Supporting Information to

Experimental and Molecular Dynamics Characterization of Dense Microemulsion Systems: Morphology, Conductivity and SAXS

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Table S1 Compositions, unit cell dimensions, and morphological classifications of the system containing 20% water obtained with AA, Standard CG and Refined CG. n_w, n_s and n_o are the number of water, surfactant and oil molecules, respectively. For CG models, n_w, is calculated by associating each W bead with 4 water molecules and each Na^+-ion bead with 3 water molecules.

	Box Size / nm^3	n_w	n_s	n_o	t / ns	Continuity	Structure
AA	14x8x9	7320	800	1776	400	XYZ	BME
Standard CG	10x10x10	7424	800	1776	1000	XY	L
Refined CG	10x10x10	7424	800	1776	1000	XYZ	BME

Table S2 The compositions, unit cell dimensions, and morphological classifications of the systems corresponding to compositions a-m depicted in Figure 2, CG standard was used. (See also Table S1.)

Water %	Box Size / nm^3	n_w	n_s	n_o	Continuity	Structure
10	10x12x10	3296	800	1776	YZ	L
15[a]	11x11x11	5216	800	1776	YZ	L
20[a]	11x11x11	7424	800	1776	YZ	L
25	13x8x13	9888	800	1776	YZ	L
b30	12x7x15	12704	800	1776	YZ	L
40	10x12x14	19744	800	1776	-	W
50	8x12x21	29632	800	1776	Y	HC
60[a, b]	27x27x27	355584	6400	14208	XYZ	IL-M

[a] Isotropic pressure coupling [b] Anisotropic pressure coupling

Table S3 The compositions, unit cell dimensions, and morphological classifications of the systems corresponding to compositions a-c-d-g depicted in Figure 2. AA simulations were carried out for at least 40 ns. (See also Table S1.)

Water %	Box Size / nm^3	n_w	n_s	n_o	Continuity	Structure
10	15x8x9	3296	800	1776	XYZ	BME
20	11x11x11	7424	800	1776	XYZ	BME
25	11x9x12	9888	800	1776	YZ	IC/L
40	10x10x16	19744	800	1776	-	FCC/IRM

Table S4 The compositions, unit cell dimensions, of the systems corresponding to compositions a-m depicted in Figure 2, when system was enlarged 8 times compared to simulations described in Table 1. Simulation time is 200 ns. (See also Table S1.)

Water %	Box Size / nm^3	n_w	n_s	n_o
10	29x16x17	26368	6400	14208
15[a]	20x20x20	41728	6400	14208
20[a]	21x21x20	59392	6400	14208
25	22x18x23	79104	6400	14208
30	22x20x23	101632	6400	14208
35	17x19x33	127744	6400	14208
40	20x20x30	157952	6400	14208
45	24x24x23	194048	6400	14208
50	25x22x25	237056	6400	14208
55	28x17x33	289792	6400	14208
60[a, b]	52x52x52	2844672	51200	113664

Table S5 The compositions, unit cell dimensions, of the systems corresponding to compositions g-i depicted in Figure 2, when system was enlarged 64 times compared to simulations described in Table 1. (See also Table S1.)

Water %	Box Size / nm^3	n_w	n_s	n_o
40	40x40x59	157952	51200	113664
50	52x43x50	237056	51200	113664

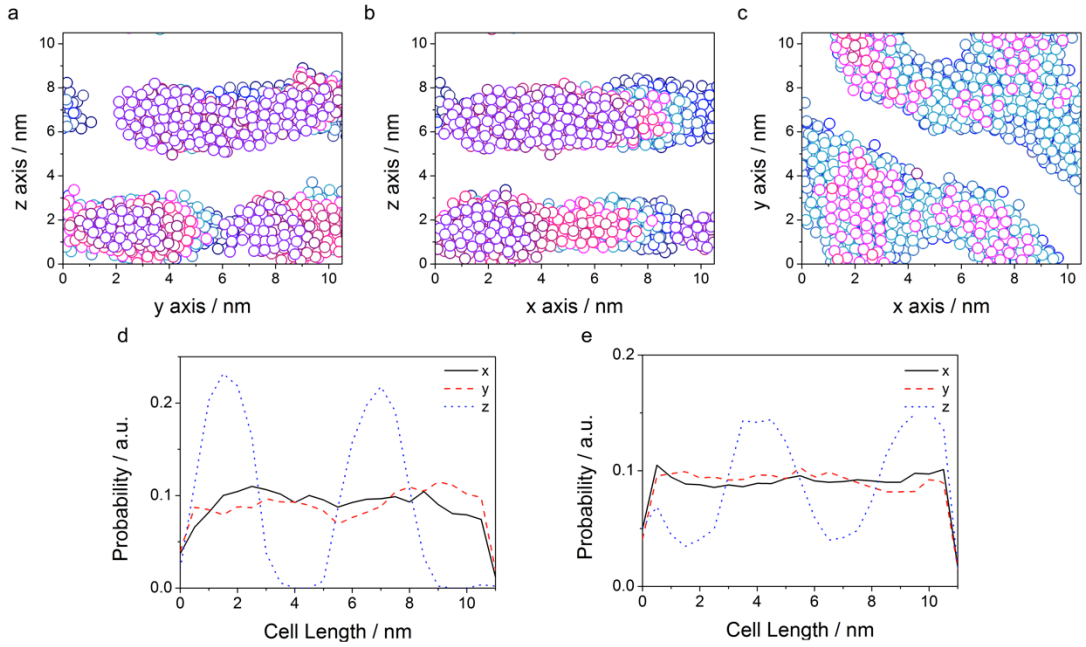

Figure S1. Slices of last frame of the 20% CG Standard simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na^+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na^+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane.

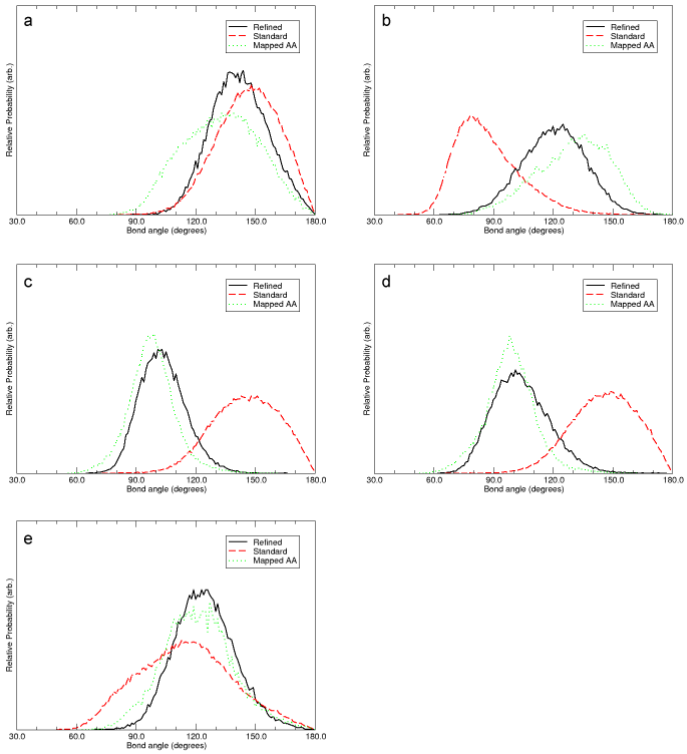

Figure S2 Bond Angle distributions for CG Standard, CG Refined and Mapped AA. Bonds refers to beads depicted in Figure 1. AOT: a) 1-2-4, b) 3-2-4, c) 3-6-7, d) 3-4-5, e) 2-3-6.

