Supplementary Material (ESI) for *Soft Matter*

Supplementary data for

Coarse-grained molecular modeling of nonionic surfactant self-assembly

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Table S1: Definition of coarse-grained segments

segments	all-atom description
W	$(H_2O)_3$
CT	$CH_3CH_2CH_2$-
CM	-$CH_2CH_2CH_2$-
CT2	CH_3CH_2-
EOT	CH_3-O-CH_2-
EO	-CH_2-O-CH_2-
OA	$HOCH_2$-

Bond stretching interaction is given by

$$U_{stretching} = k_b \left(r - r_0 \right)^2$$

Table S2: Bond stretching parameters

Pair		k_b [kcal/mol/Å^2]	r_0 [Å]
CT	CT	6.955	3.71
CM	CM	6.160	3.64
CM	CT	6.160	3.65
CT2	CM	9.000	3.13
OA	OA	63.000	2.16
EOT	EOT	5.500	3.33
EOT	EO	5.400	3.34
EO	EO	4.900	3.28
EO	OA	15.000	2.79
CT	EO	7.100	3.61
CM	EO	7.100	3.56
CT2	EO	10.000	3.07
CT	OA	6.955	3.05
CM	OA	7.500	3.01
CT2	OA	14.000	2.53

Angle bending interaction is given by

$$U_{\text{bending}} = k_\theta \left(\theta_{ijk} - \theta_0 \right)^2$$

Table S3: Angle bending parameters

Angle pair			k_θ [kcal/mol/rad^2]	θ_0 [degree]
CM	CM	CM	1.190	173.0
CM	CM	CT	1.190	175.0
CT2	CM	CM	1.600	172.0
CT2	CM	CT2	1.700	173.0
CT	CM	CT	1.093	175.5
EO	EO	EOT	3.500	135.0
EO	EO	EO	3.400	132.0
EOT	EO	EOT	3.500	134.0
OA	EO	OA	6.600	131.0
EO	EO	OA	3.000	131.0
CT	EO	EO	2.200	145.0
CT2	CM	EO	1.300	178.0

CM	EO	CM	1.800	171.0
CT2	EO	CT2	2.600	165.0
OA	EO	CT2	4.000	146.0
CM	CM	EO	1.500	172.0
CM	EO	EO	3.200	146.0
CT2	CM	OA	1.800	166.0

Nonbonded LJ interaction is given by

$$U_{\mathrm{LJ}}\left(r_{ij}\right)=\begin{cases}\dfrac{3\sqrt{3}}{2}\varepsilon_{ij}\left\{\left(\dfrac{\sigma_{ij}}{r_{ij}}\right)^{12}-\left(\dfrac{\sigma_{ij}}{r_{ij}}\right)^{4}\right\}\\ \dfrac{27}{4}\varepsilon_{ij}\left\{\left(\dfrac{\sigma_{ij}}{r_{ij}}\right)^{9}-\left(\dfrac{\sigma_{ij}}{r_{ij}}\right)^{6}\right\}\end{cases}$$

Table S4: Nonbonded interaction parameters

Nonbond pair		type	ε [kcal/mol]	σ [Å]
W	W	LJ12-4	0.8950	4.3710
CT	CT	LJ9-6	0.4690	4.5850
CT	CM	LJ9-6	0.4440	4.5455
CM	CM	LJ9-6	0.4200	4.5060
W	CT	LJ12-4	0.3600	4.4780
W	CM	LJ12-4	0.3400	4.4385
CT2	CT2	LJ9-6	0.3120	4.2210
CT2	CM	LJ9-6	0.3620	4.3635
W	CT2	LJ12-4	0.2900	4.2960
OA	OA	LJ9-6	0.4491	3.7130
EOT	EOT	LJ9-6	0.4370	4.2500
EO	EO	LJ9-6	0.4050	4.2500
EO	EOT	LJ9-6	0.4200	4.2500
EO	OA	LJ9-6	0.4400	3.8900
EO	CT	LJ9-6	0.4100	4.3400
EO	CM	LJ9-6	0.3770	4.2740
EO	CT2	LJ9-6	0.3700	4.1400
W	OA	LJ12-4	0.7000	3.9500
W	EO	LJ12-4	0.5700	4.3100

CT	OA	LJ9-6	0.4372	4.0330
CM	OA	LJ9-6	0.3650	3.9870
CT2	OA	LJ9-6	0.3800	3.8400