Supporting Information for:

Investigating anionic surfactant phase diagrams using Dissipative Particle Dynamics: development of a transferable model

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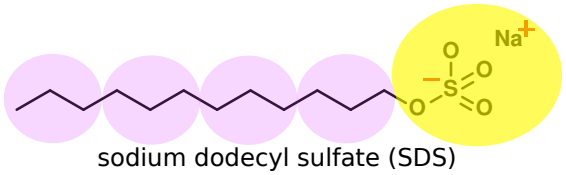
1 Coarse graining for SDS and LAS

In this supporting information we detail the coarse graining, bonding, and bond angles used for the surfactant molecules.



sodium dodecyl sulfate (SDS)

Bead number	type
1	H
2	T
3	T
4	T
5	T

(a) Beads

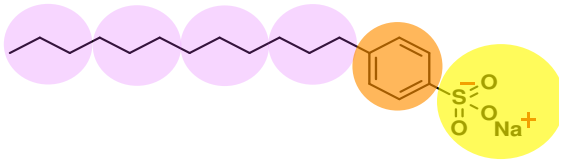
bead i	bead j
1	2
2	3
3	4
4	5

(b) Bonds

bead i	bead j	bead k
1	2	3
2	3	4
3	4	5

(c) Angles

Table S.1: SDS



sodium dodecylbenzene-1-sulfonate (DBS1)

Bead number	type
1	H
2	B
3	T
4	T
5	T
6	T

(a) Beads

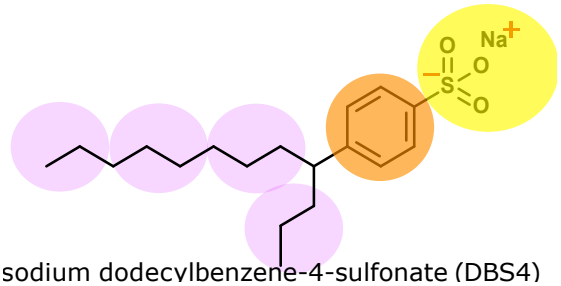
bead i	bead j
1	2
2	3
3	4
4	5
5	6

(b) Bonds

bead i	bead j	bead k
1	2	3
2	3	4
3	4	5
4	5	6

(c) Angles

Table S.2: DBS1



sodium dodecylbenzene-4-sulfonate (DBS4)

Bead number	type
1	H
2	B
3	T
4	T
5	T
6	T

(a) Beads

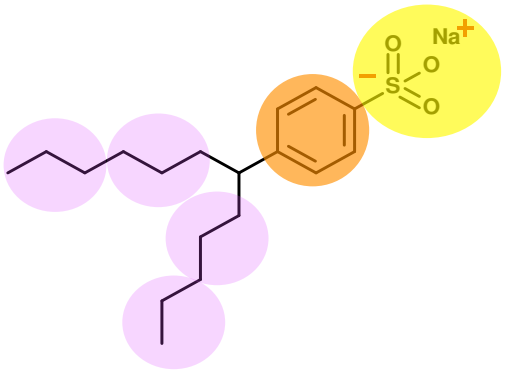
bead i	bead j
1	2
2	3
2	4
4	5
5	6

(b) Bonds

bead i	bead j	bead k
1	2	3
1	2	4
2	4	5
4	5	6

(c) Angles

Table S.3: DBS4



sodium dodecylbenzene-6-sulfonate (DBS6)

Bead number	type
1	H
2	B
3	T
4	T
5	T
6	T

(a) Beads

bead i	bead j
1	2
2	3
3	4
2	5
5	6

(b) Bonds

bead i	bead j	bead k
1	2	3
2	3	4
1	2	5
2	5	6

(c) Angles

Table S.4: DBS6

2 SDS Phase Diagram

In order to simulate the systems of interest, that is lyotropic phases, we choose to model at 80°C. Figure S1 presents a simplified representation of the phase diagram, as a function of SDS concentration and temperature. At 80° we are able to model lyotropic liquid phases without the presence of hydrated crystalline structures.

