Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information

HOW THE CHAIN CONFORMATION GOVERNS THE PACKING OF INVERTED MICELLES IN THE Fd3m-PHASE

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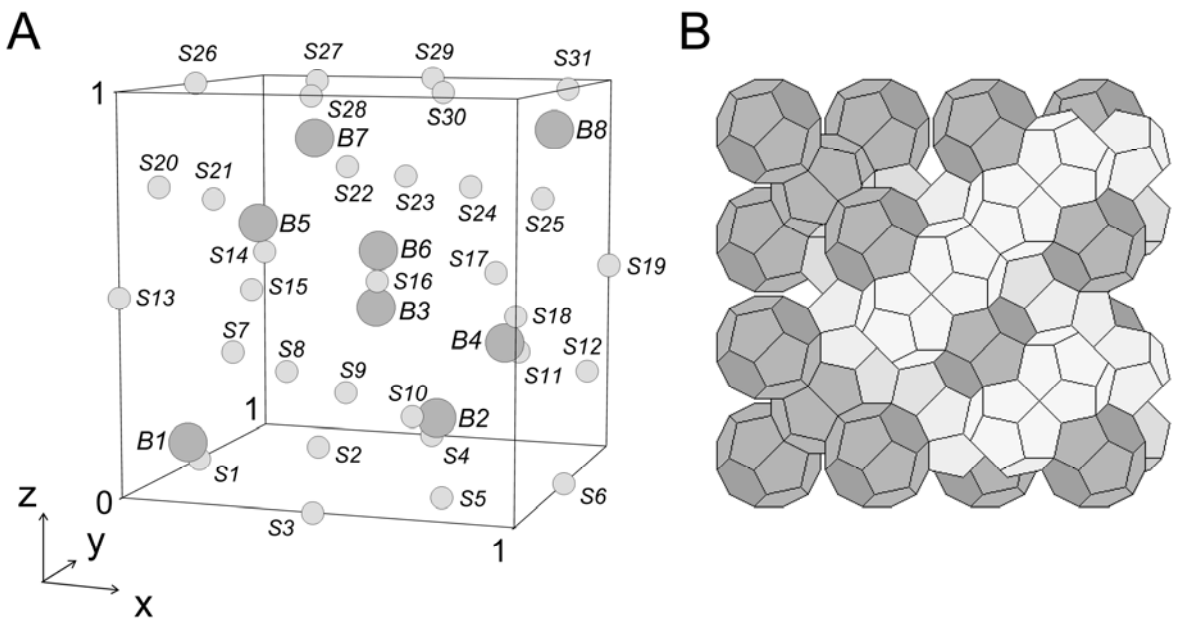


Figure S1 Schematic drawings of the structure the inverse micellar phase Fd3m. (A) Positions of the big (B) and small (S) micelles having chosen the origin at $\bar{3}\,m$. The unit cell parameter, *a*, is set to unity (for coordinates see Table S1). (B) Same structure displaying the corresponding small (5^{12}; light grey) and big cages ($5^{12}6^4$; dark grey) of each micelles. Viewing direction is along the z-axis (compare Fig. S3).

Table S1 Micelle coordinates in fractions of the unit cell parameter, *a* (refer to Fig. S1 A)

	Big micelle coordinates				**Small micelle coordinates**		
B1	0.125	0.125	0.125	*S1*	0	0.5	0
B2	0.625	0.625	0.125	*S2*	0.25	0.75	0
B3	0.375	0.875	0.375	*S3*	0.5	0	0
B4	0.875	0.375	0.375	*S4*	0.5	1	0
B5	0.125	0.625	0.625	*S5*	0.75	0.25	0
B6	0.625	0.125	0.625	*S6*	1	0.5	0
B7	0.375	0.375	0.875	*S7*	0	0.75	0.25
B8	0.875	0.875	0.875	*S8*	0.25	0.5	0.25

	S9	0.5	0.25	0.25
	S10	0.75	0	0.25
	S11	0.75	1	0.25
	S12	1	0.75	0.25
	S13	0	0	0.5
	S14	0	1	0.5
	S15	0.25	0.25	0.5
	S16	0.5	0.5	0.5
	S17	0.75	0.75	0.5
	S18	1	0	0.5
	S19	1	1	0.5
	S20	0	0.25	0.75
	S21	0.25	0	0.75
	S22	0.25	1	0.75
	S23	0.5	0.75	0.75
	S24	0.75	0.5	0.75
	S25	1	0.25	0.75
	S26	0	0.5	1
	S27	0.25	0.75	1
	S28	0.5	0	1
	S29	0.5	1	1
	S30	0.75	0.25	1
	S31	1	0.5	1

Table S2: Characteristic parameters of the regular polygons with the edge length, *s*, concerning Figure 1 and Table 1.

