Electronic Supplementary Information

Tailoring properties of SBA-15 materials by controlling conditions of hydrothermal synthesis

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Table 1S. Parameters obtained from Small Angle X-ray Scattering (SAXS) for the calcined SBA-15 samples prepared from TEOS at 100ºC.

Sample δ^a	2θ (deg.)[b]	d (nm)[c]	$I/I_0{}^d$	hkl^e	a (nm)[f]
SBA-15/6 0.084	0.87	10.15	1000	100	11.72
	1.52	5.81	25	110	11.62
	1.75	5.05	19	200	11.66
	2.32	3.80	1	210	11.61
	2.61	3.38	1	300	11.71
	3.02	2.92	1	220	11.70
	3.16	2.79	1	310	11.62
SBA-15/24 0.084	0.84	10.52	1000	100	12.15
	1.46	6.07	40	110	12.14
	1.68	5.26	22	200	12.15
	2.22	3.97	2	210	12.13
	2.52	3.51	1	300	12.16
SBA-15/48 0.085	0.83	10.62	1000	100	12.26
	1.45	6.11	48	110	12.22
	1.67	5.29	21	200	12.21
	2.21	4.00	3	210	12.23
	2.50	3.54	1	300	12.26
SBA-15/72 0.084	0.82	10.77	1000	100	12.44
	1.42	6.23	55	110	12.46
	1.64	5.38	21	200	12.42
	2.17	4.07	4	210	12.43
	2.45	3.60	1	300	12.47
SBA-15/96 0.09	0.82	10.77	1000	100	12.44
	1.42	6.23	57	110	12.46
	1.63	5.41	20	200	12.49
	2.16	4.09	4	210	12.49
	2.45	3.60	1	300	12.47
SBA-15/120 0.083	0.83	10.64	1000	100	12.28
	1.45	6.07	54	110	12.14
	1.68	5.27	16	200	12.17
	2.21	3.99	3	210	12.19

[a] δ - Full width at half maximum of the most intense peak; [b] 2θ – scattering angle; [c] d – interplanar spacing; [d] I/I_0 – relative intensity defined as the ratio of the areas of a given peak to the most intense peak multiplied by 1000; [e] hkl – Muller indexes; [f] a – unit cell parameter.

Table 2S. Parameters obtained from Small Angle X-ray Scattering (SAXS) for the calcined SBA-15* samples prepared from TEOS at 120ºC.

Sample δ^a	2θ (deg.)[b]	d (nm)[c]	I/I_0[d]	hkl[e]	a (nm)[f]
SBA-15/12* **0.084**	0.83	10.64	1000	100	12.28
	1.44	6.14	44	110	12.28
	1.65	5.34	19	200	12.33
	2.20	4.02	2	210	12.29
	2.49	3.55	1	300	12.29
	2.90	3.05	1	220	12.20
SBA-15/24* **0.081**	0.83	10.64	1000	100	12.28
	1.44	6.14	49	110	12.28
	1.65	5.34	21	200	12.33
	2.19	4.03	3	210	12.31
	2.48	3.56	1	300	12.33
SBA-15/48* **0.096**	0.84	10.52	1000	100	12.15
	1.47	6.01	56	110	12.01
	1.69	5.23	14	200	12.08
	2.22	3.97	3	210	12.14
	2.53	3.50	1	300	12.11
	2.92	3.03	1	220	12.13
SBA-15/72* **0.084**	0.82	10.77	1000	100	12.44
	1.42	6.23	66	110	12.46
	1.64	5.40	16	200	12.47
	2.16	4.09	4	210	12.49
	2.45	3.61	1	300	12.47

[a] δ - Full width at half maximum of the most intense peak; [b] 2θ – scattering angle; [c] d – interplanar spacing; [d] I/I_0 – relative intensity defined as the ratio of the areas of a given peak to the most intense peak multiplied by 1000; [e] hkl – Muller indexes; [f] a – unit cell parameter.

Table 3S. Parameters obtained from Small Angle X-ray Scattering (SAXS) for the calcined NaSBA-15 samples prepared from sodium metasilicate at 100ºC.

