Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Electronic Supporting Information

Sustainable porous carbons from tannic acid based KOH activated as high-performance CO_2 capture sorbents

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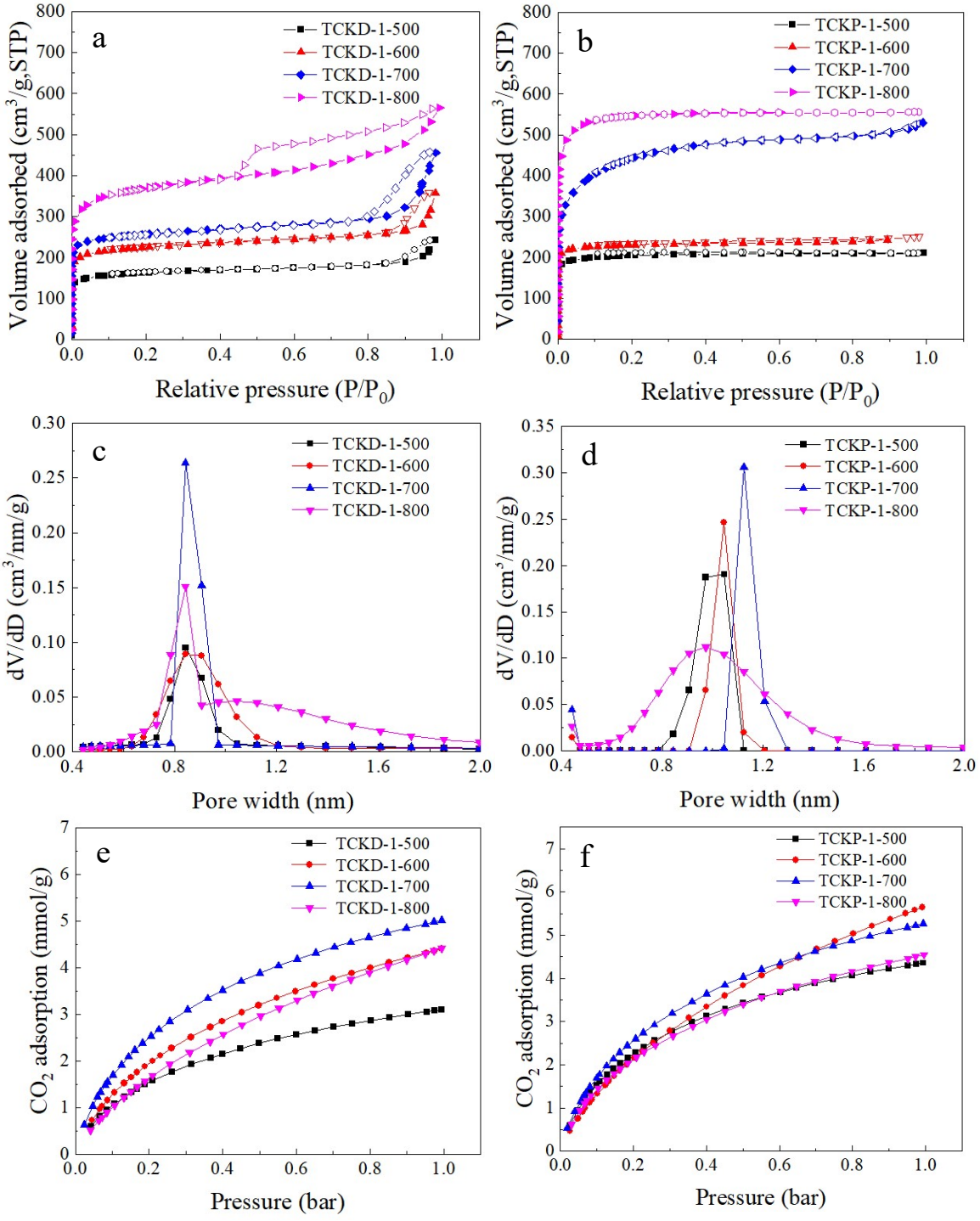

Figure S1. (a-b) Comparison of TCKs-1-Y obtained at different activation temperature by gas adsorption/desorption analysis. (a-b) N_2 sorption isotherms at -196 °C, (c-d) pore size distribution (PSD), PSD was calculated by NLDFT with the slit pore geometry assumption. (e-f) CO_2 adsorption isotherms at 0 °C