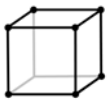
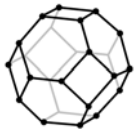
Name	Picture	Surface Area	Volume	R_o	R_i
Cube		$6 \cdot s^2$	$1 \cdot s^3$	$\frac{\sqrt{3}}{2} \cdot s$	$\frac{1}{2} \cdot s$
Rhombic Dodeca-hedron		$(8\sqrt{2}) \cdot s^2$	$\frac{16}{9}\sqrt{3} \cdot s^3$	$\frac{\sqrt{12}}{3} \cdot s$	$\frac{\sqrt{6}}{3} \cdot s$
Truncated Octa-hedron		$(6+12\sqrt{3}) \cdot s^2$	$8\sqrt{3} \cdot s^3$	$\frac{1}{2}\sqrt{10} \cdot s$	$\frac{1}{2}\sqrt{6} \cdot s$
Dodeca-hedron		$3\sqrt{25+10\sqrt{5}} \cdot s^2$	$\frac{1}{4}(15+7\sqrt{5}) \cdot s^3$	$\frac{\sqrt{3}}{4}(1+\sqrt{5}) \cdot s$	$\frac{1}{2}\sqrt{\frac{5}{2}+\frac{11}{10}\sqrt{5}} \cdot s$

Table S3: Overview of constructed cages of type 5^{12} and $5^{12}6^4$ (see Tables S4-S7).

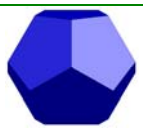
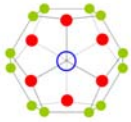
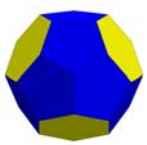
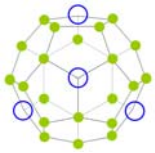
Name	Picture	Wireframe	S-S ratio	B-B ratio	S-B ratio
$W5^{12}$			1:1	1:1	1:1
$D5^{12}$			1:1	1:1	$\sqrt{2}:\sqrt{3}$
$W5^{12}6^4$			1:1	1:1	1:1
$D5^{12}6^4$			1:1	1:1	$\sqrt{2}:\sqrt{3}$

Table S4 Faces and vertices of the $W5^{12}$ cage constructed after Wigner-Seitz. The centre of the cage is placed in the origin and the unit cell parameter, *a*, is set to unity (cp. Table S3).