Sample δ^a	2θ (deg.)[b]	d (nm)[c]	I/I_0[d]	hkl[e]	a (nm)[f]
NaSBA-15/12 **0.11**	0.87	10.15	1000	100	11.72
	1.50	5.90	19	110	11.80
	1.73	5.09	14	200	11.75
NaSBA-15/24 **0.115**	0.84	10.52	1000	100	12.15
	1.46	6.03	21	110	12.14
	1.69	5.23	14	200	12.08
	2.22	3.97	1	210	12.13
	2.53	3.48	1	300	12.05
NaSBA-15/48 **0.116**	0.82	10.77	1000	100	12.44
	1.44	6.13	29	110	12.25
	1.67	5.30	14	200	12.24
	2.18	4.05	1	210	12.30
	2.44	3.62	1	300	12.54
NaSBA-15/72 **0.109**	0.83	10.64	1000	100	12.28
	1.43	6.17	32	110	12.34
	1.66	5.33	15	200	12.31
	2.20	4.02	1	210	12.29
	2.49	3.55	1	300	12.29
NaSBA-15/120 **0.116**	0.83	10.65	1000	100	12.28
	1.43	6.17	36	110	12.34
	1.65	5.35	13	200	12.33
	2.19	4.03	2	210	12.31
	2.47	3.57	1	300	12.36
NaSBA-15S/24 **0.09**	0.89	9.93	1000	100	11.46
	1.55	5.71	26	110	11.42
	1.79	4.95	14	200	11.43
	2.36	3.73	1	210	11.40
	2.68	3.30	1	300	11.43
NaSBA-15S/48 **0.096**	0.86	10.27	1000	100	11.86
	1.50	5.90	34	110	11.80
	1.72	5.13	16	200	11.85
	2.27	3.88	1	210	11.85
	2.58	3.42	1	300	11.85

[a]δ - Full width at half maximum of the most intense peak; [b]2θ – scattering angle; [c]d – interplanar spacing; [d]I/I_0 – relative intensity defined as the ratio of the areas of a given peak to the most intense peak multiplied by 1000; [e]hkl – Muller indexes; [f]a – unit cell parameter.

Table 4S. Parameters obtained from N$_2$ adsorption at -196ºC and SAXS data for the calcined SBA-15 samples prepared from TEOS at 100ºC and SBA-15S/48.

Sample	S$_{BET}$ (m^2/g)	Single point V$_S$^{a} (cm^3/g)	ā ^{b} (nm)	w$_d$ (nm)	b$_d$ (nm)	w$_{KJS}$ (nm)	V$_t$^{c} (cm^3/g)	V$_{me}$^{d} (cm^3/g)	V$_{mi}$^{e} (cm^3/g)
SBA-15/06	1012	1.14	11.66	9.39	2.27	9.45	1.16	0.91	0.20
SBA-15/24	965	1.26	12.15	10.18	1.97	10.53	1.26	1.06	0.15
SBA-15/48	890	1.29	12.24	10.49	1.75	10.74	1.28	1.11	0.11
SBA-15/72	836	1.31	12.44	10.75	1.69	11.29	1.35	1.16	0.10
SBA-15/96	809	1.35	12.47	10.82	1.65	11.44	1.33	1.19	0.09
SBA-15/120	772	1.31	12.20	10.60	1.60	11.55	1.35	1.17	0.11
SBA-15S/48	912	1.26	12.40	10.45	1.95	10.57	1.28	1.08	0.13

^{a} Single-point pore volume V$_S$ evaluated from nitrogen adsorption isotherms; ^{b}ā – average unit cell parameter; ^{c}V$_t$ - total pore volume obtained by integration of the PSD curves; ^{d}V$_{me}$ - volume of primary mesopores calculated by integration of the PSD curves from 3 to ~17 nm; ^{e}V$_{mi}$ - micropore volume calculated by integration of the PSD curves up to 3 nm. Other symbols: S$_{BET}$ - BET specific surface area, w$_d$ – mesopore width evaluated according to the formulae reported in *Langmuir*, 1997, **13**, 6267, w$_{KJS}$ - mesopore width at the maximum of the pore size distribution obtained by the KJS method (see ref given above), and b$_d$ – mesopore wall thickness expressed as follows: b$_d$ = ā - w$_d$.