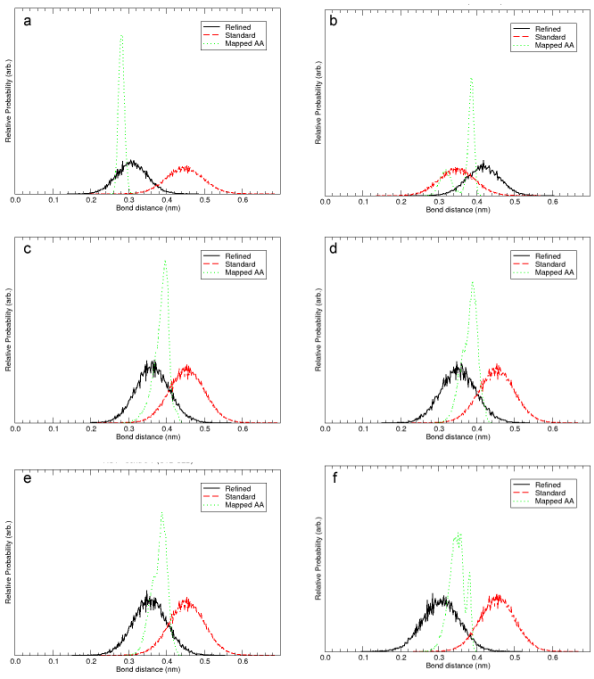

Figure S3 Bond length distributions for CG Standard, CG Refined and Mapped AA. Bonds refers to beads depicted in Figure 1. AOT: a) 1-2, b) 2-3, c) 3-6, d) 4-5, e) 6-7, n-heptane: f) 1-2

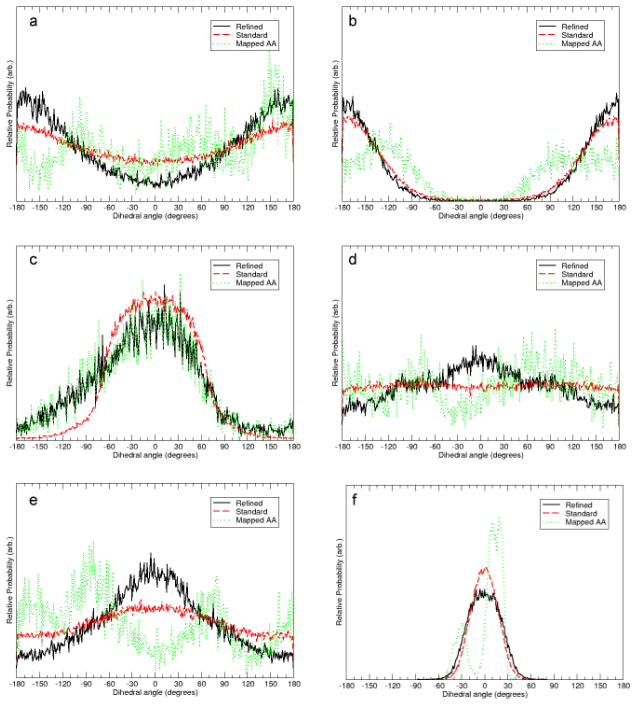

Figure S4 Dihedral Angle Distributions for CG Standard, CG Refined and Mapped AA. Bonds refers to beads depicted in Figure 1. AOT: a) 1-2-4-5, b) 1-2-3-6, c) 4-2-3-6, d) 2-3-6-7, e) 3-2-4-5, f) 2-1-3-4.

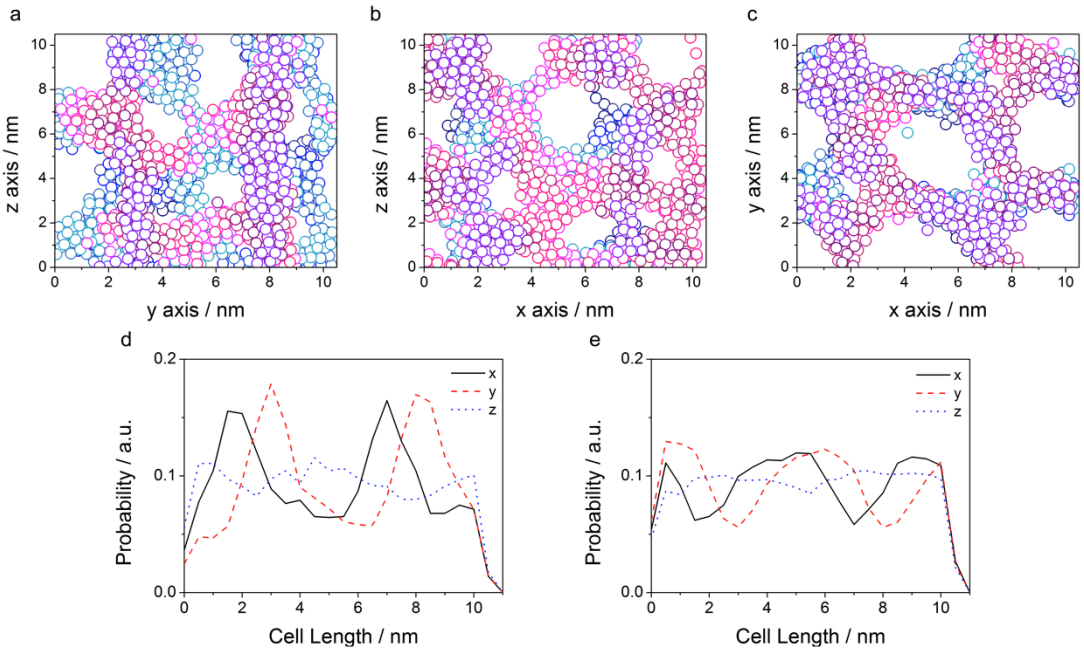

Figure S5. Slices of last frame of the 20% AA Mapped simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na^+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na^+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

