Synthesis and Study of Pyridine-based Nitrogen-rich Porous Organic Polytriazine for the Highly Efficient Capture of SO_2

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1. Instrumentation and methods

Fourier-transformed infrared (FT-IR) spectra were characterized using a Bruker TENSOR-27 infrared spectrophotometer from 4000 cm^{-1} to 400 cm^{-1} at a resolution of 4 cm^{-1}. The sample was prepared using a conventional KBr disk method. ^{1}H NMR spectra were measured on a Brucker spectrometer using tetramethylsilane (TMS) as an internal standard at 400 MHz. Solid-state ^{13}C CP/MAS NMR was recorded on a Bruker AVANCE500 NMR spectrometer operating under a magnetic field strength of 9.4 T. The ^{13}C chemical shifts were referenced externally via the resonance of tetramethylsilane (TMS) of 0 ppm. Elemental analysis was conducted using an Elementarvario EL III elemental analyzer. Thermal gravimetric analysis (TGA) was performed on a Mettler-Toledo model SDTA -854 TG A system under a N_2 atmosphere at a heating rate of 10 ^{o}C min^{-1} from room temperature to 800 ^{o}C. Wide-angle X-ray diffraction (WAXD) images were collected on a Riguku D/MAX 2550 diffractometer under Cu-K_{α} radiation, at 40 kV and 200 mA, with a 2 θ range of 5-80^{o} (scanning rate of 10^{o} min^{-1}) at room temperature. The UV-vis adsorption spectra of dye solutions were obtained by a TU-1901 spectrophotometer at room temperature. N_2 sorption isotherm measurements were characterized at Quantachrome Quadrasorb apparatus with a Micromeritics surface area and pore-size analyzer. Before measurement, the samples were degassed for 12 h at 150 ^{o}C. Nonlocal density functional theory (NL-DFT) pore-size distributions (PSDs) were determined by using the carbon/slit-cylindrical pore mode of the Quadrawin software.

Gas Adsorption and Separation Performance

The gas adsorption and separation performance of SO_2, CO_2, and N_2 were conducted on a gas adsorption analyzer (BSD-PMC, BeiShiDe Instrument Co. Ltd., China) at temperatures of 273 and 298 K over a pressure ranging from 0 to 1 bar. The calculated adsorption selectivities of SO_2/CO_2, SO_2/N_2 were based on the initial slope and IAST approaches at 273 K and 298 K, respectively.

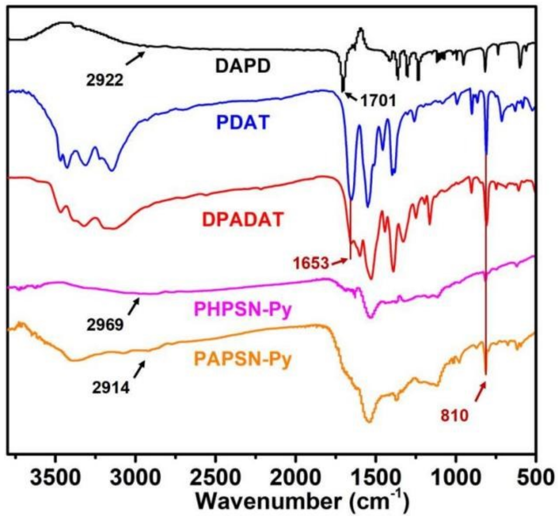

Figure S1. The comparison of the FT-IR results for the monomers and polymers.

