Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Tetraalkylammonium Interactions with Dodecyl Sulfate Micelles: a Molecular Dynamics Study

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Table S1. Bond-Stretching Parameters.

	Force constant K_b (10^6kJmol^{-1}nm^{-4})	Ideal bond length b_0(nm)
-C-C- (DS^-)	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-H (TMA^+)	12.3	0.109
-C-N- (TMA^+)	5.73	0.148
-C-N-	2.46	0.153
-C-C-	5.43	0.152

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	1110	112.0
C-N-C	1440	107.0
N-C-C	610	115.0

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-C-N	1.00	180.0
C-C-N-C	1.05	0.0

Table S4. Binding energy of the studied system.

	Binding energy (kJ/mol)			
	TMADS	TEADS	TPADS	TBADS
Binding pattern I	-437.70	-407.61	-405.47	-395.48
Binding pattern II	-510.33	-487.42	-472.92	-473.19
Binding pattern III	-367.53	-362.17	-355.43	-358.43
Binding pattern IV	-423.88	-405.25	-389.89	-368.97

Semiempirical method PM6 with the corrections called D3H4X was used for geometry optimization and binding energy calculation. PM6-D3H4X approach, which can give an accurate description of dispersion, hydrogen bonding and also halogen bonding has been tested.[1] All calculations were performed using the MOPAC 2012 program.[2]

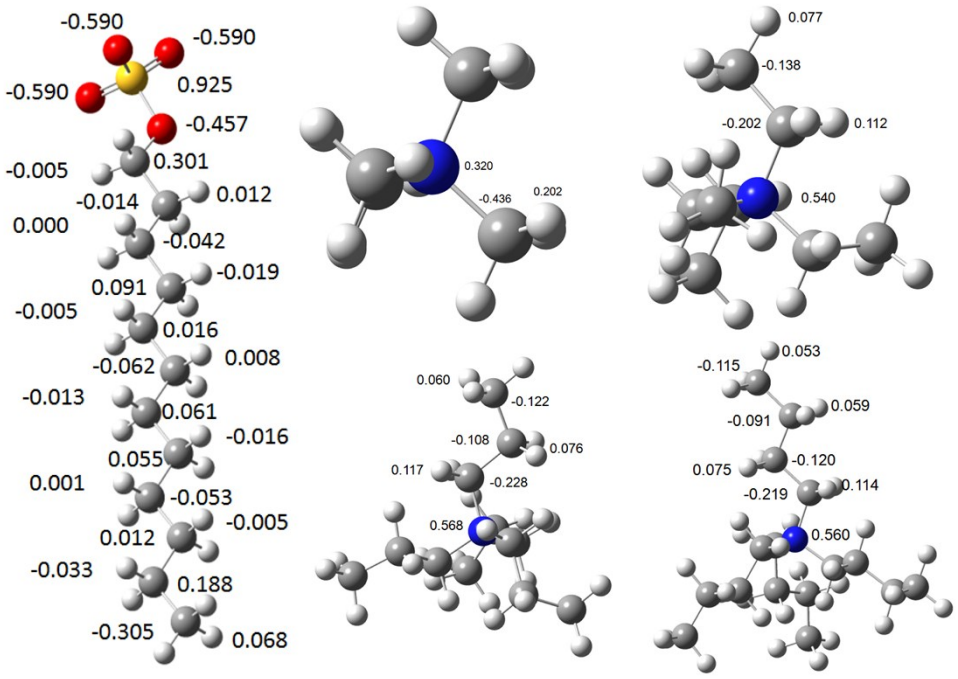

Fig. S1. Partial charges of different groups in this study

It should be noted that the partial charge of N atom of T tetramethyl-, tetraethyl-, tetrapropyl- and tetrabutylammonium (TMA^+, TEA^+, TPA^+, and TBA^+, respectively) ions is positive. In preceding paper, the charge of N atom of CTAB is zero[3] or -0.56.[4] The partial charges of N are all positive in our studied groups. The partial charges of this paper are all obtained with Automated Force Field Topology Builder (ATB) with a systemic way as described in the paper.[5-6] Initial charges were estimated using the ESP method (at B3LYP/6-31G* level) of Merz-Kollman.[7] And then then further optimized by ATB. In order to check the rationality of the partial charge, we calculated the partial charges with ESP method of Merz-Singh-Kollman scheme,[7-8] CHelp scheme,[9] and CHelpG scheme[10] at B3LYP/6-31G* level[11-12] with Gaussian 09 program.[13] The results show positive partial charge of N atom of tetraalkylammonium, except that TEA^+ and TPA^+ with Merz-Singh-Kollman scheme and TEA^+ with CHelpG scheme are slightly negative. However, the partial charge of N atom will be negative with Mulliken population analysis. Mulliken population analysis has its well-known shortcomings. For modelling purposes, especially force field charges, ESP charges are the logical choice.[14] Therefore, we believe that the positive partial charge of N atom is reasonable.