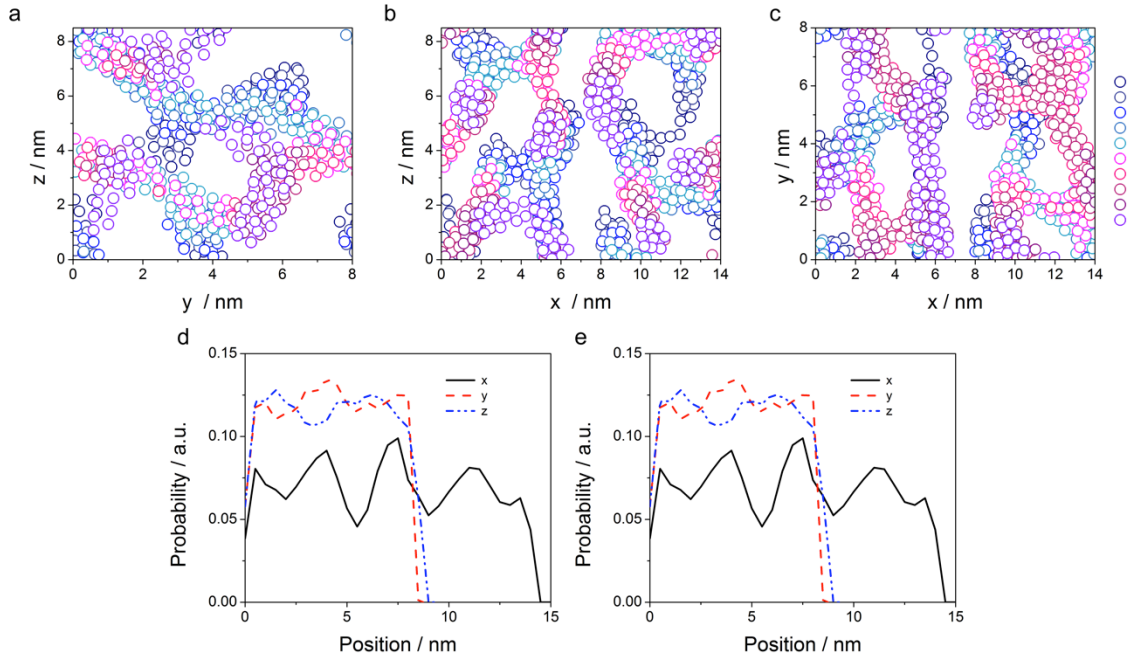

Figure S6. Slices of last frame of the 10% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na^+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na^+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

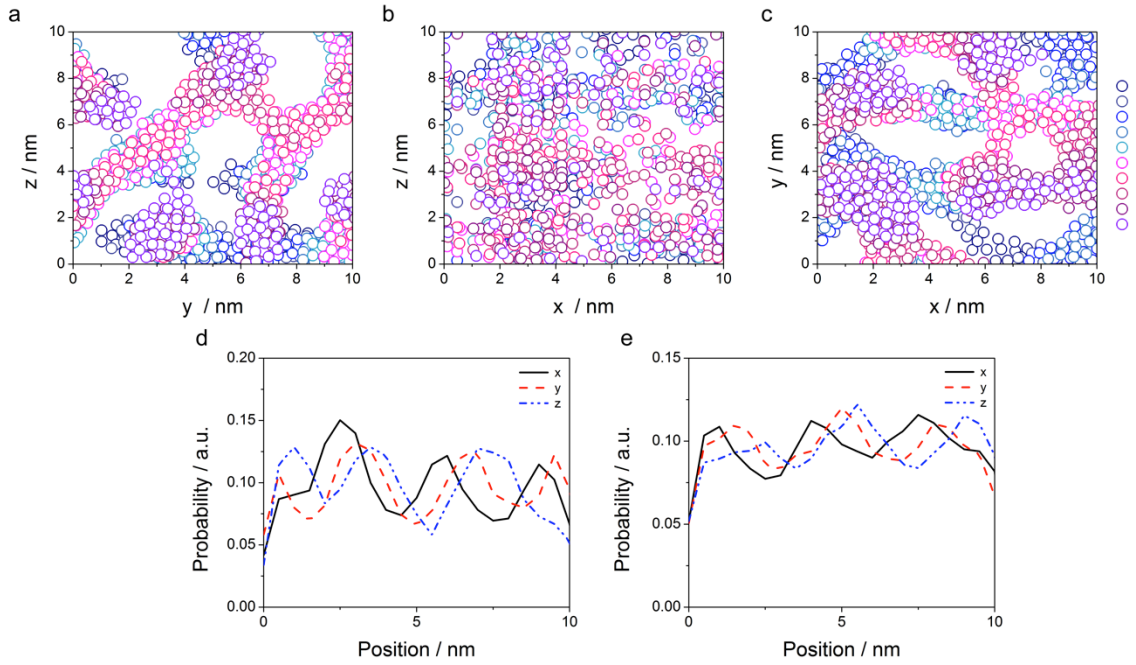

Figure S7. Slices of last frame of the 15% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na^+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na^+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

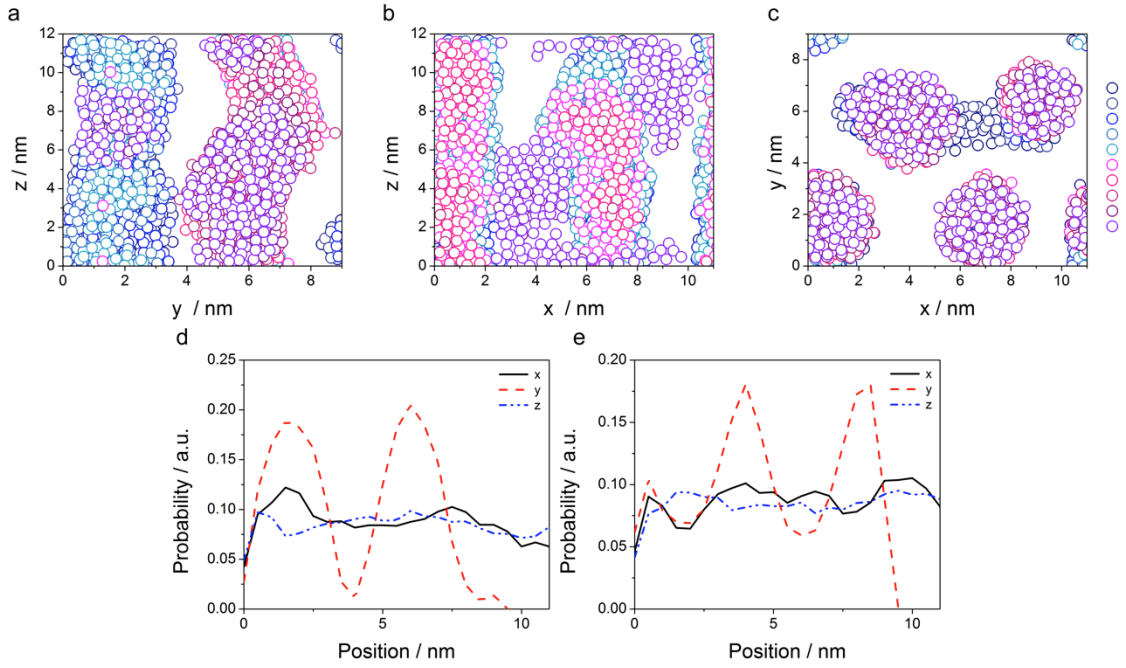

Figure S8. Slices of last frame of the 25% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na^+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na^+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane.