Faces	**x**	**y**	**z**	**length**	**area**
0	0.301511	0.301511	-0.904534	0.207289[a]	0.0427
1	-0.301511	0.904534	-0.301511	0.207289	0.0427
2	0.904534	-0.301511	-0.301511	0.207289	0.0427
3	-0.904534	0.301511	0.301511	0.207289	0.0427
4	0.301511	-0.904534	0.301511	0.207289	0.0427
5	-0.301511	-0.301511	0.904534	0.207289	0.0427
6	0.707107	0.707107	0	0.176777[b]	0.0594
7	0	0.707107	0.707107	0.176777	0.0594
8	-0.707107	0	-0.707107	0.176777	0.0594
9	0.707107	0	0.707107	0.176777	0.0594
10	0	-0.707107	-0.707107	0.176777	0.0594
11	-0.707107	-0.707107	0	0.176777	0.0594
Vertices*	**x**	**y**	**z**	**length**	**colour code**
6-7-9	0.125	0.125	0.125	0.21650635	○
8-10-11	-0.125	-0.125	-0.125	0.21650635	○
2-6-9	0.2375	0.0125	0.0125	0.23815699	●
3-8-11	-0.2375	-0.0125	-0.0125	0.23815699	●
0-8-10	-0.0125	-0.0125	-0.2375	0.23815699	●
5-7-9	0.0125	0.0125	0.2375	0.23815699	●
4-10-11	-0.0125	-0.2375	-0.0125	0.23815699	●
1-6-7	0.0125	0.2375	0.0125	0.23815699	●
2-4-9	0.197917	-0.145833	0.0520833	0.25129877	●
1-3-7	-0.145833	0.197917	0.0520833	0.25129877	●
0-1-6	0.0520833	0.197917	-0.145833	0.25129877	●
3-5-11	-0.197917	-0.0520833	0.145833	0.25129877	●
1-3-8	-0.197917	0.145833	-0.0520833	0.25129877	●
0-2-10	0.145833	-0.0520833	-0.197917	0.25129877	●
3-5-7	-0.145833	0.0520833	0.197917	0.25129877	●
0-1-8	-0.0520833	0.145833	-0.197917	0.25129877	●
2-4-10	0.145833	-0.197917	-0.0520833	0.25129877	●
4-5-11	-0.0520833	-0.197917	0.145833	0.25129877	●
0-2-6	0.197917	0.0520833	-0.145833	0.25129877	●
4-5-9	0.0520833	-0.145833	0.197917	0.25129877	●

* Each vertex was determined from the intersection of three faces, e.g. 6-7-9. [a] The B-S micelles distance equals $\sqrt{11}/8$, i.e., the faces 1-6 are placed at a distance of $\sqrt{11}/16$. [b] The S-S micelles distance equals $\sqrt{2}/4$, i.e., the faces 7-12 are placed at a distance of $\sqrt{2}/8$. Total surface area A = 0.6126 and the total volume V = 0.0387.

Table S5 Faces and vertices of the $D5^{12}$ cage constructed after Duesing [1]. The centre of the cage is placed in the origin and the unit cell parameter, *a*, is set to unity (cp. Table S3).

Faces	**x**	**y**	**z**	**length**	**area**
0	0.301511	0.301511	-0.904534	0.186349[a]	0.0441
1	-0.301511	0.904534	-0.301511	0.186349	0.0441
2	0.904534	-0.301511	-0.301511	0.186349	0.0441
3	-0.904534	0.301511	0.301511	0.186349	0.0441
4	0.301511	-0.904534	0.301511	0.186349	0.0441
5	-0.301511	-0.301511	0.904534	0.186349	0.0441
6	0.707107	0.707107	0	0.176777[b]	0.0475
7	0	0.707107	0.707107	0.176777	0.0475
8	-0.707107	0	-0.707107	0.176777	0.0475
9	0.707107	0	0.707107	0.176777	0.0475
10	0	-0.707107	-0.707107	0.176777	0.0475
11	-0.707107	-0.707107	0	0.176777	0.0475
Vertices*	**x**	**y**	**z**	**length**	**colour code**
6-7-9	0.125	0.125	0.125	0.21650635	○
8-10-11	-0.125	-0.125	-0.125	0.21650635	○
0-8-10	-0.0263903	-0.0263903	-0.22361	0.22670317	●
5-7-9	0.0263903	0.0263903	0.22361	0.22670317	●
1-6-7	0.0263903	0.22361	0.0263903	0.22670317	●
2-6-9	0.22361	0.0263903	0.0263903	0.22670317	●
3-8-11	-0.22361	-0.0263903	-0.0263903	0.22670317	●
4-10-11	-0.0263903	-0.22361	-0.0263903	0.22670317	●
3-5-7	-0.122683	0.0636586	0.186341	0.2320054	●
0-2-10	0.122683	-0.0636586	-0.186341	0.2320054	●
0-1-8	-0.0636586	0.122683	-0.186341	0.2320054	●
0-1-6	0.0636586	0.186341	-0.122683	0.2320054	●
4-5-9	0.0636586	-0.122683	0.186341	0.2320054	●
4-5-11	-0.0636586	-0.186341	0.122683	0.2320054	●
3-5-11	-0.186341	-0.0636586	0.122683	0.2320054	●
0-2-6	0.186341	0.0636586	-0.122683	0.2320054	●
2-4-9	0.186341	-0.122683	0.0636586	0.2320054	●
1-3-7	-0.122683	0.186341	0.0636586	0.2320054	●
1-3-8	-0.186341	0.122683	-0.0636586	0.2320054	●
2-4-10	0.122683	-0.186341	-0.0636586	0.2320054	●

* Each vertex was determined from the intersection of three faces, e.g. 6-7-9.

