

**Supplementary Table S1**

Proximate analyses (%), forms of sulfur (%), and vitrinite random reflectance (%) of No.11 and No.3 coals from the Sangshuping Coal Mine, Weibei Coalfield.

Sample	M <sub>ad</sub>	A <sub>d</sub>	V <sub>daf</sub>	S <sub>t,d</sub>	S <sub>o,d</sub>	S <sub>p,d</sub>	S <sub>s,d</sub>	R <sub>o</sub>
SSP11-R	2.9	68.9	58.8	25.40	6.67	16.40	2.34	nd
SSP11-1	2.2	22.7	16.9	8.80	4.34	3.55	0.90	1.32
SSP11-2	1.4	11.5	13.7	6.56	4.99	1.30	0.27	1.76
SSP11-3	1.1	8.4	14.8	5.97	5.44	0.42	0.10	1.68
SSP11-4	1.0	8.1	14.6	5.62	5.48	0.10	0.04	1.71
SSP11-P1	0.7	60.7	31.3	2.37	1.36	0.92	0.09	nd
SSP11-6	0.9	15.8	13.2	4.06	3.99	0.05	0.02	1.78
SSP11-7	0.8	18.5	27.8	4.00	3.93	0.04	0.03	0.70
SSP11-8	0.8	22.6	15.5	3.70	3.66	0.02	0.02	1.58
SSP11-9	0.8	13.3	15.2	4.00	3.95	0.03	0.02	1.70
SSP11-P2	0.6	58.0	31.2	1.69	1.48	0.15	0.06	nd
SSP11-11	0.5	12.2	15.4	4.27	4.09	0.16	0.02	1.63
SSP11-F	0.6	68.8	43.4	1.23	1.02	0.16	0.05	nd
Coal Avg.	1.0	14.8	16.3	5.41	4.53	0.71	0.18	1.54
SSP3-R	0.9	85.5	93.8	0.19	nd	nd	nd	nd
SSP3-1	0.6	21.0	18.3	0.38	nd	nd	nd	1.20
SSP3-2	0.7	14.2	17.2	0.49	nd	nd	nd	1.29
SSP3-3	1.1	9.4	16.7	0.30	nd	nd	nd	1.33
SSP3-4	0.9	9.0	15.3	0.28	nd	nd	nd	1.63
SSP3-5	3.1	7.4	13.7	0.35	nd	nd	nd	1.75
SSP3-6	1.0	8.4	15.2	0.40	nd	nd	nd	1.71
SSP3-7	1.1	9.7	15.6	0.42	nd	nd	nd	1.53

SSP3-8	1.0	15.1	16.5	0.47	nd	nd	nd	1.34
SSP3-9	1.4	17.5	16.2	0.36	nd	nd	nd	1.38
SSP3-10	0.9	10.6	15.6	0.50	nd	nd	nd	1.49
SSP3-11	1.1	10.7	18.0	0.44	nd	nd	nd	1.24
Coal Avg.	1.0	12.1	16.2	0.40	nd	nd	nd	1.44

M, moisture; A, ash yield; V, volatile matter yield; St, total sulfur; Ss, sulfate sulfur; Sp, sulfide sulfur; So, organic sulfur; ad, air-dry basis; d, dry basis; daf, dry and ash-free basis; Ro, vitrinite random reflectance; nd, not determined.

**Table S2**

Percentages of major-element oxides (%) and concentrations of trace elements ( $\mu\text{g/g}$ ) of the No.11 coal from the Sangshuping coal mine, Weibei Coalfield (on whole coal basis)