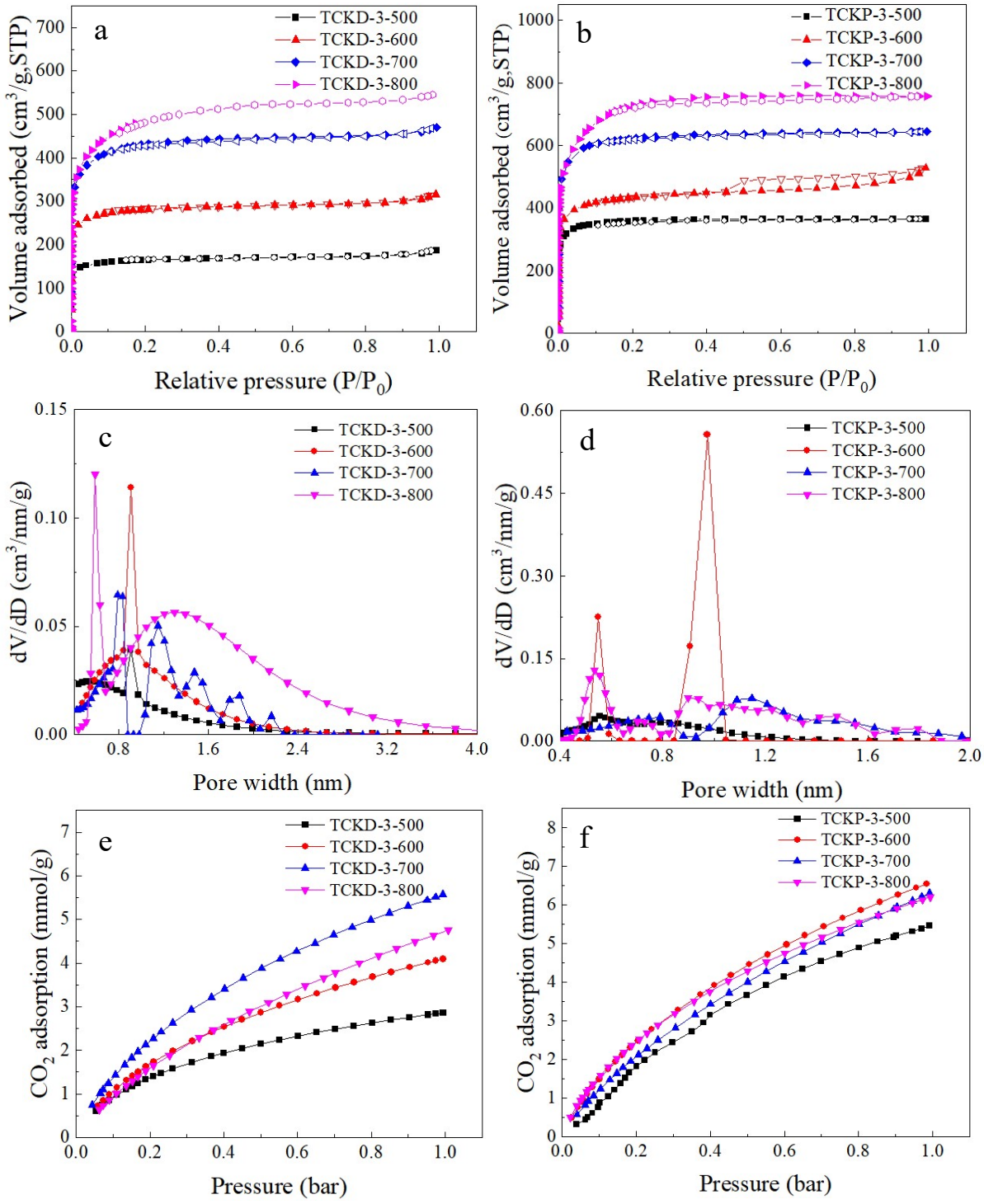

Figure S2. (a-b) Comparison of TCKs-3-Y obtained at different activation temperature by gas adsorption/desorption analysis. (a-b) N_2 sorption isotherms at -196 °C, (c-d) pore size distribution (PSD), PSD was calculated by NLDFT with the slit pore geometry assumption. (e-f) CO_2 adsorption isotherms at 0 °C

S1. Supplementary experimental section

The application of Ideal adsorbed solution theory (IAST) for calculating adsorption selectivity of CO_2/N_2

The adsorption selectivity is a significant parameter to evaluate the adsorption separation efficiency in the industrial processes. The adsorption selectivity of TCKs for CO_2/N_2 binary mixture is defined as Eq. (S1).

$$S = \frac{x_1}{x_2} \times \frac{y_2}{y_1} \quad \text{(Eq.S1)}$$

Where x_i and y_i represent the mole fraction of component i (i =1 or 2) in the adsorbed and bulk phases, respectively. In this work, component 1 represents CO_2, while component 2 represents N_2. Ideal adsorbed solution theory (IAST) is widely applied to predict the adsorption selectivities of binary gas mixtures from pure component isotherms, which is based on the principle that the adsorbate-adsorbent and adsorbate-adsorbate interactions are sufficiently ideal. In addition, an appropriate model used to fit pure-component isotherm is important to compute the integration required by IAST. Although there are no constraints on the choice of IAST models, the data should be fit precisely over the full range of pressure.

In this work, the experimentally measured loadings for CO_2 were measured as a function of the absolute pressure at two different temperatures 273 and 298 K. The CO_2 isotherm for were fitted with the Single-site Langmuir-Freundlich model.

$$q = q_{sat} \frac{bp^v}{1 + bp^v} \quad \text{(Eq.S2)}$$

Where q is the adsorbed amount in equilibrium with the concentration of adsorbate in the gas phase (mmol/g), p is the equilibrium pressure of the bulk gas with the adsorbed phase (kPa); q_{sat} is the saturation capacities of CO_2 or N_2 (mmol/g); b is the affinity coefficients of CO_2 or N_2 (1/kPa), respectively; and v is equal to $1/n_1$, t is equal to $1/n_2$, where n_1 and n_2 are the corresponding deviations from an ideal homogeneous surface. The Single-site Langmuir-Freundlich model was combined with the Ideal adsorbed solution theory (IAST) to predict the adsorption isotherms of the mixture and calculate the selectivity of the adsorbate.