[a] The B-S micelles distance equals $\sqrt{11}/8$, i.e., the faces 1-6 are placed at a distance of $\frac{\sqrt{2}}{\sqrt{2}+\sqrt{3}} \cdot \sqrt{11}/8$. [b] The S-S micelles distance equals $\sqrt{2}/4$, i.e., the faces 7-12 are placed at a distance of $\sqrt{2}/8$. Total surface area A = 0.5497 and the total volume V = 0.0332.

Table S6 Faces and vertices of the $W5^{12}6^4$ cage constructed after Wigner-Seitz. The centre of the cage is placed in the origin and the unit cell parameter, *a*, is set to unity (cp. Table S3).

Faces	x	y	z	length	Area
0	0.57735	0.57735	-0.57735	0.216506[a]	0.0423
1	-0.57735	0.57735	0.57735	0.216506	0.0423
2	0.57735	-0.57735	0.57735	0.216506	0.0423
3	-0.57735	-0.57735	-0.57735	0.216506	0.0423
4	-0.301511	0.904534	-0.301511	0.207289[b]	0.0427
5	0.301511	0.904534	0.301511	0.207289	0.0427
6	-0.301511	0.301511	-0.904534	0.207289	0.0427
7	-0.904534	0.301511	-0.301511	0.207289	0.0427
8	0.904534	0.301511	0.301511	0.207289	0.0427
9	0.301511	0.301511	0.904534	0.207289	0.0427
10	0.301511	-0.301511	-0.904534	0.207289	0.0427
11	0.904534	-0.301511	-0.301511	0.207289	0.0427
12	-0.904534	-0.301511	0.301511	0.207289	0.0427
13	-0.301511	-0.301511	0.904534	0.207289	0.0427
14	0.301511	-0.904534	-0.301511	0.207289	0.0427
15	-0.301511	-0.904534	0.301511	0.207289	0.0427
Vertices*	**x**	**y**	**z**	**length**	**colour code**
10-11-14	0.1375	-0.1375	-0.1375	0.23815699	
5-8-9	0.1375	0.1375	0.1375	0.23815699	
4-6-7	-0.1375	0.1375	-0.1375	0.23815699	
12-13-15	-0.1375	-0.1375	0.1375	0.23815699	
0-10-11	0.177083	0.0208334	-0.177083	0.25129864	
0-5-8	0.177083	0.177083	-0.0208334	0.25129864	
2-13-15	0.0208334	-0.177083	0.177083	0.25129864	
3-10-14	-0.0208334	-0.177083	-0.177083	0.25129864	
1-4-7	-0.177083	0.177083	0.0208334	0.25129864	
0-4-6	0.0208334	0.177083	-0.177083	0.25129864	
1-5-6	-0.0208334	0.177083	0.177083	0.25129864	
2-11-14	0.177083	-0.177083	0.0208334	0.25129864	
1-12-13	-0.177083	0.0208334	0.177083	0.25129864	
3-6-7	-0.177083	-0.0208334	-0.177083	0.25129864	
3-12-15	-0.177083	-0.177083	-0.0208334	0.25129864	
2-8-9	0.177083	-0.0208334	0.177083	0.25129864	
0-4-5	0.0729167	0.229167	-0.0729167	0.25129864	
3-7-12	-0.229167	-0.0729167	-0.0729167	0.25129864	
2-9-13	0.0729167	-0.0729167	0.229167	0.25129864	
1-4-5	-0.0729167	0.229167	0.0729167	0.25129864	
0-8-11	0.229167	0.0729167	-0.0729167	0.25129864	
3-14-15	-0.0729167	-0.229167	-0.0729167	0.25129864	
0-6-10	0.0729167	0.0729167	-0.229167	0.25129864	
2-8-11	0.229167	-0.0729167	0.0729167	0.25129864	
1-9-13	-0.0729167	0.0729167	0.229167	0.25129864	
2-14-15	0.0729167	-0.229167	0.0729167	0.25129864	
3-6-10	-0.0729167	-0.0729167	-0.229167	0.25129864	
1-7-12	-0.229167	0.0729167	0.0729167	0.25129864	

* Each vertex was determined from the intersection of three faces, e.g. 10-11-14.