Li	342	163	61.0	83.7	105	583	93.4	214	79.1	457	90.8	1467	111	31.8	12	33		
Be	3.66	2.05	1.65	0.87	0.93	4.4	1.18	1.78	1.21	2.89	1.53	3.54	1.40	2.11	1.6	2.3		
B	19.8	10.5	1.75	8.41	6.62	22.3	22.6	15.5	12.5	26.6	6.25	46.8	10.5	53.0	52	34		
Sc	2.29	6.34	2.17	<dl	0.90	14.7	5.41	3.20	2.69	4.76	10.0	10.61	4.39	4.38	3.9	16		
V	238	157	14.3	7.88	56.5	87.4	32.7	22.1	29.5	29.2	51.9	45.6	46.4	35.1	25	121		
Cr	114	77.2	9.66	2.77	21.4	76.9	19.0	10.4	11.1	15.8	18.9	28.5	21.3	15.4	16	92		
Co	19.0	11.2	<dl	11.2	7.08	5.1	17											
Ni	24.8	15.1	0.05	1.81	5.67	17.9	1.08	3.82	4.16	13.9	4.38	9.89	4.50	13.7	13	50		
Cu	33.4	27.7	11.6	3.88	8.90	47.7	10.6	17.2	16.8	44.2	19.2	65.6	14.5	17.5	16	39		
Zn	35.5	71.3	33.4	3.95	3.40	9.49	4.03	6.15	8.23	2.49	10.4	8.41	17.6	41.4	23	75		
Ga	12.6	15.4	6.49	5.89	36.2	16.1	9.62	22.2	15.7	7.83	28.5	27.6	17.5	6.55	5.8	16		
Ge	3.83	5.76	1.58	2.19	3.77	3.14	1.11	4.74	1.44	2.20	2.95	<dl	2.94	2.78	2.2	1.3		
As	27.7	13.2	3.14	1.67	1.32	6.66	1.11	1.56	0.65	5.47	1.65	5.29	3.04	3.79	8.3	5.6		
Se	7.08	5.52	4.55	1.55	1.11	8.16	3.14	4.68	4.20	7.09	3.29	5.60	3.51	2.47	1.3	0.15		
Rb	96.5	34.8	3.35	3.88	3.04	12.6	6.71	3.10	3.45	24.9	2.15	10.7	7.57	9.25	14	98		
Sr	585	93.4	45.5	66.2	71.0	53.7	74.8	383	68.8	27.7	110	242	114	140	110	270		
Y	10.85	11.8	8.34	5.41	8.6	19.6	12.1	13.7	15.8	13.0	37.2	30.9	14.1	18.2	8.4	26		
Zr	138	84.1	38.2	26.5	69.7	274	75.6	102	122	140	176	193	86.7	89.5	36	16		
Nb	14.5	10.7	4.25	1.53	9.54	46.1	3.40	9.11	7.79	18.1	7.50	22.7	6.73	9.44	3.7	12		
Mo	3.77	21.5	6.78	3.39	4.10	12.6	0.00	1.38	0.80	<dl	2.81	<dl	5.09	3.08	2.2	1.56		
Cd	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.25	0.22	0.64			
Sn	1.41	1.91	1.10	<dl	3.97	4.64	0.00	2.29	2.93	0.80	7.64	6.34	2.83	2.11	1.1	3.5		
Sb	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.84	0.92	0.81			
Cs	8.01	5.07	<dl	<dl	<dl	1.33	<dl	<dl	<dl	1.59	<dl	1.28	5.1	1.13	1	5.5		
Ba	88.1	55.6	3.28	1.83	3.13	18.7	3.38	8.41	2.52	8.64	4.73	15.8	10.4	159	150	510		

