Supporting Information for

A molecular dynamics study on two promising green surfactant micelles of Choline Dodecyl Sulfate and laurate

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Detailed force field parameters for all the studied systems are shown as follows:

Table S1 to S5 show the bonded and nonbonded parameters, and Fig. S1 show Partial atomic charges of dodecyl sulfate (DS^-), laurate (C12) and choline (Ch^+).

Table S1 Bond-Stretching Parameters

	Force constant K_b (10^6kJmol^{-1}nm^{-4})	Ideal bond length b_0(nm)
-C-C- (DS^-,C12)	7.15	0.153
-C-H	12.1	0.110
-C-O-	6.10	0.144
-S-O	8.37	0.150
-S-O-	3.38	0.164
-C-N-	3.73	0.151
-C-C-	5.43	0.152
-C-O	1.31	0.127
-O-H	7.96	0.097

Table S2 Bond-Angle Bending Parameters

	Force constant K_θ (kJmol^{-1})	Ideal bond angle ϑ_0 (degree)
C-C-H	842	109.0
C-C-C	530	111.0
H-C-H	987	107.0
C-O-S	50	115.0
O-C-C	320	109.5
O-S-O	503	106.8
N-C-H	443	108.5
C-N-C	1680	109.0
N-C-C	610	115.0
O-C-O	770	126.0
C-O-H	450	109.5

Table S3 Dihedral-angle parameters

	Force constant K_ζ (kJmol^{-1}degree^{-2})	Ideal dihedral angle ζ_0 (degree)
C-C-C-H	3.77	0.0
C-C-O-S	1.26	0.0
C-O-S-O	1.05	0.0
C-C-C-C	3.77	0.0
C-C-N-C	1.05	0.0
C-C-O-H	1.26	0.0
O-C-C-N	5.92	0.0
C-N-C-H	1.05	0.0

Table S4 Improper (harmonic) dihedral-angle parameters

	Force constant K_ζ (kJmol^{-1}degree^{-2})	Ideal improper dihedral angle ζ_0(degree)
C-C-O-O	167.36	0.0

Table S5 Normal van der Waals Parameters

Atom type	[C6(I,I)]$^{1/2}$ [(kJmol^{-1}nm^6)$^{1/2}$]	[C12(I,I)]$^{1/2}$ [10^{-3}(kJmol^{-1}nm^{12})$^{1/2}$]
OM	0.04756	0.8611
HC	0.009200	0.1230
SDmso	0.10277	4.6366
C	0.04838	2.222