[a] The B-B micelles distance equals $\sqrt{3}/4$, i.e., the faces 1-4 are placed at a distance of $\sqrt{3}/8$. [b] The B-S micelles distance equals $\sqrt{11}/8$, i.e., the faces 5-28 are placed at a distance of $\sqrt{11}/16$. Total surface area A = 0.6813 and the total volume V = 0.0476.

Table S7 Faces and vertices of the $D5^{12}6^4$ cage constructed after Duesing [1]. The centre of the cage is placed in the origin and the unit cell parameter, *a*, is set to unity (cp. Table S3).

Faces	x	y	z	length	area
0	0.57735	0.57735	-0.57735	0.216506[a]	0.0632
1	-0.57735	0.57735	0.57735	0.216506	0.0632
2	0.57735	-0.57735	0.57735	0.216506	0.0632
3	-0.57735	-0.57735	-0.57735	0.216506	0.0632
4	-0.301511	0.904534	-0.301511	0.228229[b]	0.0441
5	0.301511	0.904534	0.301511	0.228229	0.0441
6	-0.301511	0.301511	-0.904534	0.228229	0.0441
7	-0.904534	0.301511	-0.301511	0.228229	0.0441
8	0.904534	0.301511	0.301511	0.228229	0.0441
9	0.301511	0.301511	0.904534	0.228229	0.0441
10	0.301511	-0.301511	-0.904534	0.228229	0.0441
11	0.904534	-0.301511	-0.301511	0.228229	0.0441
12	-0.904534	-0.301511	0.301511	0.228229	0.0441
13	-0.301511	-0.301511	0.904534	0.228229	0.0441
14	0.301511	-0.904534	-0.301511	0.228229	0.0441
15	-0.301511	-0.904534	0.301511	0.228229	0.0441
Vertices*	**x**	**y**	**z**	**length**	**colour code**
10-11-14	0.15139	-0.15139	-0.15139	0.26221517	○
5-8-9	0.15139	0.15139	0.15139	0.26221517	○
4-6-7	-0.15139	0.15139	-0.15139	0.26221517	○
12-13-15	-0.15139	-0.15139	0.15139	0.26221517	○
2-9-13	0.0613414	-0.0613414	0.252317	0.26681380	●
2-14-15	0.0613414	-0.252317	0.0613414	0.26681380	●
3-14-15	-0.0613414	-0.252317	-0.0613414	0.26681380	●
1-4-5	-0.0613414	0.252317	0.0613414	0.26681380	●
0-4-5	0.0613414	0.252317	-0.0613414	0.26681380	●
3-6-10	-0.0613414	-0.0613414	-0.252317	0.26681380	●
0-6-10	0.0613414	0.0613414	-0.252317	0.26681380	●
3-7-12	-0.252317	-0.0613414	-0.0613414	0.26681380	●
0-8-11	0.252317	0.0613414	-0.0613414	0.26681380	●
1-9-13	-0.0613414	0.0613414	0.252317	0.26681380	●
1-7-12	-0.252317	0.0613414	0.0613414	0.26681380	●
2-8-11	0.252317	-0.0613414	0.0613414	0.26681380	●
2-11-14	0.188659	-0.188659	-0.00231717	0.26681380	●
1-4-7	-0.188659	0.188659	-0.00231717	0.26681380	●
0-5-8	0.188659	0.188659	0.00231717	0.26681380	●
0-10-11	0.188659	-0.00231717	-0.188659	0.26681380	●
2-8-9	0.188659	0.00231717	0.188659	0.26681380	●
3-12-15	-0.188659	-0.188659	0.00231717	0.26681380	●
0-4-6	-0.00231717	0.188659	-0.188659	0.26681380	●
3-10-14	0.00231717	-0.188659	-0.188659	0.26681380	●
2-13-15	-0.00231717	-0.188659	0.188659	0.26681380	●
3-6-7	-0.188659	0.00231717	-0.188659	0.26681380	●
1-12-13	-0.188659	-0.00231717	0.188659	0.26681380	●
1-5-9	0.00231717	0.188659	0.188659	0.26681380	●