Table S1. Single-site Langmuir-Freundlich parameters for adsorption of CO_2 in different TCKP-2-600 and TCKD-2-700.

Sample	q_{sat} mmol/g	b_0 Pa^{-v}	v dimensionless
TCKP-2-600	6.37828	1.26621	1.00928
TCKD-2-700	6.84578	0.91067	1.19419

Table S2. Single-site Langmuir-Freundlich parameters for adsorption of N_2 in different TCKP-2-600 and TCKD-2-700.

Sample	q_{sat} mmol/g	b_0 Pa^{-v}	v dimensionless
TCKP-2-600	3.91529	0.12787	0.96746
TCKD-2-700	4.23783	0.06446	1.00227

Table S3. CO_2 adsorption performance of TCKP-2-600 and other adsorbents.

Biomass	Sample	Preparation method	CO_2 uptake (mmol/g at 1 bar)		S_{BET} (m^2/g)	V_{mic} (cm^3/g)	CO_2/N_2 Selectivity	Serial number	References
			0 °C	25 °C					
Olive stones	OS	single-step activation	4.8	3.0	1113	0.37	18	S1	[1]
Almond shells	AS	single-step activation	3.7	2.7	822	0.33	20	S2	[1]
Pomegranate peels	PP	single-step activation	6.03	4.11	585	0.20	15.1	S3	[2]
Carrot peels	CP	single-step activation	5.64	4.18	1379	0.51	8.1	S4	[2]
Fern leaves	FL	single-step activation	4.52	4.12	1593	0.54	5.6	S5	[2]
Rice Husk	-	single-step activation	-	3.10	1492	0.34	7.6	S6	[3]
Coffee grounds	CG800-1	single-step activation	7.18	4.54	1692	0.68	17	S7	[4]
Amazonian nutshells	BNS	single-step activation	5.14	3.67	1532	0.44	46.9	S8	[5]
Arundo donax	KLB2	single-step activation	6.3	3.6	1122	0.50	-	S9	[6]
Coconut Shell	C-600-3	carbonization and KOH activation	6.04	4.23	1172	0.43	22	S10	[7]
Microcrystalline cellulose	ACel-ac	carbonization and KOH activation	5.8	3.7	753	0.27	-	S11	[8]
Chestnut shell	WS-600-0.6	carbonization and KOH activation	5.23	3.61	1255	0.48	16	S12	[9]
Vine shoots	BC-CO_2-0.1-800	carbonization and CO_2 activation	3.45	1.10	374	0.112	55.2	S13	[10]
Vine shoots	AC-KOH-W-2-600	carbonization and KOH activation	6.04	1.21	1305	0.451	44.2	S14	[10]
Vine shoots	AC-KOH-D-5-700	carbonization and KOH activation	6.08	1.98	1439	0.493	58.8	S15	[10]
Wheat	MCC-K3	carbonization and KOH activation	5.7	3.48	1438	0.581	16	S16	[11]
Lotus seed	LSB3-800	carbonization and KOH activation	6.8	3.1	2230	0.67	-	S17	[12]
Peanut shell	PC680	carbonization and KOH activation	7.25	4.41	1713	0.73	7.9	S18	[13]
Fungi	PC-2	carbonization and KOH activation	5.5	3.4	1742	-	18.5	S19	[14]
Sawdust	AS-2-600	carbonization and KOH activation	6.1	4.8	1260	0.55	5.4	S20	[15]
Coffee grounds	NCLK3	carbonization and KOH activation	4.7	3.0	840	0.36	13	S21	[16]
Africa palm Shells	C600K3	carbonization and KOH activation	6.3	4.4	1250	0.55	-	S22	[17]
Polyurethane foam	PUF-400-KOH-1-700	N-doped activated	6.67	4.33	1516	0.57	12	S23	[18]
Fir bark	ACBK3	N-doped activated	7.0	5.2	1377	0.51	32.3	S24	[19]
Rice husk	CAC-5	N-doped activated	5.83	3.68	1495	0.447	15.3	S25	[20]
Phenolic resin	RUK-600-3	N-doped activated	7.13	4.61	1404	0.53	12	S26	[21]
Arundo donax	NDAB3-500	N-doped activated	3.6	2.1	1863	0.32	-	S27	[22]
Alligator Weed	NAB800-2	N-doped activated	6.4	5.4	3031	0.58	-	S28	[23]
Lotus stalk	LSC-500-1	N-doped activated	5.62	3.88	1113	0.41	22	S29	[24]
Tannic acid	TCKP-2-600	carbonization and KOH activation	7.03	4.29	1845	0.74	20.3		**This work**

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