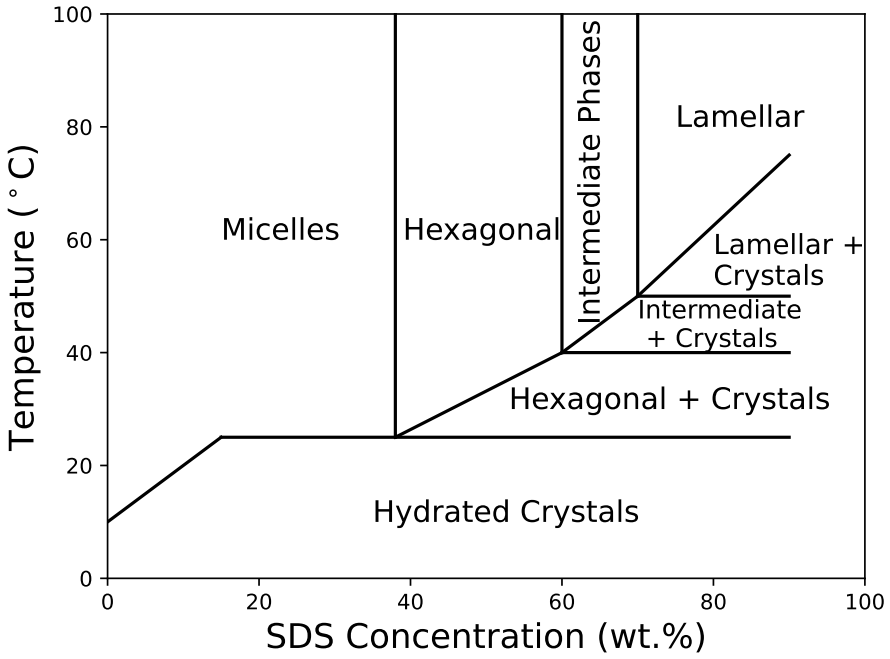


Fig. S1: Simplified schematic phase diagram for SDS aqueous solutions, adapted from Kékicheff *et al.*[1].

3 Lamellar layer spacing for LAS

Fig. S2 shows a plot of the lamellar layer spacings (presented in Table 5 in the main text) in order to highlight the change in spacing as a function of concentration. There is generally a decrease in spacing with concentration. One exception to this is the spacing calculated at 50% for DBS6, which experimentally is close to the region of the phase diagram in which two lamellar phases coexist.

