-1.055457000	2.048168000	1.634346000
C	-1.654039000	-0.433836000	0.599763000
H	-1.158156000	-0.996698000	1.406370000
H	-2.532545000	0.071745000	1.049823000
C	-2.110504000	-1.401388000	-0.480314000
H	-2.720697000	-2.192281000	-0.022258000
H	-2.727337000	-0.915843000	-1.250205000
H	-1.254098000	-1.883874000	-0.974024000
S	1.316167000	-0.555454000	-0.397392000
O	2.087566000	0.669444000	-0.613302000
O	1.459351000	-1.193535000	0.912190000

N-ethyl-*N*-methylethanamine

E = -253.1167972

N	0.002783000	0.371870000	-0.190165000
C	-0.561972000	1.699928000	-0.115224000
H	0.045678000	2.403462000	-0.703925000
H	-1.577286000	1.717320000	-0.535726000
H	-0.622379000	2.090253000	0.927099000
C	1.390436000	0.350657000	0.242281000
H	1.872508000	1.256571000	-0.158228000
H	1.473100000	0.428574000	1.351901000

C	-0.818196000	-0.620172000	0.482837000
H	-0.242427000	-1.555028000	0.543937000
H	-1.025299000	-0.318828000	1.537224000
C	-2.128789000	-0.920155000	-0.233179000
H	-2.652058000	-1.751725000	0.261713000
H	-2.813821000	-0.059459000	-0.234622000
H	-1.933166000	-1.201742000	-1.278390000
C	2.171585000	-0.860793000	-0.250352000
H	1.811484000	-1.803132000	0.188293000
H	2.091707000	-0.942965000	-1.344278000
H	3.234087000	-0.763178000	0.017978000

N-ethyl-*N*-methylethanamine-SO_2

E = -801.7888257

N	0.717785000	0.018308000	0.389995000
C	1.615197000	-0.684312000	-0.531773000
H	1.514425000	-0.204713000	-1.516714000
H	2.666754000	-0.532549000	-0.210627000
C	0.545725000	-0.642794000	1.673691000
H	-0.110930000	-0.026620000	2.303491000
H	0.052328000	-1.614352000	1.539461000
H	1.511103000	-0.784964000	2.195349000
C	1.051877000	1.434010000	0.573091000
H	0.239107000	1.868167000	1.175460000
H	1.983239000	1.514890000	1.169978000
C	1.189921000	2.238541000	-0.709526000

H	1.322200000	3.298366000	-0.450283000
H	2.057475000	1.937949000	-1.313924000
H	0.282661000	2.163100000	-1.325986000
S	-1.496912000	-0.011028000	-0.512775000
O	-1.893403000	-1.298142000	0.061823000
O	-1.953421000	1.180294000	0.204111000
C	1.329169000	-2.171932000	-0.678978000
H	0.268517000	-2.356244000	-0.900251000
H	1.932717000	-2.575029000	-1.504399000
H	1.589765000	-2.738019000	0.226378000

triethylamine

E = -292.4337314

N	0.000403000	0.000036000	0.059334000
C	-0.314619000	-1.364258000	0.451843000
H	0.611525000	-1.956787000	0.407994000
H	-0.650401000	-1.411189000	1.513091000
C	-1.023108000	0.954992000	0.453450000
H	-1.999160000	0.448499000	0.414125000
H	-0.892320000	1.271397000	1.513569000
C	1.339400000	0.408929000	0.452545000
H	1.389075000	1.507402000	0.411405000
H	1.548127000	0.139090000	1.513111000
C	2.429186000	-0.149890000	-0.452859000
H	3.419626000	0.210982000	-0.136739000
H	2.458762000	-1.249874000	-0.434698000

H	2.254613000	0.163675000	-1.492455000
C	-1.085495000	2.177483000	-0.452797000
H	-0.147234000	2.752464000	-0.437196000
H	-1.272126000	1.868739000	-1.491738000
H	-1.892160000	2.855575000	-0.135576000
C	-1.345602000	-2.027270000	-0.452119000
H	-1.528164000	-3.065681000	-0.136661000
H	-2.312714000	-1.502440000	-0.431509000
H	-0.988841000	-2.032020000	-1.492441000

triethylamine-SO_2

E = -841.1047165

N	0.712741000	-0.003634000	0.233580000
C	1.667104000	-0.672224000	-0.660061000
H	1.632891000	-0.148720000	-1.626397000
H	2.694967000	-0.541353000	-0.263385000
C	0.473456000	-0.760452000	1.470192000
H	0.001397000	-1.709290000	1.178801000
H	1.448578000	-1.004528000	1.939767000
C	1.047421000	1.403212000	0.481646000
H	0.181177000	1.855789000	0.982969000
H	1.903070000	1.455688000	1.185531000
C	1.351301000	2.227432000	-0.760315000
H	1.459423000	3.280256000	-0.463909000
H	2.283672000	1.930059000	-1.260403000
H	0.524409000	2.176197000	-1.483066000