La	88.3	20.2	5.97	6.01	3.90	58.1	20.4	42.2	3.10	16.6	12.1	118	14.2	22.5	11	32
Ce	132	41.6	13.5	13.3	9.50	92.4	25.5	68.3	7.25	39.6	29.8	191	26.1	46.7	23	63
Pr	14.0	4.47	1.44	1.38	1.17	10.8	2.55	7.62	0.99	5.05	3.91	18.3	2.94	6.42	3.5	8.7
Nd	48.9	16.9	5.34	5.00	4.95	35.6	8.90	26.4	4.31	18.0	16.7	60.1	11.1	22.3	12	29
Sm	10.3	3.95	1.43	1.23	1.53	5.53	2.44	5.21	1.96	4.67	6.58	13.7	3.04	4.07	2	5.7
Eu	1.23	<dl	1.17	1.59	1.17	0.84	0.47	1.3								
Gd	5.75	3.08	1.25	1.17	1.55	4.23	2.66	4.13	2.58	3.65	7.57	9.51	3.00	4.65	2.7	6.3
Tb	<dl	1.37	1.26	1.37	0.62	0.32	0.89									
Dy	2.66	2.57	1.52	1.05	1.77	4.27	2.56	3.21	3.27	2.87	7.77	6.74	2.96	3.74	2.1	4.8
Ho	<dl	<dl	<dl	<dl	<dl	0.81	<dl	<dl	<dl	<dl	1.29	1.17	1.29	0.96	0.54	1.3
Er	1.62	1.43	0.87	<dl	1.01	2.59	1.33	1.60	1.74	1.48	3.63	3.52	1.45	1.79	0.93	2.7
Tm	<dl	0.64	0.31	0.33												
Yb	1.77	1.46	0.90	<dl	0.83	2.69	1.19	1.48	1.52	1.36	3.08	3.19	1.31	2.08	1	2.5
Lu	<dl	0.38	0.2	0.48												
Hf	4.50	2.51	1.06	0.88	1.90	9.08	2.27	3.23	3.68	5.04	5.50	6.65	2.63	3.71	1.2	4.5
Ta	<dl	<dl	<dl	<dl	<dl	2.56	<dl	<dl	<dl	0.97	<dl	1.70	<dl	0.62	0.28	1.4
W	0.84	0.89	0.92	1.51	2.45	5.94	<dl	1.50	<dl	3.03	0.00	2.17	1.21	1.08	1.1	2.03
Tl	1.53	1.34	<dl	1.34	0.47	0.63	0.75									
Pb	136	24.1	5.90	3.79	2.63	14.5	2.00	3.90	6.61	16.1	7.16	17.8	7.01	15.1	7.8	17
Bi	<dl	<dl	<dl	<dl	<dl	2.21	<dl	<dl	<dl	0.97	<dl	0.94	<dl	0.79	0.97	0.29
Th	17.7	7.78	3.85	2.45	3.85	41.6	3.69	7.24	3.75	25.0	15.2	27.6	5.98	5.84	3.3	9.1
U	7.47	11.4	3.40	0.96	3.58	6.83	2.65	3.19	4.65	3.85	6.99	9.84	4.60	2.43	2.4	2.5

<dl, under detected limit; nd, no data; <sup>a</sup>Dai et al., 2012b; <sup>b</sup>Ketris and Yudovich, 2009; <sup>c</sup>Grigoriev, 2009.

**Table S3**

Percentages of major-element oxides (%) and concentrations of trace elements ( $\mu\text{g/g}$ ) of the No.3coal from the Sangshuping coal mine, Weibei Coalfield (on whole coal basis)