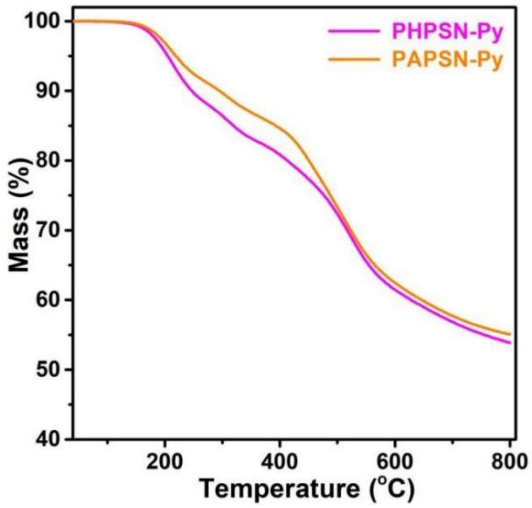

Figure S2. The TGA curves of PHPSN-Py and PAPSN-Py

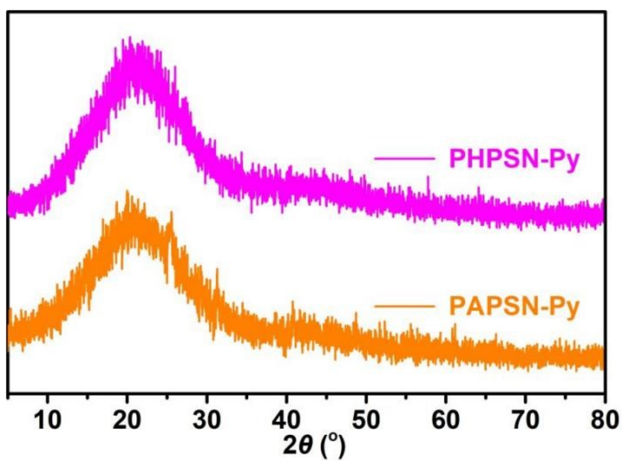

Figure S3. The WAXD for these two polymers

Table S1. The chemical composition of PHPSN-Py and PAPSN-Py

Samples	Measured value (wt%)			Theoretical value (wt%)		
	C	H	N	C	H	N
PHPSN-Py	57.82	3.40	17.53	56.96	3.30	17.41
PAPSN-Py	54.04	3.27	19.76	53.64	3.15	19.64

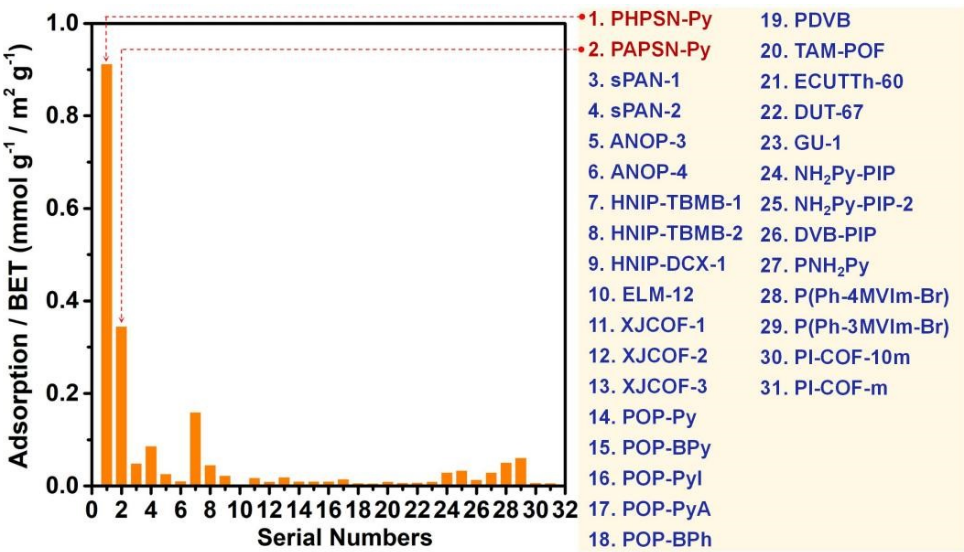

Figure S4. The capacity per unit surface area for PHPSN-Py and PAPSN-Py at 298 K and 1 bar.