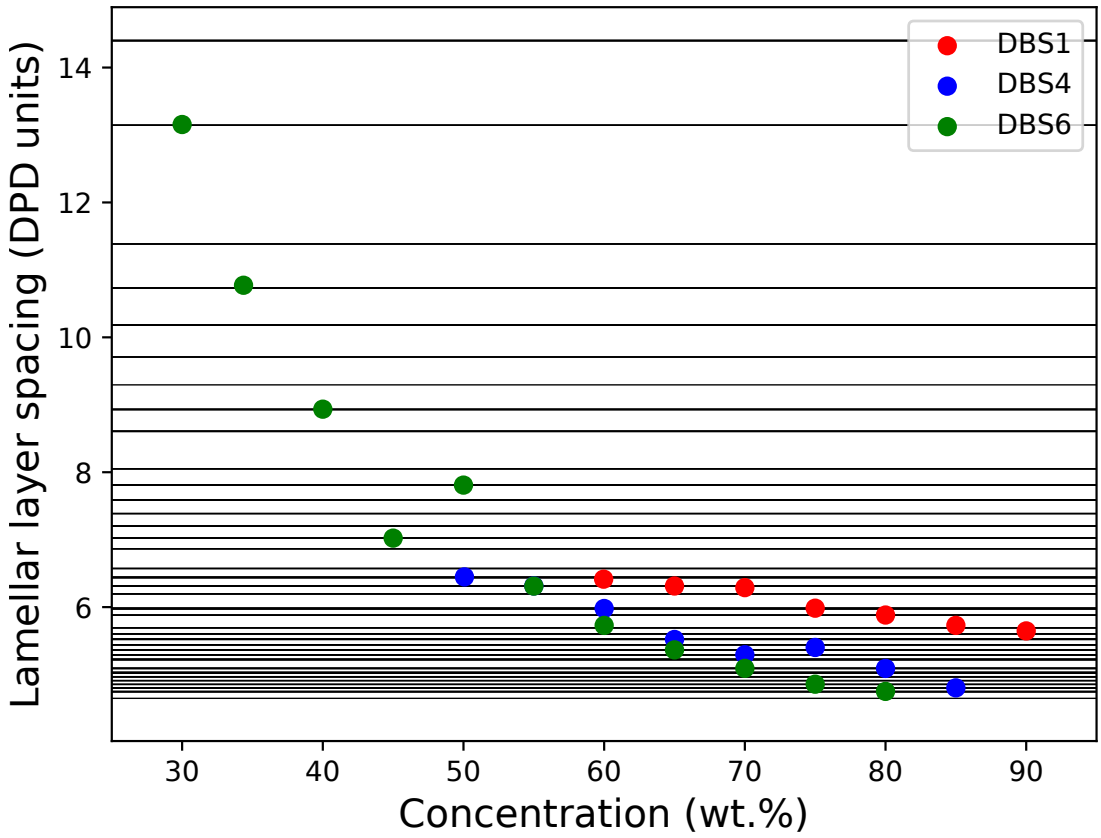


Fig. S2: Lamellar layer spacing of LAS isomers. Also shown are horizontal lines indicating the available spacings, obtained from Eq. 11 in the main article.

4 Extension to LAS - a_{ij} parameters

bead	molecule	δ^{D}	δ^{P}	δ^{H}	V_{m} (cm^3/mol)
H	dimethyl sulphate	17.7	17.0	9.7	94.7
T	propane	13.4	0	0	89.5
W	water	15.5	16.0	42.3	54.0
B	benzene	18.4	0.0	2.0	89.4

Table S.5: Hanson solubility parameters (units $\mathrm{MPa}^{1/2}$)[2] used in calculation of benzene bead interactions.

Equation 7 (see main article) can be used along with the values in Table S.5 in order to calculate the Flory-Huggins parameters χ (see Table 4 in main article). The bead with greater abundance is taken as bead i in any bead pairing.

4.1 a_{BW}

The interaction between benzene and water (a_{BW}) is determined via a comparison with the interaction of tail and head beads with water (a_{TW} and a_{HW}). This is calculated using the following relation:

$$\frac{a_{\mathrm{TW}} - a_{\mathrm{BW}}}{a_{\mathrm{TW}} - a_{\mathrm{HW}}} = \frac{\chi_{\mathrm{TW}} - \chi_{\mathrm{BW}}}{\chi_{\mathrm{TW}} - \chi_{\mathrm{HW}}}. \tag{1}$$

This produces a value of $a_{\mathrm{BW}} = 40.4$ which we round to the nearest integer as $a_{\mathrm{BW}} = 40$.

4.2 a_{BH}

For the interaction of benzene with the head groups, we compare with the a_{HT} interaction and self-interaction value of $a_{ii} = 25$, calculating as

$$\frac{a_{\mathrm{BH}} - a_{ii}}{a_{\mathrm{TH}} - a_{ii}} = \frac{\chi_{\mathrm{BH}} - \chi_{ii}}{\chi_{\mathrm{TH}} - \chi_{ii}}. \tag{2}$$

Using that $\chi_{ii} = 0$, we find a value of $a_{\mathrm{BH}} = 44.18$, which is approximated to $a_{\mathrm{BH}} = 45$ for simplicity.

4.3 a_{BT}

The Flory-Huggins parameter for benzene-tail interactions is calculated to be very small ($\chi_{ii} = 0.792$), as expected because benzene is very soluble in hydrocarbon solvents. Hence we have approximated the benzene-tail interaction to be comparable to the (tail-tail) self-interaction, i.e. $a_{\mathrm{BT}} = a_{ii} = 25$.

References

[1] P. Kékicheff, C. Grabielle-Madelmont and M. Ollivon, *Journal of colloid and interface science*, 1989, **131**, 112–132.

[2] C. M. Hansen, *Hansen solubility parameters: A user's handbook.*, CRC Press, 6000 Broken Sound Parkway NW, Suite 300, Boca Raton, FL 33487-2742, 2007.