Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Prediction of Striped Cylindrical Micelles (SCM) Formed by Dodecyl-β-D-maltoside (DDM) Surfactants

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Bead-pairs	σ (nm)	ε (kJ/mol)
C_1-C_1	0.47	3.5
P_1-P_1	0.47	4.5
P_2-P_2	0.47	4.5
P_4-P_4	0.47	5.0
N_a-N_a	0.47	4.0
Q_a-Q_a	0.47	5.0
C_1-P_1	0.47	2.7
C_1-P_2	0.47	2.3
C_1-P_4	0.47	2.0
C_1-N_a	0.47	2.7
C_1-Q_a	0.62	2.0
P_1-P_2	0.47	4.5
P_1-P_4	0.47	4.5
P_1-N_a	0.47	4.5
P_1-Q_a	0.47	5.0
P_2-P_4	0.47	4.5
P_2-N_a	0.47	4.5
P_2-Q_a	0.47	5.0
P_4-N_a	0.47	4.0
P_4-Q_a	0.47	5.6
N_a-Q_a	0.47	4.0

Table S1: Interaction parameters for various MARTINI bead pairs.

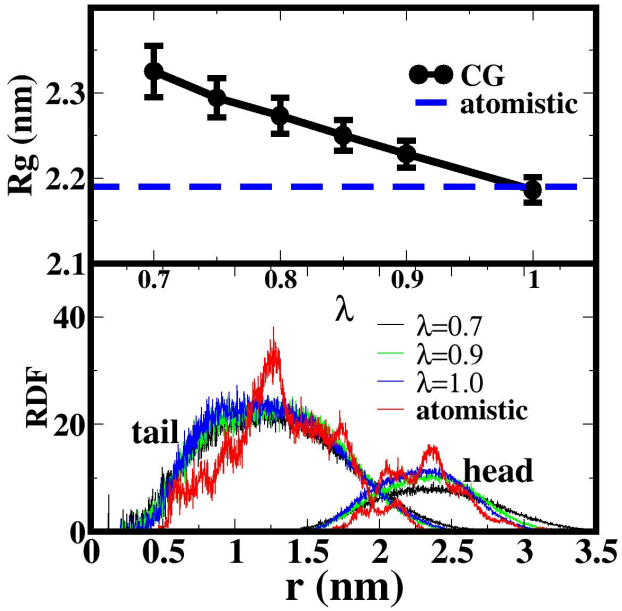

Figure S1: (a) *Upper panel*: Radius of gyration (Rg) of DDM micelle as a function of λ obtained from CG simulation (see main text for details). Dotted line shows the Rg of the micelle obtained from atomistic simulation. *Lower panel*: Radial Distribution function (RDF) of the center of mass of the surfactant tails and heads with respect to the micelle center obtained for different CG and atomistic simulations.

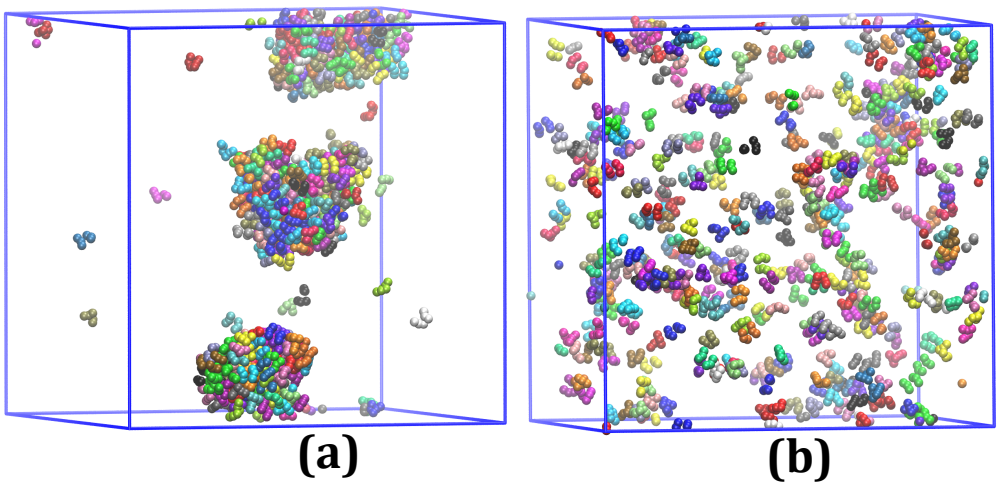

Figure S2: (a) Maltose molecules form unphysical clusters with original MARTINI force field ($\lambda = 1.0$). Structure obtained after 300 ns long simulations (b) However, maltose molecules remain well dispersed in the solution with the force field for $\lambda = 0.9$. See main

text for details. The concentration of the maltose molecules in these systems is 100mM. Structure obtained after 1000 ns long simulations.

