

Supporting information section for

“Wall thickness prediction in precipitated precursors of mesoporous materials”

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In all cases, the chain length is equal to 11.7 Å, which corresponds to an alkyl chain with 8 units. The mean charge of the ions in the inter-cylinder area was considered to be equal to 1. The Bjerrum Length is equal to 7.2 Å.

rh = head group size (Å)

The radius of the head group surfactant may vary from 1 Å in the case of amine to about 8 Å for EO. Tests with the head group size varying within this realistic range are given in the next table.

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Effect of head group size

r_h	A	λ	Π_0	I	$t_{\text{calc}} (\text{\AA})$
1	0.6	1.9	$4 \cdot 10^8$	2	9
2					10.2
4					11.7
6					12.8
8					13.6

A = Hamaker constant (kT)

Depending on the nature of the surfactant, the Hamaker constant may vary from 0.6 $k_B T$ for the hydrocarbon surfactant to about 1.7 $k_B T$ in case of a fluorocarbon surfactant. The Hamaker constant is directly implied in the Van Der Waals attractive potential. Increasing this constant leads to an increase of this attractive force and thus to a decrease in the expected wall thickness. This explains the thinner wall obtained when using a fluorocarbon surfactant.

Effect of the Hamaker constant

r_h	A	λ	Π_0	I	$t_{\text{calc}} (\text{\AA})$
4	0.5	1.9	$4 \cdot 10^8$	2	12.2
	0.6				11.7
	0.8				11.0

1	10.4
1.4	9.5
1.7	9

$\lambda = \text{decay length (\AA)}$

According to the literature, the decay length varies from 1.8 to 2.2 Å^{47, 48}. This parameter has an effect on the repulsive hydration force. An increase in the decay length leads to an increase of this attractive potential and then to an increase in the expected wall thickness.

Effect of decay length

r_h	A	λ	Π_0	I	$t_{\text{calc}} (\text{\AA})$
4	0.6	1.8	4e8	2	10.9
		1.9			11.7
		2.0			12.5
		2.1			13.4
		2.2			14.3

Π_0 = osmotic pressure (Pa)

According to the literature, the osmotic pressure may vary between $4 \cdot 10^8$ to $4 \cdot 10^9$ Pa^{47 48}. This parameter has an effect on the repulsive hydration force. An increase in the osmotic pressure leads to an increase in the repulsive potential and then to an increase of the expected wall thickness. In the case of a non-ionic surfactant, this osmotic pressure is higher than in the case of an ionic surfactant. This difference explains the thicker walls observed when using a non-ionic rather than an ionic surfactant.

Effect of osmotic pressure

r_h	A	λ	Π_0	I	t_{calc} (Å)
4	0.6	1.9	4e8	2	11.7
			6e8		12.6
			8e8		13.2
			1e9		13.7
			2e9		15.3
			4e9		16.9

I = ionic strength

The ionic strength is difficult to evaluate because it depends on the salt concentration and also on the silica concentration during the synthesis of mesoporous materials. Many variations of this parameter are available. To evaluate the effect of this parameter on the expected wall thickness, the range tested is 0.5 to 3 mol/L. This parameter impacts the electrostatic force.

When the ionic strength is too high, the repulsive potential becomes negligible compared with the two other contributions. This explains why for a high ionic strength, the expected wall thickness is no longer affected by this parameter.

Effect of the ionic strength

r_h	A	λ	Π_0	I	$t_{\text{calc}} (\text{\AA})$
4	0.6	1.9	4e8	0.8	15.1
				1	13.6
				1.5	12.2
				2	11.7
				2.5	11.5
				3	11.5