* Each vertex was determined from the intersection of three faces, e.g. 10-11-14. [a] The B-B micelles distance equals $\sqrt{3}/4$, i.e., the faces 1-4 are placed at a distance of $\sqrt{3}/8$. [b] The B-S micelles distance equals $\sqrt{11}/8$, i.e., the faces 5-28 are placed at a distance of $\frac{\sqrt{3}}{\sqrt{2}+\sqrt{3}} \cdot \sqrt{11}/8$. Total surface area A = 0.7823 and the total volume V = 0.0585.

The following three figures are supporting Figures 3 and 4 of the article. Displaying larger areas, they serve to understand the 3D arrangement of cages in the viewing direction [-110], [001] and [111].

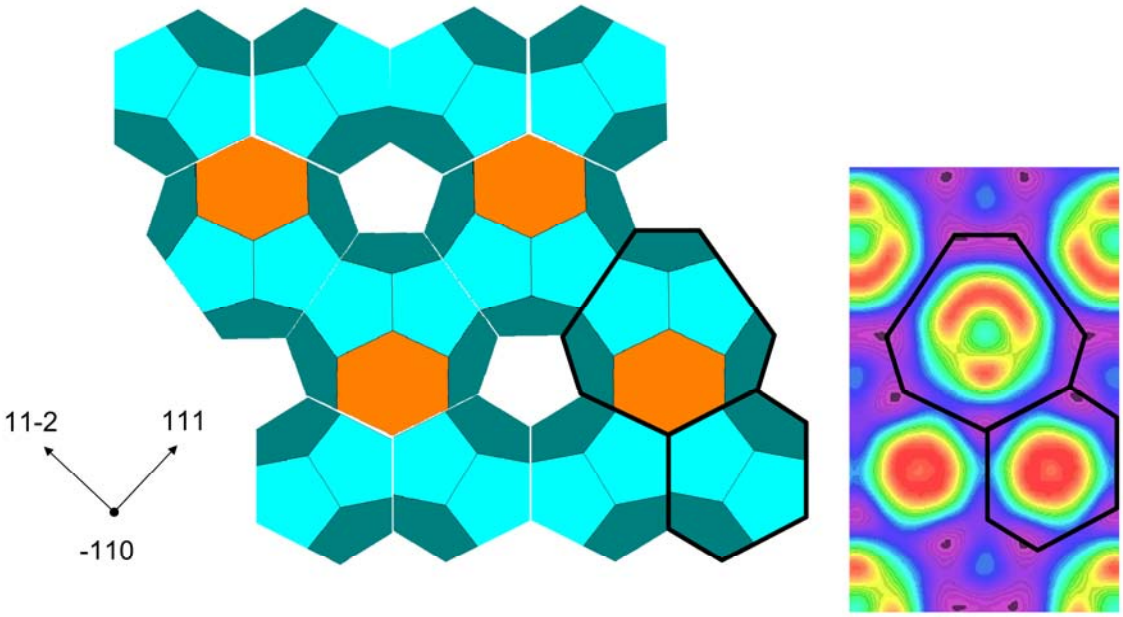


Figure S2 Schematic view of the packing of the cages viewed in [-110]-direction. On the right hand side the corresponding electron density map of the -110-plane of MO/OA (1:4 wt/wt)[2] is shown. The cross-section of the 5^{12} and $5^{12}6^4$ cages with the -110-plane are displayed with black boarders, both, in the scheme and the electron density map.

