Supporting information

X-ray Diffraction Structure Analysis of MCM-48 Mesoporous Silica

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Table 1S. Observed (F_o) and calculated (F_c) structure factors for the calcined MCM-48 sample C-SY for different structure models.^a The reliability factors R_F are given in the bottom row.

Structure model:		A		B		C	
hkl	$ F_o $	$ F_c $	$\Delta F $	$ F_c $	$\Delta F $	$ F_c $	$\Delta F $
112	101.0	100.0	1	99.1	1.9	100.0	1
022	57.1	53.8	3.3	58.2	-1.1	57.5	-0.4
123	10.0	10.6	-0.6	10.1	-0.1	10.1	-0.1
004	33.0	33.4	-0.4	33.0	0	32.2	0.8
024	27.0	26.5	0.5	27.0	0	26.2	0.8
233	34.1	33.4	0.7	33.7	0.4	34.0	0.1
224	18.7	17.7	1	18.1	0.6	18.2	0.5
134	12.4	12.1	0.3	11.9	0.5	12.6	-0.2
125	3.0	3.3	-0.3	3.4	-0.4	3.1	-0.1
044	2.6	3.5	-0.9	3.3	-0.7	3.1	-0.5
116	6.6	6.9	-0.3	7.4	-0.8	6.8	-0.2
235	3.3	3.4	-0.1	3.3	0	3.4	-0.1
026	1.7	1.9	-0.2	1.5	0.2	1.9	-0.2
145	4.0	4.1	-0.1	4.1	-0.1	4.0	0
136	3.8	3.9	-0.1	3.7	0.1	3.9	-0.1
444	8.1	8.1	0	8.0	0.1	8.3	-0.2
345	5.8	5.6	0.2	5.2	0.6	5.8	0
046	2.7	2.7	0	2.8	-0.1	2.7	0
127	0.3	0.3	0	0.4	-0.1	0.3	0
255	2.4	2.3	0.1	2.2	0.2	2.5	-0.1
336	1.5	1.5	0	1.2	0.3	1.6	-0.1
246	1.0	1.2	-0.2	0.9	0.1	1.2	-0.2
R_F :		0.030		0.025		0.016	

^a The following structure models were checked: A, simplified model with wall of uniform density and thickness; B, model with ~10% thicker flat wall segments; C, model with ~10% denser flat wall segments.

Figure 1S. Expected (001) section of the difference density map for the case of the local thickening of flat wall segments calculated based on the structure factors from Table S1 for models A and B.

Figure 2S. Variation of reliability factor of full-profile refinement (for calcined sample C-SY) with wall thickness parameter.