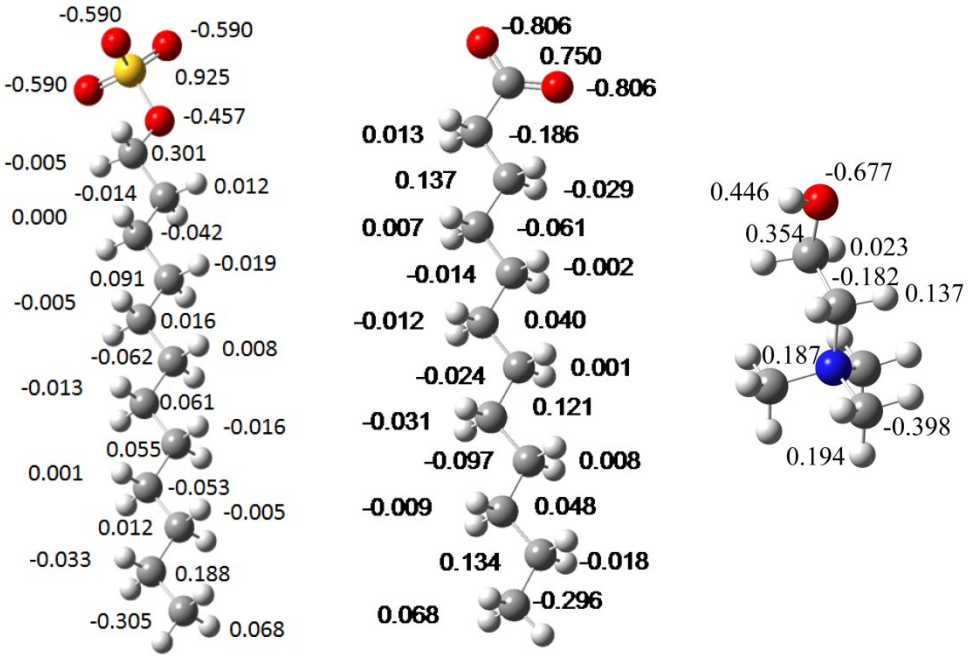

Figure S1 Partial charges of different groups in this study

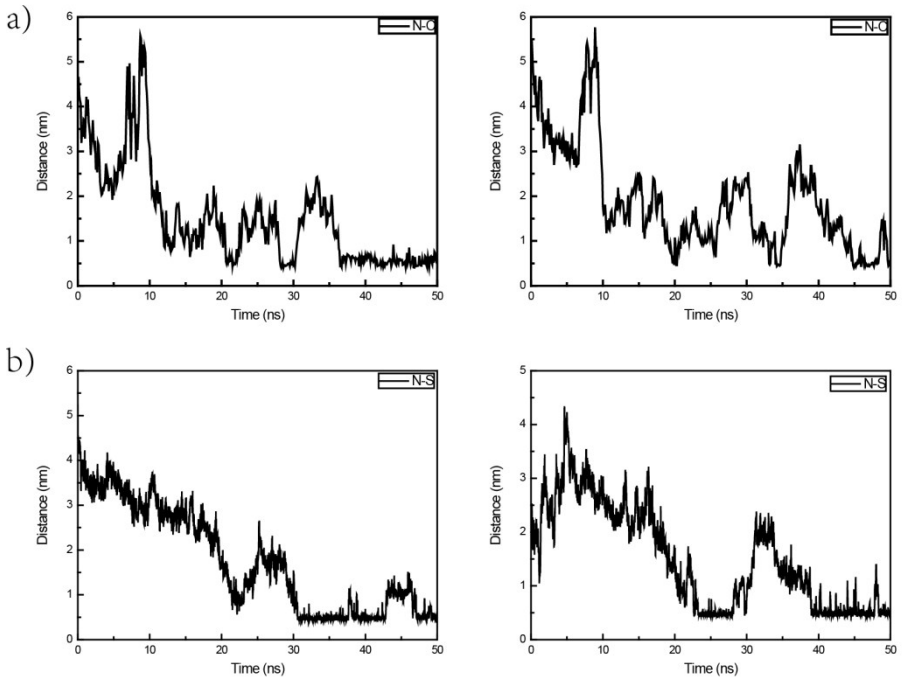

Fig. S2 The representative evolution of the distance between the head group and choline during simulations for a) ChC12 and b) ChDS. Since not all choline ions are absorbed, the result obtained here is the distance between one Ch^+ ion and one surfactant molecule. For each system, two Ch^+ molecules, absorbed in the last frame, are randomly selected via the VDW visual. And corresponding head groups are defined based on the selected Ch^+ molecules individually. The label N-S in the top two figures means the distance between N of Ch^+ ion and S of DS^-, and label N-C in the below means the distance between N of Ch^+ ion and C of C12.

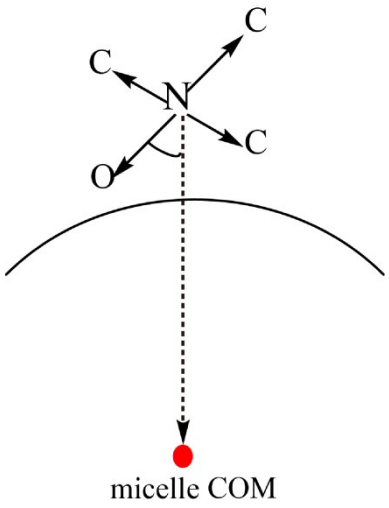

Fig. S3 Representative diagram of angle between the vectors N-micelle center of mass (COM) and N-terminal groups (including methyl groups and hydroxyl (OH) group). In the diagram, the labeled angle between N- micelle COM and N-OH is used as an example.