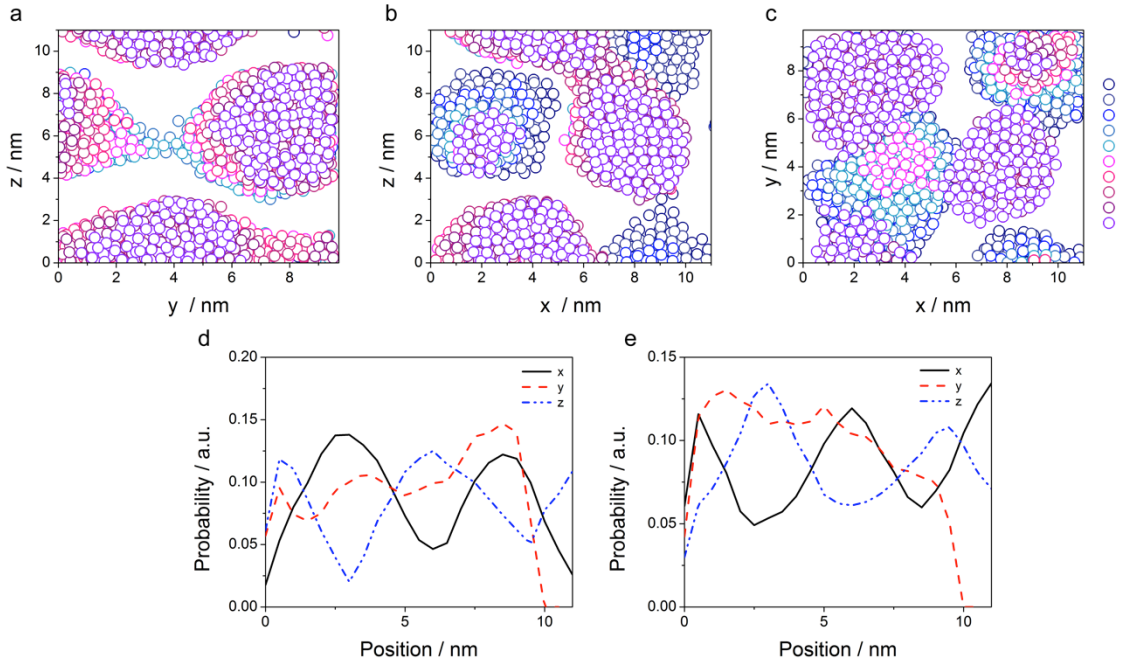

Figure S9. Slices of last frame of the 30% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na^+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na^+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

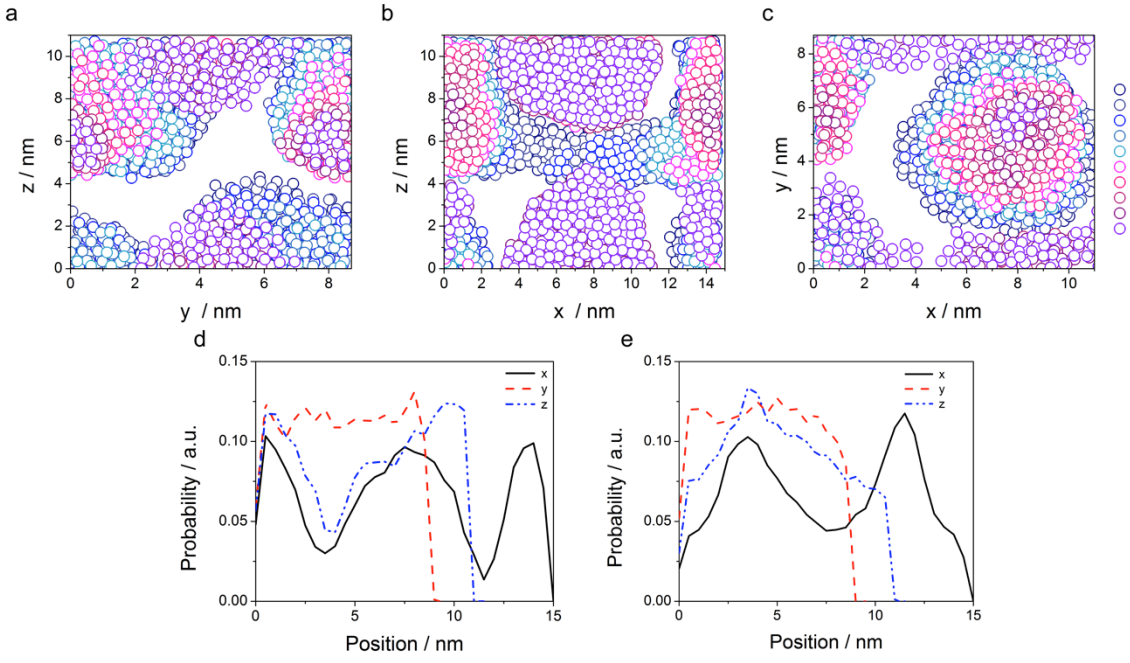

Figure S10. Slices of last frame of the35 % CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

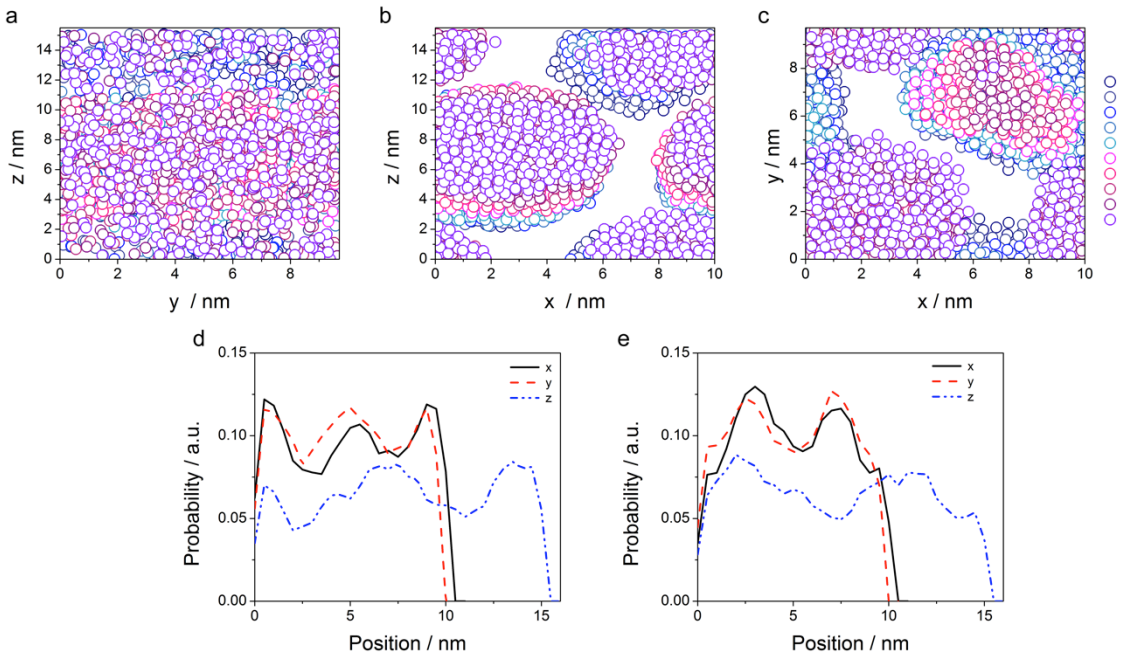

Figure S11. Slices of last frame of the 40% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

