Supplementary Material

Multiscale Simulation of Surfactant-Aquaporin Complex Formation and Water Permeability

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Table S1. The number of atoms (N) and the net charge (Z) of each AqpZ monomer at different

pH values

pH	N	Z
4	2144	10
7	2134	0

Molecule model for SDS

Tables S2 to S5 give the force-field parameters for the bonded and non-bonded interactions of

SDS molecules, i.e., parameters appeared in the potential function:

$$V(r_1, r_2, r_3, \mathsf{K}, r_N) =$$

$$\left.\begin{array}{l} \displaystyle\sum_{Bonds} \frac{1}{4} K_b (b^2 - b_0^{\,2})^2 + \sum_{angles} \frac{1}{2} K_\theta (\cos(\theta) - \cos(\theta_0))^2 \\[2em] + \displaystyle\sum_{\substack{\Pr oper \\ dihedral}} K_\phi (1 + \cos(n\phi - \phi_S)) \end{array}\right\} \text{Bonded interactions}$$

$$+ \left.\begin{array}{l} \displaystyle\sum_i \sum_{j>i} \left(\frac{C^{12}{}_{ij}}{r_{ij}^{12}} - \frac{C^6{}_{ij}}{r_{ij}^6} \right) \\[2em] + \displaystyle\sum_i \sum_{j>i} \left(\frac{q_i q_j}{4\pi\varepsilon_o \varepsilon_r r_{ij}} \right) \end{array}\right\} \text{Non - bonded interactions}$$

Table S2. Covalent bond parameters between atoms of type i and type j from the SDS molecule.

Here b_0 stands for bond length and k_b for harmonic vibration constant.

type i	type j	b_0 (nm)	k_b (kJ mol^{-1} nm^{-2})
S	OM	0.150	376 650.0
S	OS	0.136	376 560.0
OS	CH2	0.143	251 040.0
CH2	CH2	0.153	334 720.0

Table S3. Angle parameters for SDS. Here θ_0 is the equilibrium bond angle, and k_θ is the bond angle harmonic vibrational constant.

type i	type j	type k	f	θ_0 (deg)	k_θ (kJ mol^{-1} rad^{2})
OM	S	OM	1	109.5	520.00
OS	S	OM	1	109.5	520.00
CH2	OS	S	1	120.0	397.50
CH2	CH2	OS	1	109.5	460.24
CH2	CH2	CH2	1	111.0	460.24
CH2	CH2	CH3	1	111.0	460.24

Table S4. Parameters for the dihedral angles

type i	type j	type k	type l	f	φ (deg)	k_φ (kJ mol^{-1})	n
X	OS	S	X	1	0.0	3.766	3
X	OS	CH2	X	1	0.0	3.766	3
X	CH2	CH2	X	1	0.0	5.858	3

Table S5. Parameters for the atomic partial charges and the Lennard-Jones (LJ) potential.

atomic type	q, e	C^6	C^{12}
Na$^+$	+1.000	7.2063121e-5	2.1025000e-8
OM	−0.654	2.2619536e-3	7.4149321e-7
S	+1.284	9.9840064e-3	1.3075456e-5
OS	−0.459	2.2619536e-3	1.5055290e-6
CH2 (next to OS)	+0.137	7.1048041e-3	2.5775929e-5
CH2 (in the tail)	0.000	7.1048041e-3	2.5775929e-5
CH3	0.000	9.9161764e-3	3.3570436e-5

Gauche defect probability of SDS adsorbed on AqpZ

The conformation of SDS molecule is characterized by the dihedral angle formed by 4 carbon

atoms in the SDS tail. The distribution of the dihedral angle is used to compute the gauche defect

probability, namely, the probability of the hydrocarbon tail's having a kink. A hydrocarbon

sequence i-j-k-l is defined to have a kink if the dihedral angle formed by the form atoms is
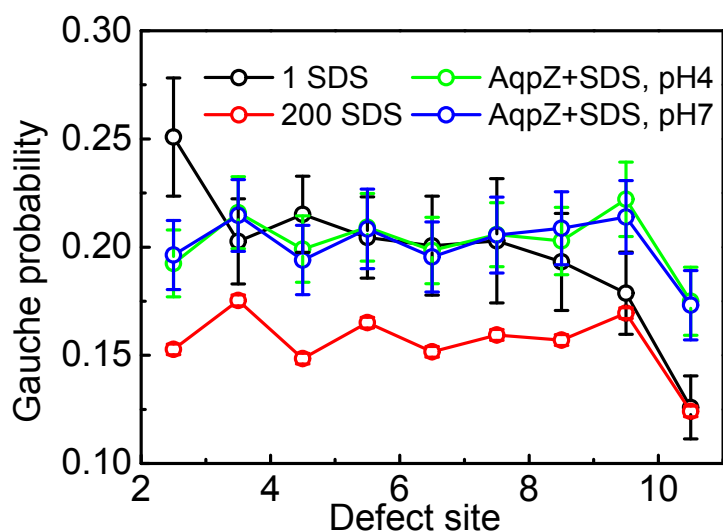
between 30 and 150 degrees.

Figure S1. Gauche defect probability for hydrocarbon tail in systems of one SDS, 200 SDS molecules, SDS adsorbed on AqpZ at pH 4 and 7. The carbon site numbering starts from the C atom next to the SO_4 head group and is plotted so that, for example, 2.5 refers to the bond between second and third carbon atom in the tail.

We studied the probability of gauche defect for SDS adsorption on AqpZ and the results were

given in Figure S1.   For SDS molecules adsorbed at the AqpZ surface, the gauche-defect

probability is changed mainly at the tail end of SDS molecules. While gauche defect probability

at the head end is between that for a single SDS molecule and the average for 200 SDS

molecules. It is should be emphasized that the gauche-defect probability for SDS molecules at the AqpZ surface is similar to that of a single SDS molecules and higher than that in a micelle of 200 SDS molecules. As a result, the behavior of SDS at the AqpZ surface is totally different from that in micelle.   This is consistent with the RDF in the main text that the SDS tails are much closer to the AqpZ surface than SDS heads.