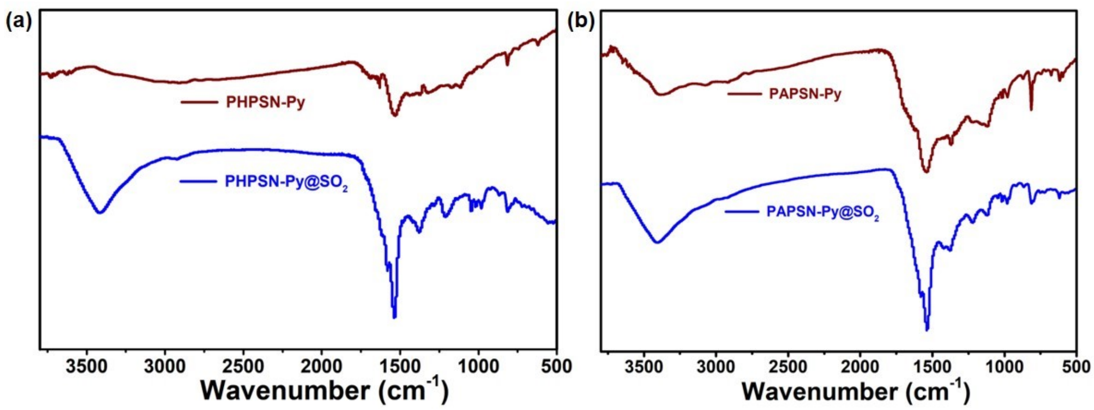

Figure S5. The FT-IR spectra of these two polymers before and after SO_2 adsorption testing.

Table S2. SO_2 uptake and SO_2/CO_2 selectivity in PHPSN-Py and PAPSN-Py and some reported porous materials.

Materials	S_{BET} m^2/g	SO_2 (mmol/g, 100 KPa)		SO_2/CO_2 (10:90, 298 K, 100 KPa)	References
		273 K	298 K		
PHPSN-Py	8	11.1	7.3	86	This work
PAPSN-Py	22	119	7.6	89	This work
HNIP-TBMB-1	45	-	7.20	91	1
HNIP-TBMB-2	155	-	7.07	50	1
HNIP-DCX-1	207	-	4.80	23	1
XJCOF-1	467	11.8	8.4	118	2
XJCOF-2	961	11.1	9.2	39	2
XJCOF-3	503	11.9	9.6	42	2
ANOP-3	287	12.5	7.7	64.7	3
ANOP-4	1016	21.9	10.9	50.5	3
NPC-1-800	773.8	-	1.68	-	4
NPC-1-900	1656.2	-	1.85	-	4
NPC-1-1000	1635.2	-	1.39	-	4
NPC-1-1100	1613.5	-	1.26	-	4
NPC-2-800	931.6	-	1.45	-	4
NPC-2-900	1452.3	-	1.60	-	4
NPC-2-1000	1398.3	-	1.35	-	4
NPC-2-1100	1335.2	-	1.22	-	4
BC-3-650	1449	-	10.7	32	5
BC-4-650	1244	-	9.1	21	5
BC-5-650	1195	-	7.9	22	5
DUT-67	1178	10.3	9.1	37	6
DUT-67-HCl	1349	10.6	9.3	33	6
TAM-POF	974	13.0	9.45	90	7
sPAN-1	113	8.45	5.56	37.6	8
sPAN-2	65	9.36	5.64	50.3	8
GC-2	507	-	10.2	-	9
GC-4	474	-	11.6	-	9
ECUTTh-60	472	4.00	3.35	27(1:99)	10
GU-1	777	8.13	7.60[a]	15.9	11
BIDC-2-700	1200	-	10.25	-	12
BIDC-0.5-750	1580	-	15.78	-	12
BIDC-3-800	3750	-	21.42	-	12
ELM-12	706	-	2.73	30	13
POP-Py	1074	-	10.8	31	14
POP-BPy	1164	-	12.2	29.8	14
POP-PyI	1087	-	11.0	19.5	14
POP-PyA	536	-	8.1	25.0	14

POP-BPh	965	-	6.5	17.8	14
PDVB	639	-	3.8	19.5	14
Fe-soc-MOF	1470	-	11.7	32	15

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