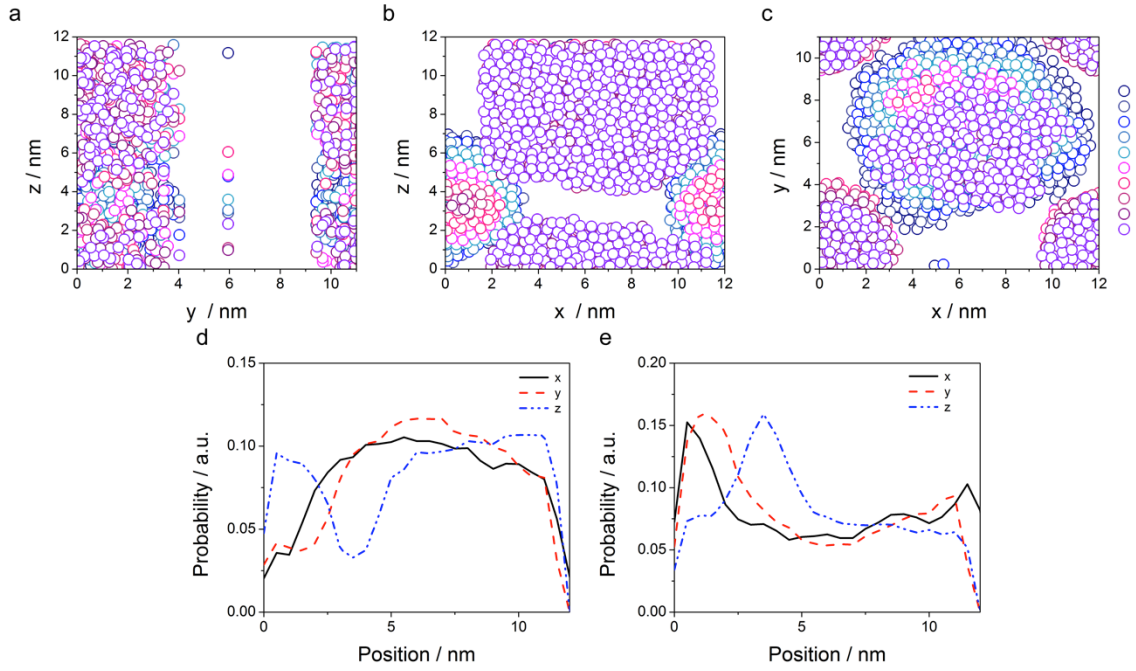

Figure S12. Slices of last frame of the 45% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

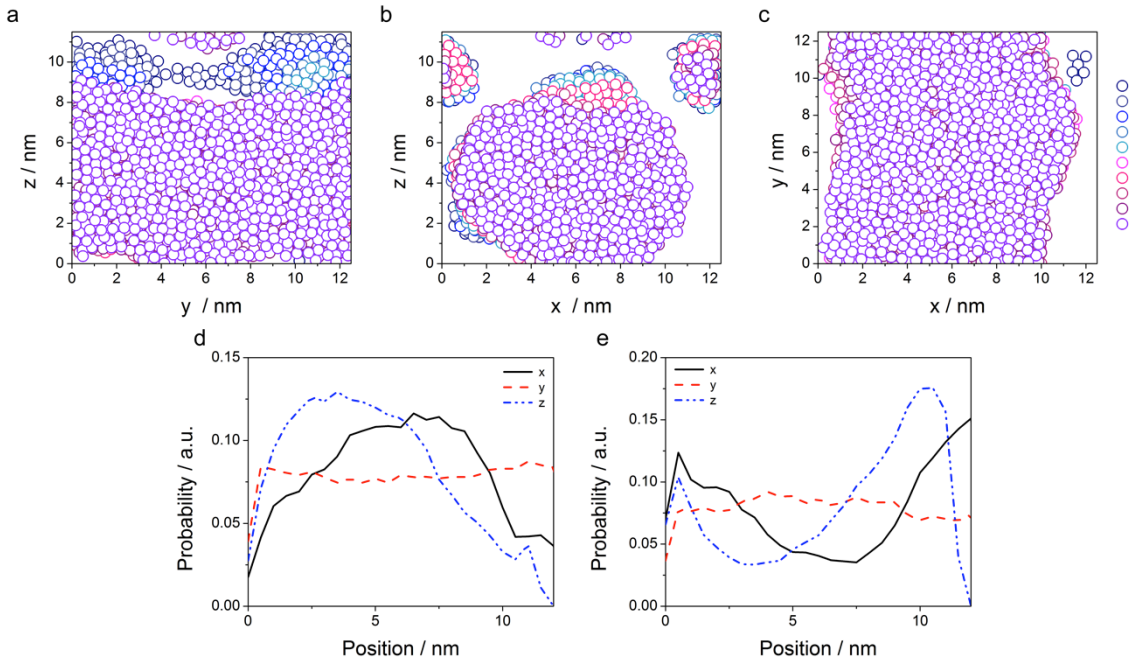

Figure S13. Slices of last frame of the 50% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

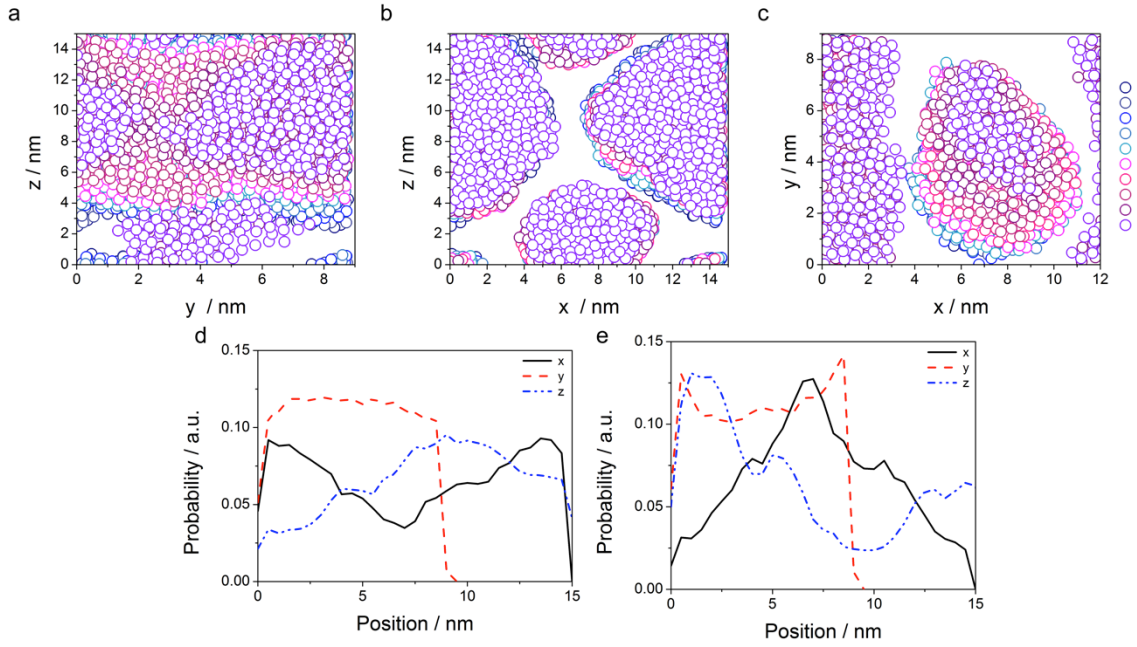

Figure S14. Slices of last frame of the 55% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