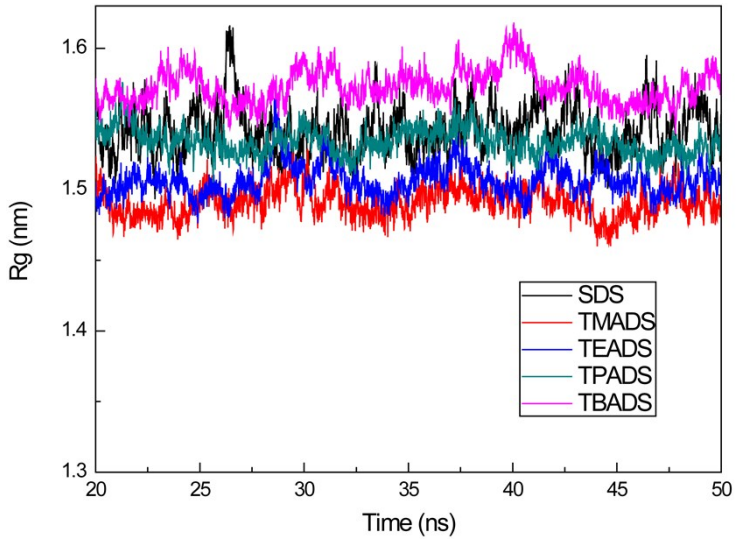

Fig. S2. Radius of gyration of the studied system with time evolution

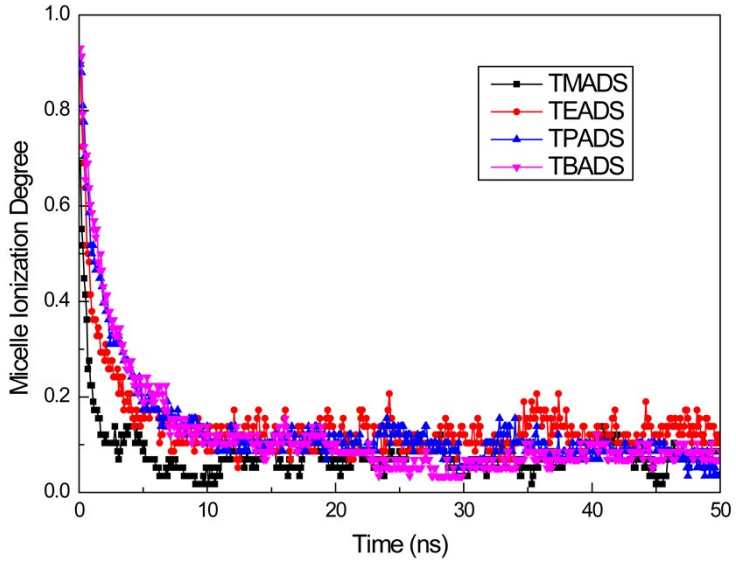

Fig. S3. Micelle ionization degree of TAADS with time evolution

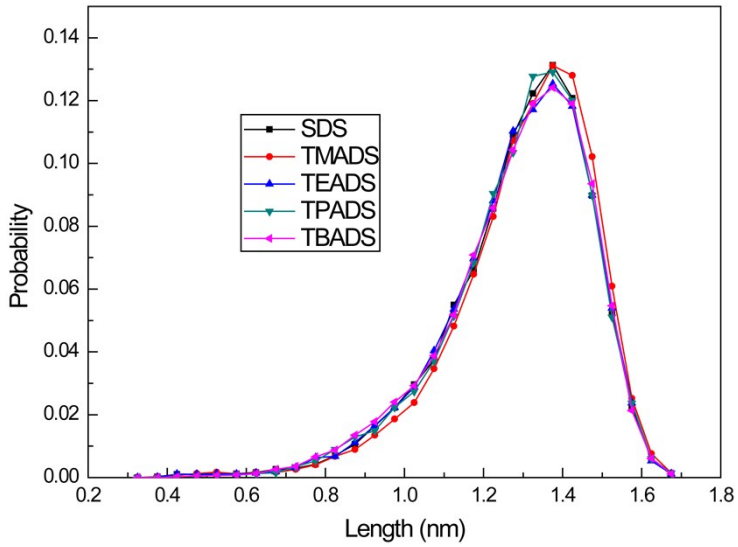

Fig. S4. The length distributions of the individual methyl groups of different systems with respect to the headgroup position.

Notes and references

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