%	SSP3-R	SSP3-1	SSP3-2	SSP3-3	SSP3-4	SSP3-5	SSP3-6	SSP3-7	SSP3-8	SSP3-9	SSP3-10	SSP3-11	Coal avg.	Chinese Coal <sup>a</sup>	world Coal <sup>b</sup>	Word Clays <sup>c</sup>
SiO <sub>2</sub>	40.6	9.80	5.91	2.71	3.79	1.40	2.39	3.35	5.46	7.17	2.47	2.25	4.25	8.47	nd	nd
TiO <sub>2</sub>	1.21	0.40	0.28	0.07	0.25	0.07	0.08	0.11	0.17	0.16	0.04	0.07	0.15	0.33	nd	nd
Al <sub>2</sub> O <sub>3</sub>	36.2	6.03	9.42	3.42	3.02	2.22	2.72	3.23	4.90	5.48	2.93	2.70	4.19	5.98	nd	nd
Fe <sub>2</sub> O <sub>3</sub>	0.49	0.36	0.24	0.14	0.08	0.17	0.68	0.43	0.60	0.63	0.63	0.73	0.43	4.85	nd	nd
MgO	0.09	0.04	0.06	0.09	0.08	0.07	0.33	0.27	0.20	0.33	0.26	0.42	0.20	0.22	nd	nd
CaO	0.05	1.39	1.29	1.59	0.38	1.31	1.35	1.12	1.52	0.88	1.74	2.50	1.37	1.23	nd	nd
MnO	0.001	0.005	0.004	0.005	0.001	0.004	0.02	0.01	0.01	0.01	0.01	0.02	0.01	0.02	nd	nd
Na <sub>2</sub> O	0.24	0.03	0.04	0.02	0.02	0.04	0.04	0.04	0.05	0.07	0.04	0.04	0.04	0.16	nd	nd
K <sub>2</sub> O	0.84	0.04	0.06	0.01	0.01	0.02	0.03	0.04	0.14	0.31	0.06	0.04	0.07	0.19	nd	nd
P <sub>2</sub> O <sub>5</sub>	0.11	0.02	0.03	0.02	0.02	0.11	0.35	0.09	0.36	0.02	0.67	0.01	0.15	0.09	nd	nd
SiO <sub>2</sub> /Al <sub>2</sub> O <sub>3</sub>	1.12	1.62	0.63	0.79	1.26	0.63	0.88	1.04	1.11	1.31	0.84	0.83	1.00	1.42	nd	nd
$\mu\text{g/g}$																
Li	313	76.3	116	39.4	32.7	42.5	60.3	70.1	149	158	88.4	89.2	83.8	31.8	12	33
Be	7.60	12.8	13.4	1.25	<dl	<dl	0.88	0.87	1.19	1.16	<dl	<dl	4.50	2.11	1.6	2.3
B	59.9	2.51	3.09	3.29	6.36	47.6	37.7	31.9	33.8	17.9	56.4	40.4	25.5	53.0	52	34
Sc	10.28	4.41	<dl	<dl	<dl	<dl	<dl	0.93	2.11	2.78	<dl	<dl	2.56	4.38	3.9	16
V	82.7	42.2	24.3	7.34	10.4	7.10	7.38	10.7	12.6	12.51	6.37	11.2	13.8	35.1	25	121
Cr	33.5	22.2	12.4	2.68	14.8	4.49	6.88	5.96	5.91	4.88	3.95	3.94	8.01	15.4	16	92
Co	26.0	11.2	32.0	14.3	4.13	2.47	1.29	0.88	<dl	1.05	1.04	1.42	6.98	7.08	5.1	17

	23.0	13.7	34.1	14.3	6.57	6.31	3.39	2.63	1.86	2.82	2.56	2.35	8.23	13.7	13	50
Ni	23.0	13.7	34.1	14.3	6.57	6.31	3.39	2.63	1.86	2.82	2.56	2.35	8.23	13.7	13	50
Cu	13.3	23.9	21.7	6.35	10.7	7.55	9.14	10.1	10.0	10.0	10.8	7.37	11.6	17.5	16	39
Zn	18.6	7.21	23.52	8.67	10.0	22.7	19.4	26.91	14.4	29.8	28.6	70.9	23.8	41.4	23	75
Ga	42.9	8.89	18.2	4.28	2.78	2.30	2.22	3.55	7.17	11.2	3.95	4.43	6.27	6.55	5.8	16
Ge	2.05	4.95	19.63	<dl	<dl	<dl	<dl	<dl	0.83	1.07	<dl	<dl	6.62	2.78	2.2	1.3
As	18.6	2.37	2.53	0.67	0.32	0.69	2.30	0.95	1.63	2.11	0.50	2.26	1.49	3.79	8.3	5.6
Se	<dl	1.93	6.27	1.53	0.26	<dl	<dl	2.47	2.44	2.63	0.90	0.96	2.16	2.47	1.3	0.15
Rb	32.2	1.12	1.86	<dl	<dl	0.98	1.63	2.03	6.82	14.91	3.20	1.56	3.79	9.25	14	98
Sr	292	74.7	143	102	89.6	238	348	239	411	108	347	124	202	140	110	270
Y	13.0	18.5	18.9	8.43	10.8	8.55	10.6	6.48	13.5	8.12	16.3	4.58	11.3	18.2	8.4	26
Zr	149	94.5	85.3	19.9	48.7	16.4	13.5	34.6	61.3	55.4	12.9	25.2	42.5	89.5	36	16
Nb	45.7	10.7	9.42	1.67	4.42	1.97	1.48	4.25	7.34	7.23	1.13	2.50	4.74	9.44	3.7	12
Mo	2.43	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.86	<dl	1.47	1.17	3.08	2.2	1.56
Cd	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.25	0.22	0.64
Sn	3.05	1.27	1.67	<dl	<dl	<dl	<dl	<dl	1.98	2.24	<dl	<dl	1.79	2.11	1.1	3.5
Sb	2.95	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.84	0.92	0.81
Cs	1.51	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.79	<dl	<dl	0.79	1.13	1	5.5
Ba	140	64.8	52.4	27.6	25.4	38.2	38.5	39.6	56.8	54.0	54.2	29.8	43.7	159	150	510
La	110	13.2	30.4	20.5	18.5	29.5	27.6	20.6	39.1	3.33	23.6	1.40	20.7	22.5	11	32
Ce	198	27.80	52.6	33.1	33.9	40.7	46.1	37.2	70.5	9.36	48.2	4.82	36.7	46.7	23	63
Pr	17.7	3.16	5.29	3.27	3.51	3.55	4.00	3.25	6.44	1.13	4.92	<dl	3.85	6.42	3.5	8.7
Nd	57.3	11.3	18.3	11.4	12.4	12.	13.2	10.1	21.0	4.66	18.1	2.96	12.3	22.3	12	29
Sm	10.6	2.83	3.85	2.27	2.68	2.55	2.61	1.77	4.19	1.62	4.28	0.99	2.69	4.07	2	5.7
Eu	1.74	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.84	0.47	1.3
Gd	7.37	2.86	3.61	1.98	2.25	2.25	2.42	1.40	3.57	1.33	3.87	0.85	2.40	4.65	2.7	6.3