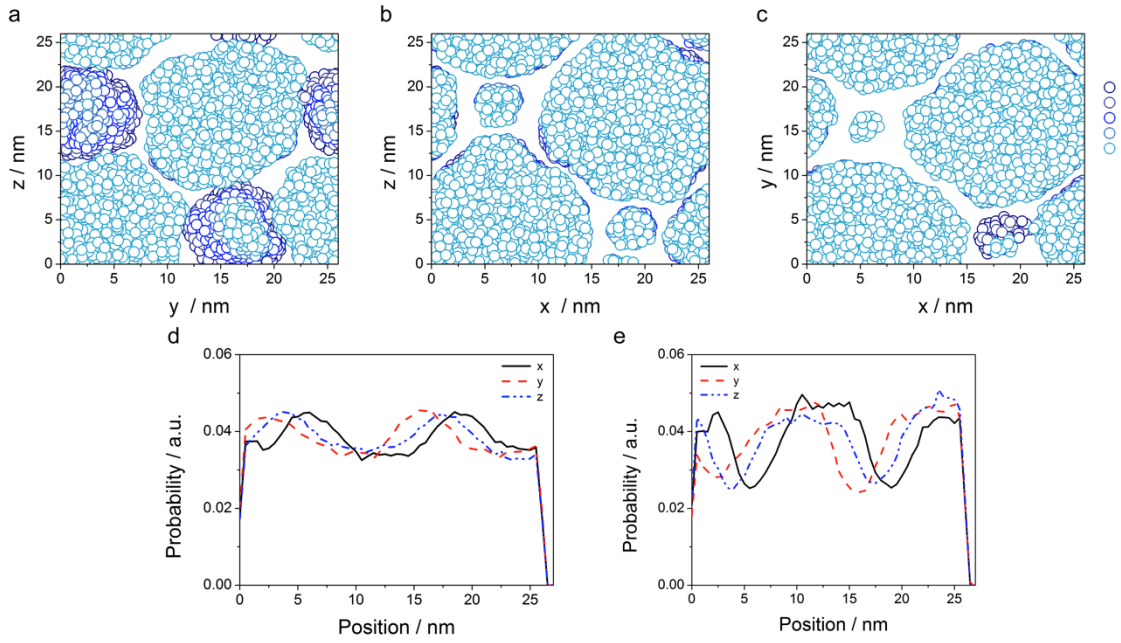

Figure S15. Slices of last frame of the 60% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

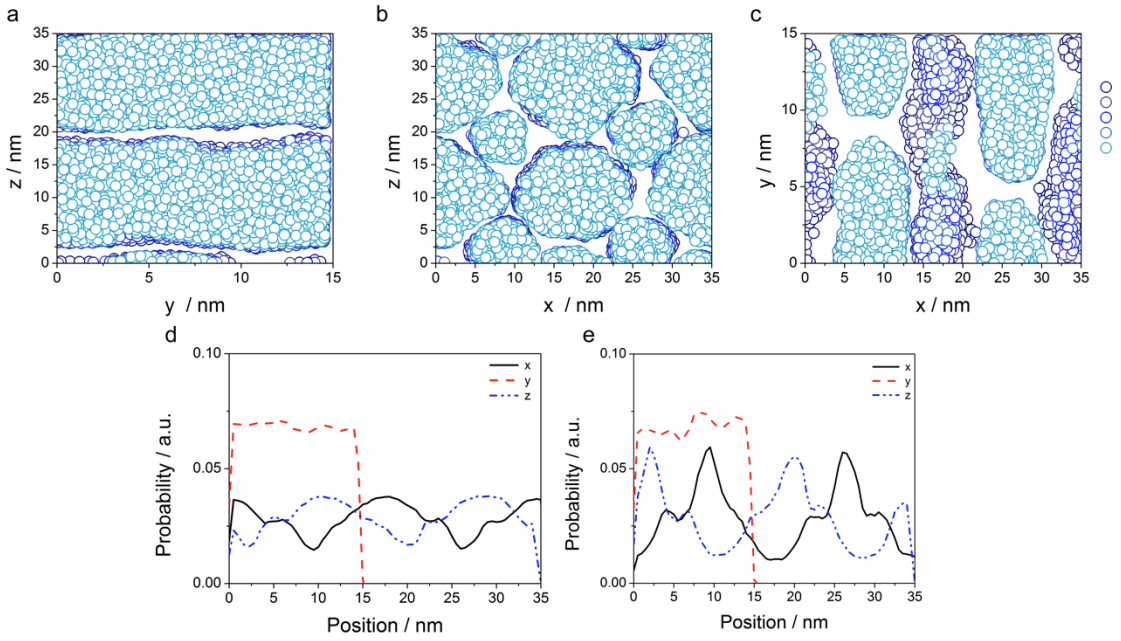

Figure S16. Slices of last frame of the 60*% CG simulation of planes perpendicular to a) x axis, b) y axis, c) z axis. Just hydrophilic beads are represented, water, Na+ and AOT head-group. Distribution of coordinates for d) hydrophilic beads, water, Na+ and AOT head group, e) hydrophobic beads, AOT apolar tail and n-heptane

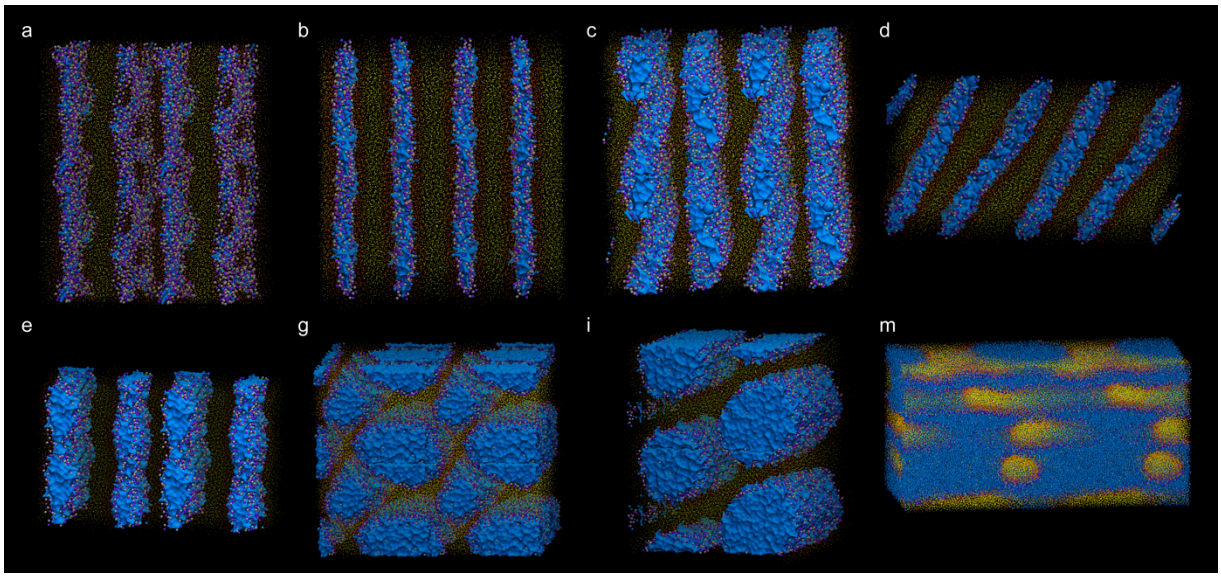

Figure S17. Snapshot at the end of 1μs simulations for the system water /Na-AOT/n-heptane using the Standard CG model. Water – Light blue, n-Heptane – yellow, Na^+ - blue, AOT head group – purple, AOT tail – orange. Compositions corresponding to points depicted in Figure 2. Details of the simulation are reported in Table S2.

