Table S1 Modelling Parameters (Eqs. 1-3).

Sample	r^S (±0.5 Å)	r_{hs} (±0.1 Å)	ϕ_{hs} (±0.02)
H-MAA/C8/1.0	7.0	11.0	0.36
S-MAA-8-M/C16/1.0	12.0	15.1	0.31
S-MAA-8-M/C16/0.9	11.0	15.8	0.32
S-MAA-8-M/C16/0.7	10.9	16.4	0.32
S-MAA-8-M/C12/1.0	8.8	12.7	0.24
S-MAA-8-M/C12/0.9	9.0	15.0	0.35
S-MAA-8-M/C12/0.8	9.5	14.2	0.30
S-MAA-8-M/C12/0.7	9.1	13.3	0.25
S-MAA-8-M/C12/0.6	9.9	14.7	0.35
S-MAA-8-M/C12/0.4	9.8	14.2	0.34
S-MAA-8-M/C12/0.2	7.8	13.7	0.24
S-MAA-8-M/C8/1.0	6.0	9.7	0.27
S-MAA-8-M/C8/0.9	6.7	9.0	0.26
S-MAA-15/C16/0.2	11.5	15.0	0.24
S-MAA-15/C16/0.15	9.5	17.6	0.36
S-MAA-15/C16/0.1	9.7	14.8	0.21
S-MAA-15/C12/1.0	8.2	12.3	0.28
S-MAA-15/C12/0.8	7.2	13.3	0.34
S-MAA-15/C12/0.6	7.5	12.9	0.28
S-MAA-15/C12/0.4	8.1	13.4	0.33
S-MAA-15/C12/0.1	8.2	14.4	0.34
S-MAA-15/-C8/1.0	6.6	9.4	0.24
S-MAA-15/C8/0.8	6.7	9.7	0.26
S-MAA-15/C8/0.6	6.5	8.8	0.22
S-MAA-3/C12/1.0	9.2	14.2	0.37
S-MAA-3/C12/0.9	7.4	14.0	0.32
S-MAA-3/C12/0.8	8.7	14.4	0.40
S-MAA-3/C12/0.7	8.6	14.3	0.37
S-MAA-3/C8/1.0	6.1	15.4	0.33
S-MAA-3/C8/0.9	6.1	14.8	0.37
S-MAA-3/C8/0.8	6.1	15.0	0.33
S-MAA-3/C8/0.7	6.1	14.3	0.34

Table S2 Modelling Parameters (Eqs. 1-5).

Sample	$R_{AmphComb}$ (±1Å)	R_{hs} (±5Å)	Φ_{hs} (±0.05)	s^a (±0.1)
S-MAA-8-M/C12/0.6	84	124	0.45	0.11
S-MAA-8-M/C12/0.4	83	123	0.48	0.10
S-MAA-8-M/C12/0.2	86	130	0.46	0.15
S-MAA-8-M/C8/0.7	83	141	0.42	0.17
S-MAA-8-M/C8/0.6	83	145	0.44	0.17
S-MAA-8-M/C8/0.5	83	133	0.41	0.13
S-MAA-8-M/C8/0.4	83	127	0.40	0.13
S-MAA-8-M/C8/0.3	70	119	0.45	0.15
S-MAA-8-M/C8/0.2	70	115	0.40	0.14
S-MAA-8-M/C8/0.1	60	110	0.40	0.15
S-MAA-3/C12/1.0	68	141	0.35	0.10
S-MAA-3/C12/0.9	67	144	0.30	0.10
S-MAA-3/C12/0.8	66	139	0.36	0.15
S-MAA-3/C8/1.0	68	125	0.34	0.14
S-MAA-3/C8/0.9	57	116	0.33	0.13
S-MAA-3/C8/0.8	56	117	0.33	0.15
S-MAA-3/C8/0.7	56	111	0.33	0.10

[a] relative standard deviation, $s = \sigma/R_{AmphComb}$.