Supporting Information file for

Counterion adsorption and electrostatic potential in sodium and choline dodecyl sulfate micelles - a molecular dynamics simulation study

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Table S1 – Partial charges and Lennard-Jones parameters for dodecyl sulfate.

Atom	q (e)	ε (kJ/mol)	σ (nm)
S	1.284	1.046000	0.355
O (bonded only to S)	-0.654	0.711280	0.296
O (C-O-S)	-0.459	0.711280	0.300
C (from CH_2 bonded to head)	0.017	0.276144	0.350
C (from other CH_2)	-0.120	0.276144	0.350
C (from terminal CH_3)	-0.180	0.276144	0.350
H	0.060	0.125520	0.250

Table S2 – Partial charges and Lennard-Jones parameters for choline.

Atom	q (e)	ε (kJ/mol)	σ (nm)
O	-0.683	0.711280	0.312
N	-0.008	0.711280	0.325
C (CH_3 bonded to N)	0.090	0.276144	0.350
C (CH_2 bonded to N)	0.150	0.276144	0.350
C (CH_2 bonded to O)	0.145	0.276144	0.350
H (bonded to C)	0.060	0.125520	0.250
H (bonded to O)	0.418	0.000000	0.000

Table S3 – Partial charges and Lennard-Jones parameters for sodium (Åqvist parameters).

Atom	q (e)	ε (kJ/mol)	σ (nm)
Na	1.000	0.011598	0.333045

Table S4 – Partial charges and Lennard-Jones parameters for water (SPC model).

Atom	q (e)	ε (kJ/mol)	σ (nm)
O	-0.820	0.650194	0.316557
H	0.410	0.000000	0.000000

Table S5 – Parameters for Ryckaert-Bellemans function used to describe dihedral angles of the choline cation that were reparametrized from the original OPLS-AA force field (values in kJ/mol).

Dihedral	C_0	C_1	C_2	C_3	C_4	C_5
N-C-C-O	223.27236776	-2.43302684	2.02582148	0.76256715	0.61590863	0.38680925
C-C-O-H	83.57190464	1.84400893	-3.76911786	-4.22542943	6.64022733	3.14606529

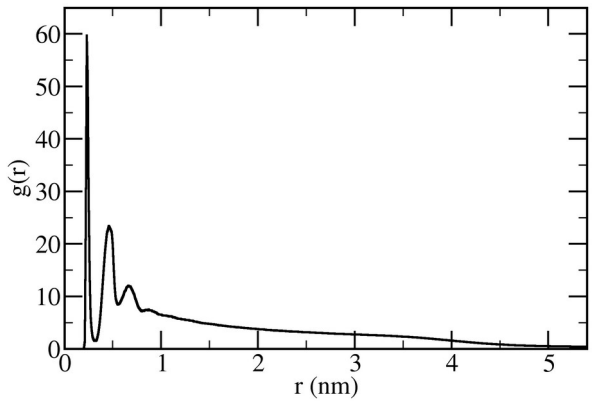

Figure S1 – Radial distribution function between oxygen atoms of the surfactant and sodium counterions in SDS simulation.

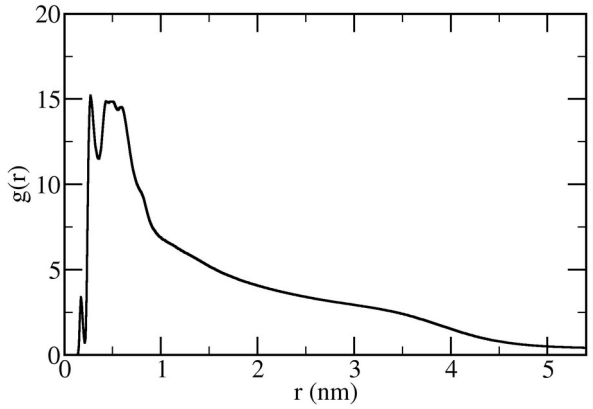

Figure S2 – Radial distribution function between oxygen atoms of the surfactant and hydrogen atoms of the choline cation in ChDS simulation. The first small and sharp peak occurs at 0.28 nm and corresponds to the hydrogen of choline OH group making a hydrogen bond with the surfactant. The criteria for the aggregation, however, was based on the second minimum at *ca.* 0.4 nm which also include hydrogen groups of CH_3 and CH_2 groups in contact with the surfactant head.

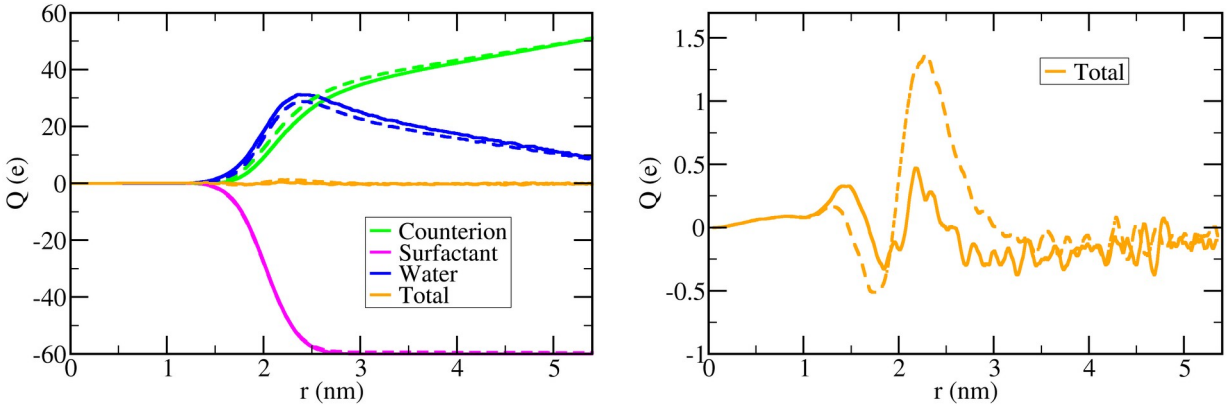

Figure S3 – Time-averaged value of the accumulated charge at each distance *r* from the micelle center of mass with results from SDS system represented as solid lines and for ChDS system as dashed lines. Left: Components from each species, Right: Zoom at the the total accumulated charge. A running average was performed at every 10-points of the total accumulated charge curves for better visualization.