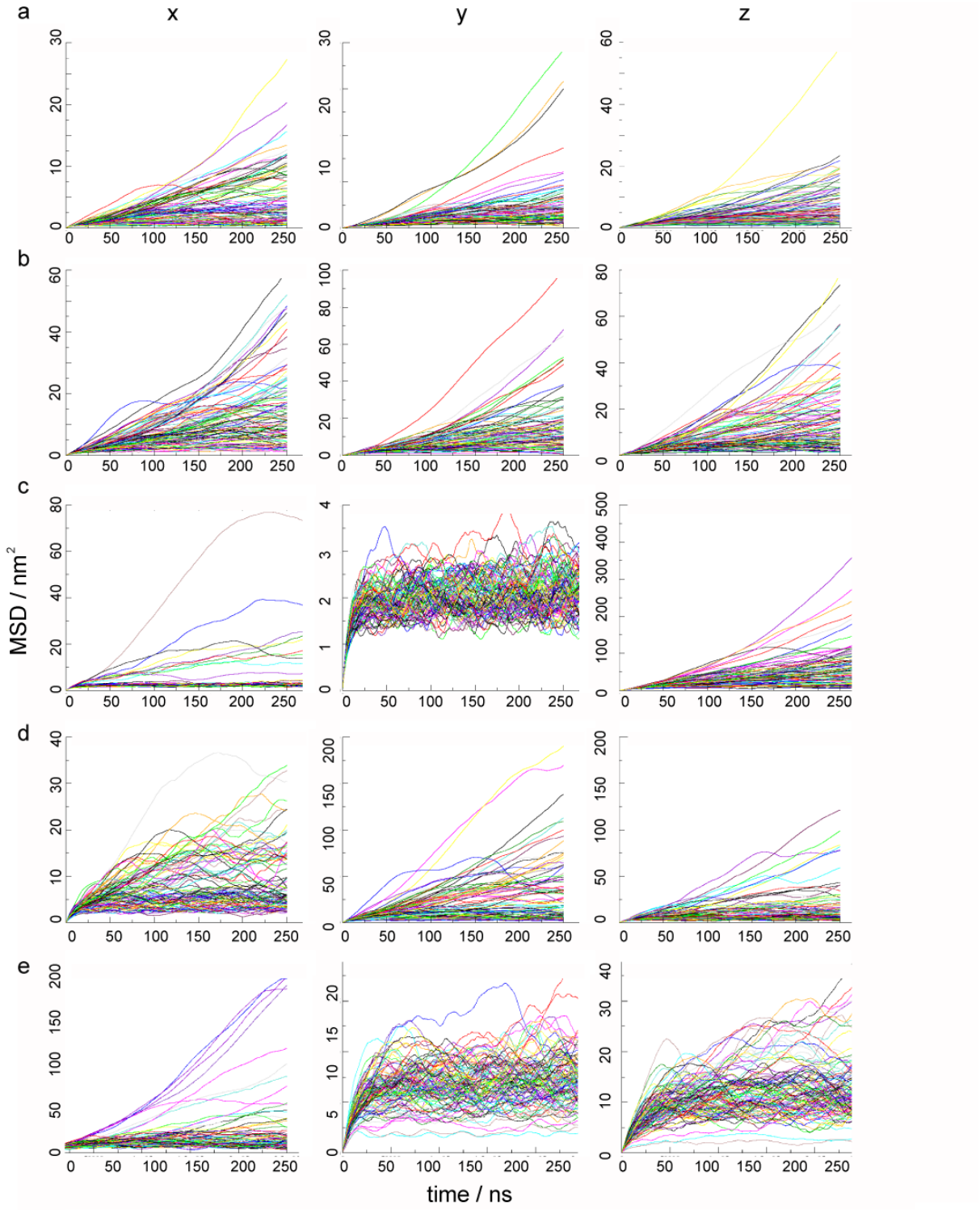

Figure S18. MSD curves for 100 Na^+ beads for the system containing a) 10%, b) 15%, c) 25%, d) 30%, e) 35% water.

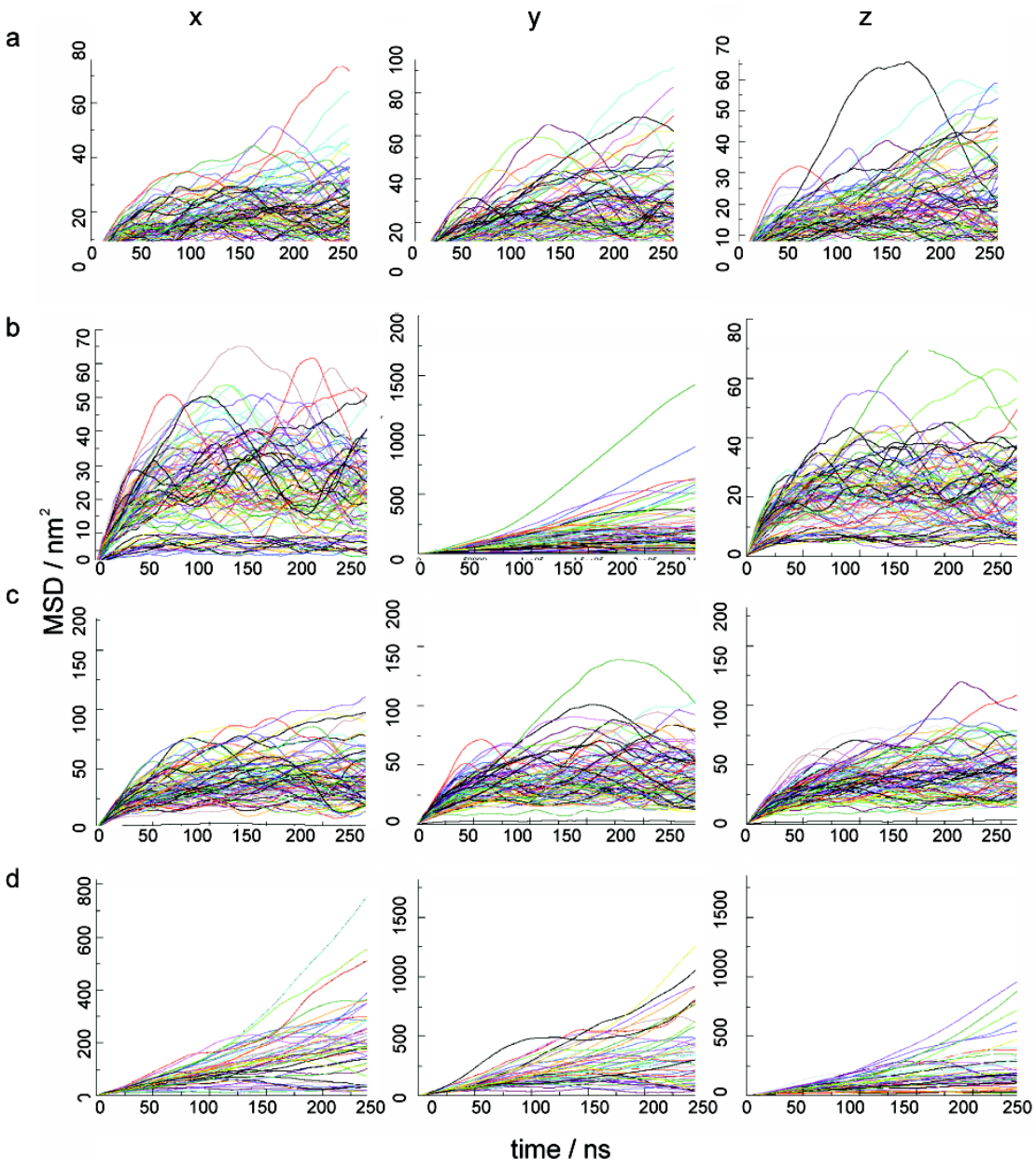

Figure S19. MSD curves for 100 Na^+ beads for the system containing a) 45% b) 55%, c) 60%, simulation m, d) 60% , simulation m*, water.