S	-1.369669000	0.003504000	-0.909714000
O	-1.890975000	-1.228379000	-0.311443000
O	-1.875081000	1.256604000	-0.343376000
C	1.393600000	-2.150820000	-0.901699000
H	0.347316000	-2.326519000	-1.189503000
H	2.040195000	-2.504480000	-1.717195000
H	1.610466000	-2.767983000	-0.019007000
C	-0.439335000	-0.077836000	2.479102000
H	0.023777000	0.801161000	2.948946000
H	-1.386573000	0.226348000	2.013713000
H	-0.672083000	-0.794929000	3.278872000

CO_2

E = -188.6055421

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.158564000
O	0.000000000	0.000000000	-1.158564000

N,N-dimethylethanamine-CO_2

E = -402.4128763

N	-0.622630000	-0.523658000	-0.107019000
C	-0.950914000	-1.136575000	1.162145000
H	-0.192169000	-1.891976000	1.413045000
H	-0.948242000	-0.391742000	1.969756000
H	-1.946832000	-1.633574000	1.154708000
C	-0.479591000	-1.515824000	-1.150809000

H	-0.148655000	-1.036490000	-2.084888000
H	0.279128000	-2.258842000	-0.861682000
H	-1.426649000	-2.059823000	-1.364103000
C	-1.533368000	0.539757000	-0.502142000
H	-1.212524000	0.887406000	-1.497099000
H	-2.569359000	0.146708000	-0.627024000
C	-1.551849000	1.731598000	0.443507000
H	-2.175390000	2.532597000	0.020486000
H	-1.970097000	1.480992000	1.429424000
H	-0.536013000	2.128534000	0.584533000
O	2.274733000	-0.539431000	0.716153000
O	1.778985000	1.278647000	-0.634358000
C	1.978300000	0.355726000	0.040234000

N-ethyl-*N*-methylethanamine-CO_2

E = -441.7295949

N	0.623480000	0.165891000	0.392572000
C	1.559368000	-0.437127000	-0.545599000
H	1.333812000	-0.041476000	-1.545874000
H	2.604996000	-0.126768000	-0.312110000
C	0.822824000	-0.278566000	1.756736000
H	0.067118000	0.182458000	2.408718000
H	0.702009000	-1.367366000	1.837453000
H	1.829164000	-0.013969000	2.151638000
C	0.615598000	1.621826000	0.329861000
H	-0.109345000	1.969981000	1.083047000

H	1.604036000	2.036287000	0.636839000
C	0.227722000	2.203289000	-1.023377000
H	0.062713000	3.286198000	-0.926452000
H	1.007858000	2.062006000	-1.785113000
H	-0.699433000	1.747779000	-1.402083000
O	-1.833435000	-0.858845000	-1.181768000
O	-2.322166000	-0.125660000	0.962664000
C	1.482988000	-1.955934000	-0.615801000
H	0.450428000	-2.280623000	-0.810432000
H	2.115452000	-2.321043000	-1.438019000
H	1.835838000	-2.442189000	0.305278000
C	-2.029200000	-0.482899000	-0.101497000

triethylamine-CO_2

E = -481.0449936

N	0.646150000	0.013029000	0.150437000
C	1.504982000	-0.663615000	-0.816467000
H	1.438850000	-0.113543000	-1.765426000
H	2.572439000	-0.604757000	-0.497201000
C	0.622152000	-0.689941000	1.428241000
H	0.266311000	-1.712369000	1.239317000
H	1.653775000	-0.786701000	1.841497000
C	1.006392000	1.418269000	0.306052000
H	0.279985000	1.875041000	0.992297000
H	2.005351000	1.514814000	0.793120000
C	0.995494000	2.230773000	-0.982083000

H	1.086419000	3.299611000	-0.739795000
H	1.827773000	1.979612000	-1.655068000
H	0.048739000	2.086228000	-1.522277000
O	-2.136410000	-1.204477000	-0.572610000
O	-2.188778000	1.112774000	-0.571073000
C	1.144324000	-2.117368000	-1.094444000
H	0.072181000	-2.218486000	-1.315127000
H	1.713052000	-2.474684000	-1.965359000
H	1.386382000	-2.784587000	-0.254802000
C	-0.277559000	-0.073224000	2.491459000
H	0.114840000	0.874003000	2.887619000
H	-1.290073000	0.115256000	2.103726000
H	-0.368201000	-0.767382000	3.339491000
C	-2.117346000	-0.044835000	-0.563693000

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