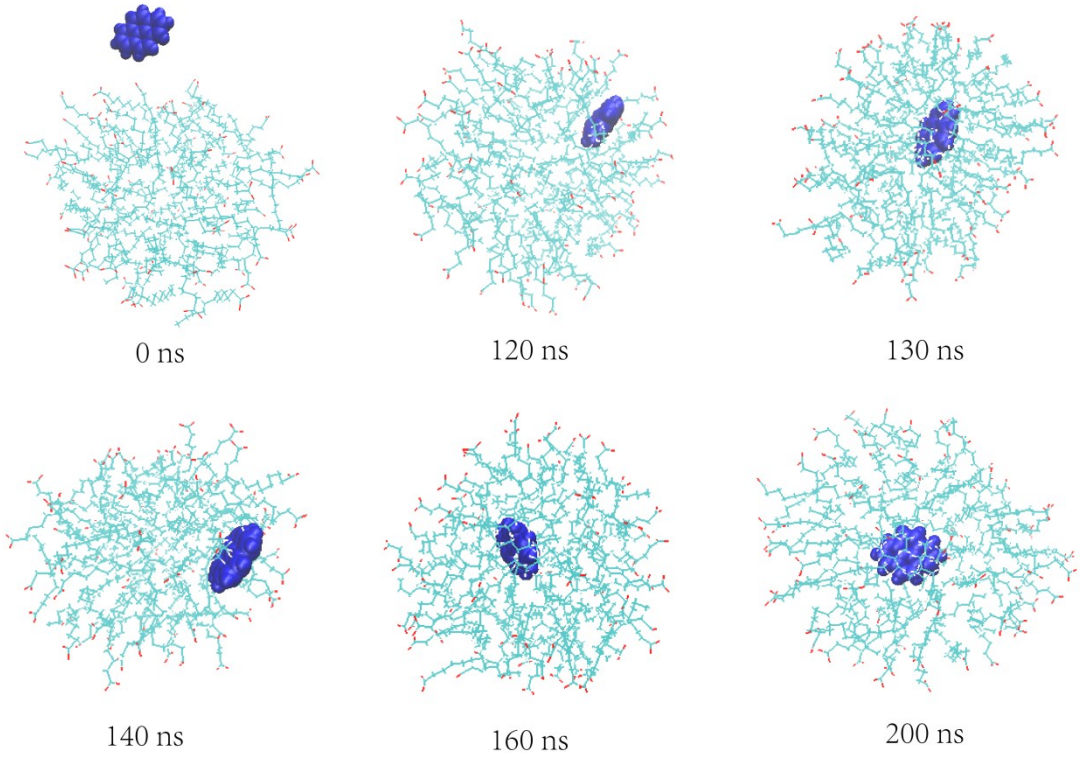

Fig. S4 Representative snapshots for Choline laurate with pyrene (ChCPy) system at specific time, especially the time when the distance between pyrene center and micelle center shows large fluctuation. It is noted that ChCPy system is used as an example here. The initial and final locations are also shown as contrast. For clear representation, only laurate (C12) and pyrene (Py) molecules are included. Deep blue: Py molecule; Red: O atom; Turquoise: C atom of C12.

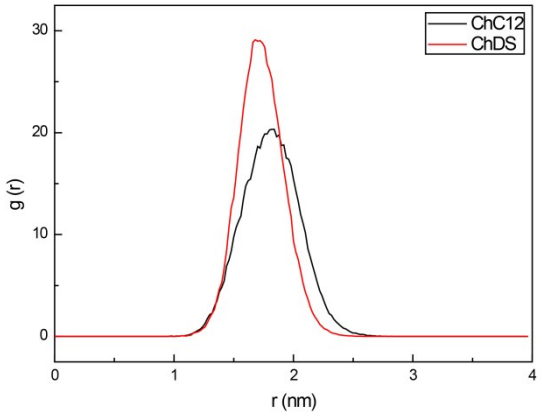

Fig. S5 Radical distribution functions (g(r)) of head groups for the two micelles. The C atom of head group for ChC12 and S atom for ChDS are chosen to obtain the plots.