Table 5S. Parameters obtained from N$_2$ adsorption at -196ºC and SAXS data for the calcined SBA-15* samples prepared from TEOS at 120ºC and SBA-15S/48.

Sample	S$_{BET}$ (m^2/g)	Single point V$_S$^{a} (cm^3/g)	ā ^{b} (nm)	w$_d$ (nm)	b$_d$ (nm)	w$_{KJS}$ (nm)	V$_t$^{c} (cm^3/g)	V$_{me}$^{d} (cm^3/g)	V$_{mi}$^{e} (cm^3/g)
SBA-15/12*	848	1.29	12.28	10.62	1.66	11.08	1.29	1.14	0.09
SBA-15/24*	834	1.30	12.30	10.65	1.65	11.03	1.29	1.14	0.08
SBA-15/48*	718	1.35	12.10	10.76	1.34	11.65	1.37	1.22	0.04
SBA-15/72*	695	1.30	12.47	10.99	1.48	11.77	1.33	1.20	0.04
SBA-15S/48	912	1.26	12.40	10.45	1.95	10.57	1.28	1.08	0.13

^{a} Single-point pore volume V$_S$ evaluated from nitrogen adsorption isotherms; ^{b}ā – average unit cell parameter; ^{c}V$_t$ - total pore volume obtained by integration of the PSD curves; ^{d}V$_{me}$ - volume of primary mesopores calculated by integration of the PSD curves from 3 to ~17 nm; ^{e}V$_{mi}$ - micropore volume calculated by integration of the PSD curves up to 3 nm. Other symbols: S$_{BET}$ - BET specific surface area, w$_d$ – mesopore width evaluated according to the formulae reported in *Langmuir*, 1997, **13**, 6267, w$_{KJS}$ - mesopore width at the maximum of the pore size distribution obtained by the KJS method (see ref given above), and b$_d$ – mesopore wall thickness expressed as follows: b$_d$ = ā - w$_d$.

Table 6S. Parameters obtained from N$_2$ adsorption at -196ºC and SAXS data for the calcined NaSBA-15 samples prepared from sodium metasilicate at 100ºC, NaSBA-15S/24 and NaSBA-15S/48.

Sample	S$_{BET}$ (m^2/g)	Single point V$_S$^{a} (cm^3/g)	ā ^{b} (nm)	w$_d$ (nm)	b$_d$ (nm)	w$_{KJS}$ (nm)	V$_t$^{c} (cm^3/g)	V$_{me}$^{d} (cm^3/g)	V$_{mi}$^{e} (cm^3/g)
NaSBA-15/12	876	1.01	11.76	9.26	2.50	9.43	1.02	0.80	0.16
NaSBA-15/24	905	1.10	12.11	9.81	2.30	10.05	1.12	0.89	0.16
NaSBA-15/48	887	1.18	12.37	10.36	2.01	10.68	1.20	0.99	0.13
NaSBA-15/72	805	1.13	12.30	10.26	2.04	10.77	1.12	0.97	0.11
NaSBA-15/120	760	1.15	12.32	10.41	1.91	11.01	1.16	1.01	0.09
NaSBA-15S/24	761	0.91	11.43	9.09	2.34	8.80	0.91	0.76	0.12
NaSBA-15S/48	820	1.06	11.84	9.73	2.11	9.84	1.06	0.90	0.12

^{a} Single-point pore volume V$_S$ evaluated from nitrogen adsorption isotherms; ^{b}ā – average unit cell parameter; ^{c}V$_t$ - total pore volume obtained by integration of the PSD curves; ^{d}V$_{me}$ - volume of primary mesopores calculated by integration of the PSD curves from 3 to ~17 nm; ^{e}V$_{mi}$ - micropore volume calculated by integration of the PSD curves up to 3 nm. Other symbols: S$_{BET}$ - BET specific surface area, w$_d$ – mesopore width evaluated according to the formulae reported in *Langmuir*, 1997, **13**, 6267, w$_{KJS}$ - mesopore width at the maximum of the pore size distribution obtained by the KJS method (see ref given above), and b$_d$ – mesopore wall thickness expressed as follows: b$_d$ = ā - w$_d$.