Tb	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.62	0.32	0.89	
Dy	2.92	2.95	3.04	1.51	1.84	1.38	1.64	1.18	2.52	1.59	2.97	0.86	1.95	3.74	2.1	4.8	
Ho	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.00	<dl	<dl	0.96	0.54	1.3	
Er	1.84	1.79	1.76	<dl	1.03	<dl	0.85	<dl	1.38	1.09	1.58	<dl	1.35	1.79	0.93	2.7	
Tm	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.00	<dl	<dl	<dl	<dl	0.00	0.64	0.31	0.33
Yb	2.04	1.86	1.58	<dl	1.06	<dl	<dl	<dl	1.17	1.24	1.39	<dl	1.38	2.08	1	2.5	
Lu	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.38	0.2	0.48	
Hf	7.29	2.72	2.77	<dl	1.41	<dl	<dl	1.34	2.65	2.50	<dl	1.06	2.06	3.71	1.2	4.5	
Ta	3.37	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.76	<dl	<dl	0.76	0.62	0.28	1,4	
W	1.42	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.83	1.11	<dl	0.89	0.94	1.08	1.1	2.03	
Tl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.47	0.63	0.75	
Pb	38.3	37.5	54.0	17.0	9.7	11.5	10.5	23.6	15.3	19.9	11.9	18.1	20.8	15.1	7.8	17	
Bi	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.79	0.97	0.29	
Th	50.0	13.4	12.14	1.99	5.71	1.28	1.46	4.11	13.7	10.10	2.09	3.01	6.28	5.84	3.3	9.1	
U	10.5	3.26	3.46	0.59	0.92	<dl	<dl	1.86	3.63	2.95	1.10	0.86	2.07	2.43	2.4	2.5	

<dl, under detected limit; nd, no data; <sup>a</sup> Dai et al., 2012b; <sup>b</sup>Ketris and Yudovich, 2009; <sup>c</sup> Grigoriev, 2009.

Table S4

Semi-quantitative compositions of mineralogical phases in the studied samples determined by XRD (%), on whole-coal basis).

SSPP11-5	<dl	53.81	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	0.48	6.25	<dl	<dl	0.05	<dl
SSPP11-6	<dl	12.52	<dl	<dl	<dl	<dl	<dl	<dl	<dl	<dl	3.29	<dl	<dl	0.01	<dl	
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Ms, muscovite; Kln, kaolinite; Clc, clinochlore; Pas, palygorskite; Qtz, quartz; Ank, ankerite; Cal, calcite; Dol, dolomite; Py, pyrite; Gp, gypsum; Mic, microcline; Tol, tobellite; Szm, szomolnokite; Men, melanterite; Fap, fluorapatite; Ant, anatase; <dl, under detected limit.