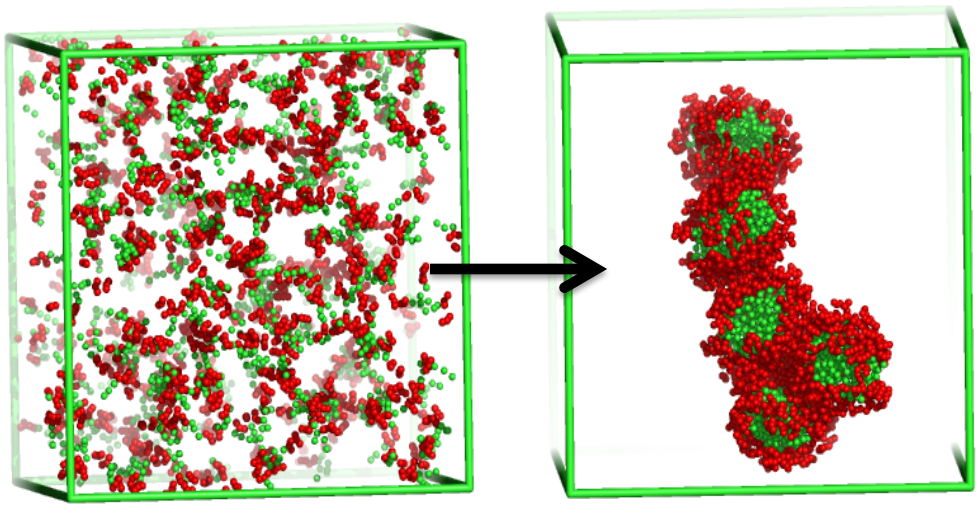

Figure S3: Formation of the SCM structure with the CG force field for $\lambda = 0.9$.

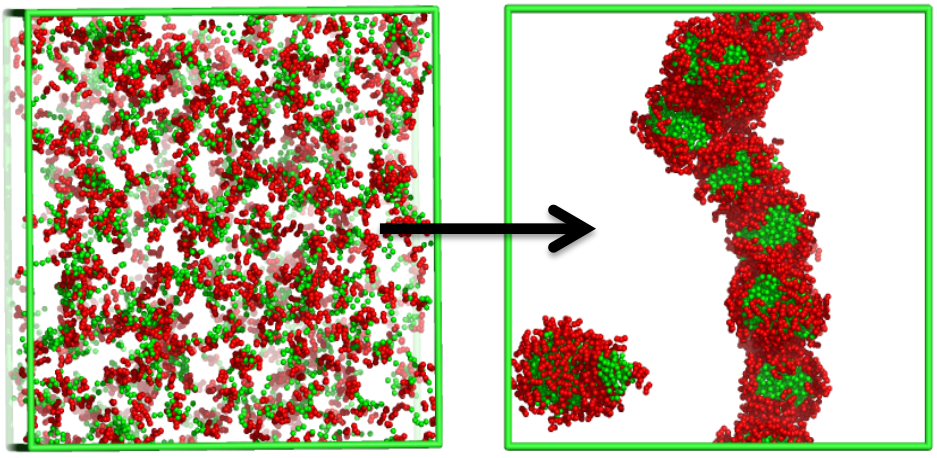

Figure S4: Formation of the SCM structure in a system containing 100mM DDM surfactants, with a total of 960 surfactants in the simulation box.

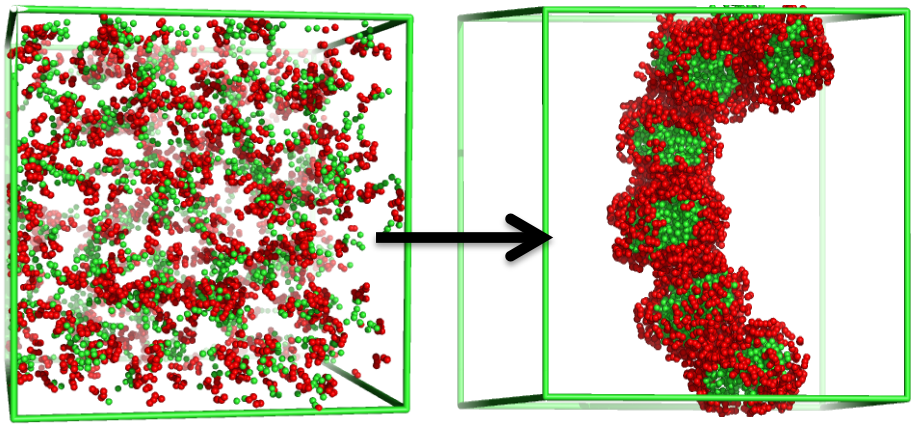

Figure S5: Formation of the SCM structure in a system containing 125mM DDM surfactants, with a total of 600 surfactants in the simulation box.