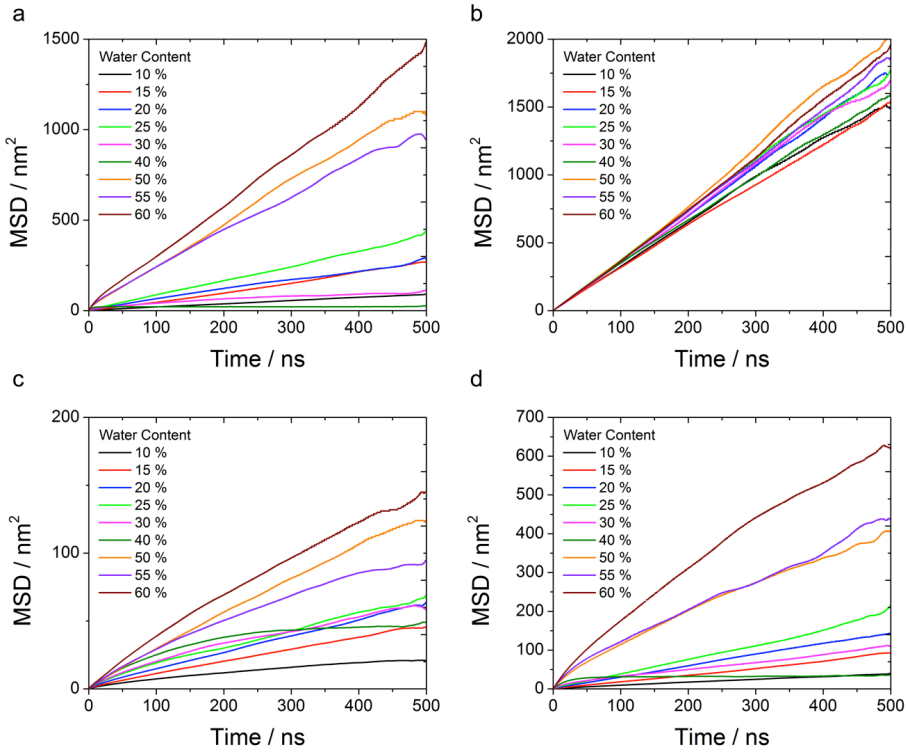

Figure S20. MSD calculated for a) AOT^-, b) n-heptane, c) Na^+ and d) water.

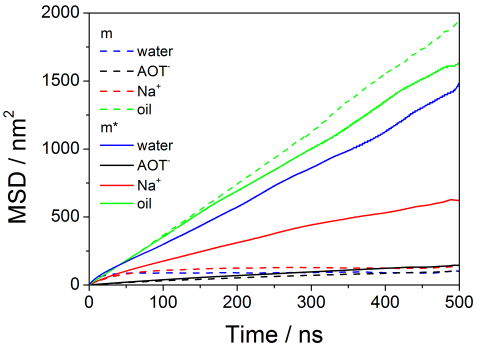

Figure S21. MSD curves for all the species for the simulation containing 60% water, with different starting point. From a random distribution, system m, and from adding water to 55% final snapshot of simulation.

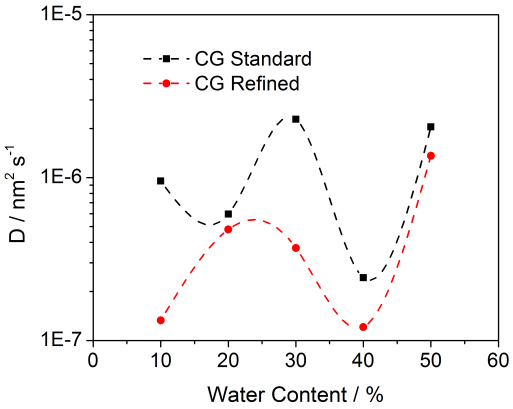

Figure S22. Diffusion coefficients calculated with CG refined and standard simulations.

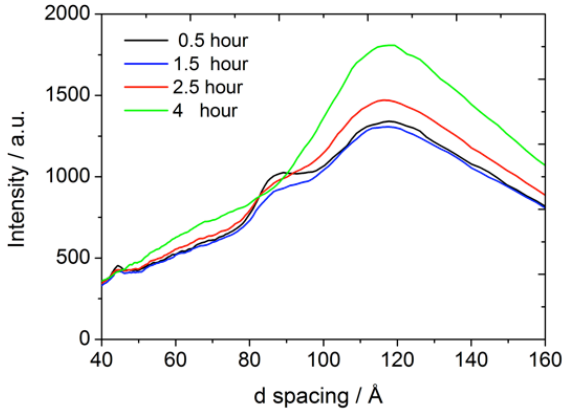

Figure S23. SAXS of 60% water content microemulsion changing with time

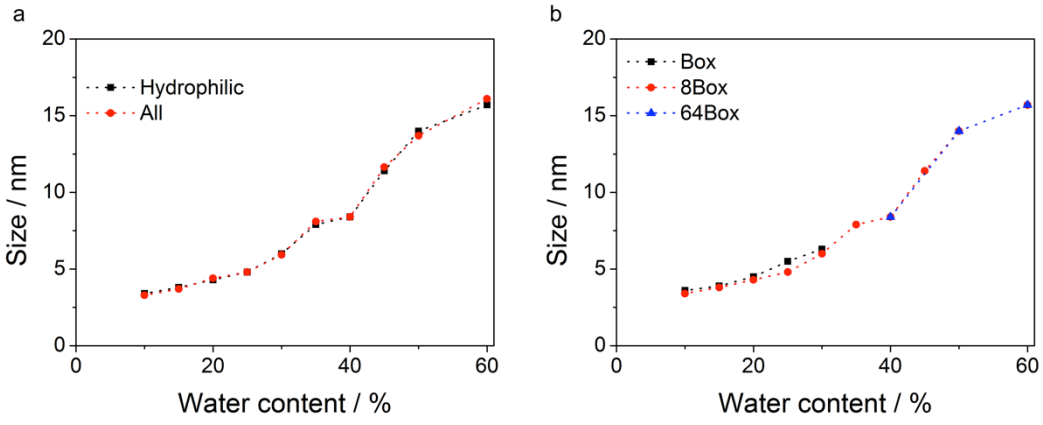

Figure S24. a) Peak position calculated from the scattering function with the simplified and exact approach. B) Peak position calculated from the scattering function for different box sizes.

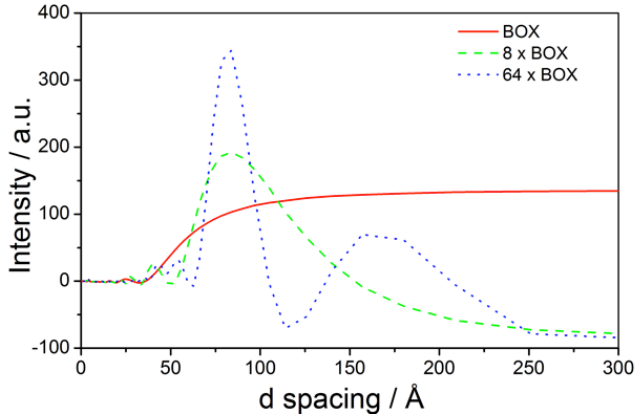

Figure S25. Scattering function for end-configuration of CG simulations of different box size (single, 8 times and 64 times) for system g, containing 40% water.