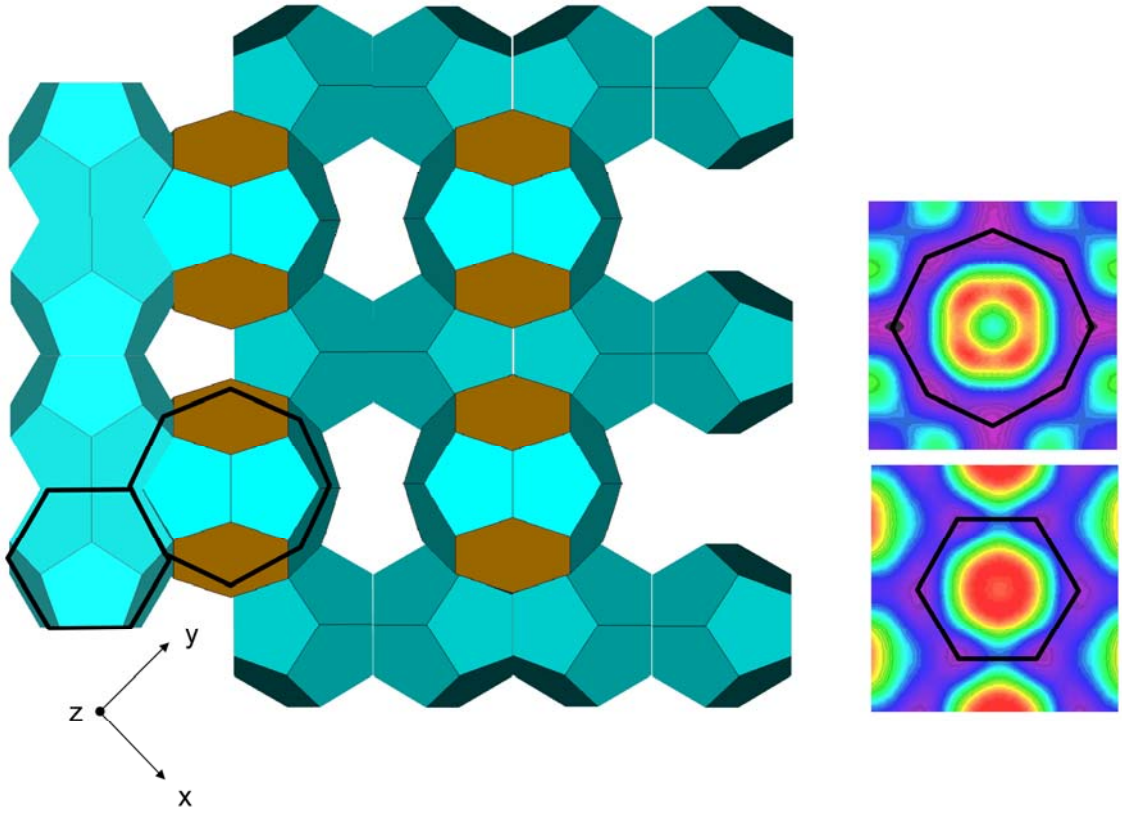


Figure S3 Schematic view of the packing of the cages viewed in [001]-direction. On the right hand side the corresponding electron density maps cutting a big micelle in its centre (top) and a small micelle in its centre (bottom) are shown. The latter two planes are 0.125 *a* apart (see Table S1). The corresponding cross-section of the 5^{12} and $5^{12}6^4$ cages perpendicular to the z-axis are displayed with black boarders, both, in the scheme and the electron density map.

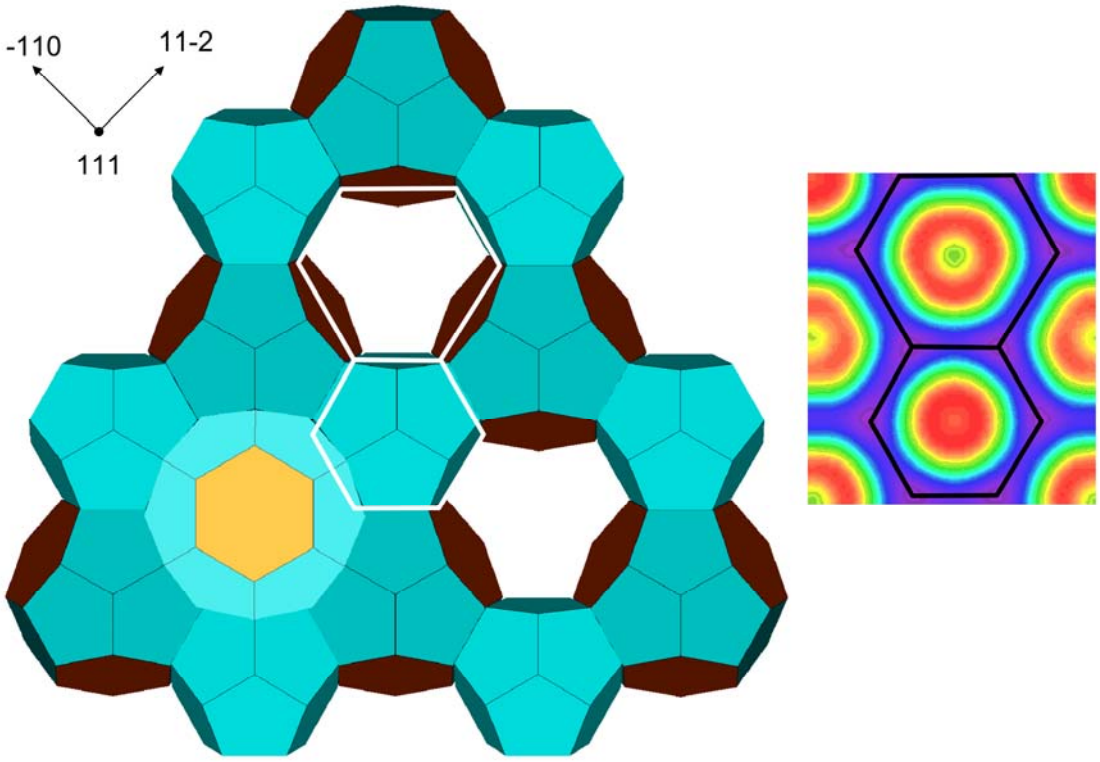


Figure S4 Schematic view of the packing of the cages viewed in [111]-direction. On the right hand side the corresponding electron density map of the 111-plane is shown. Note, that while the small micelle is cut in its centre the big one is not. The corresponding cross-section of the 5^{12} and $5^{12}6^4$ cages with the 111-plane are displayed, both, in the scheme and the electron density map.

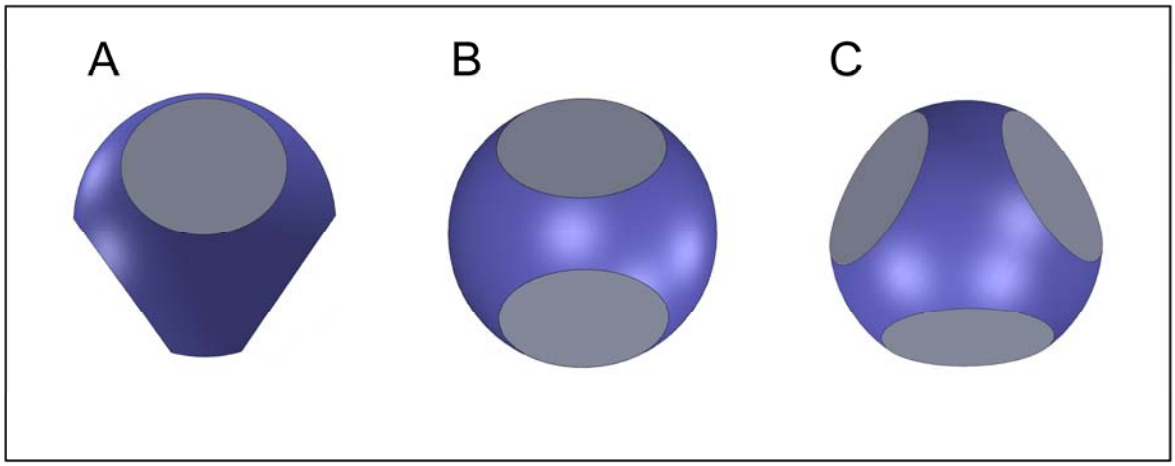


Figure S5 Model of the polar body of the big micelles viewed in [-110] (A),[001] (B), and [111]-direction (C).

See also **3D animation** of the polar/apolar interface ***Big Micelle Polar Body MOOA.avi***

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