

Supporting information for:

Influence of Lipid Bilayer Head Group Polarity on

Micelle Behavior and Surfactant Transfer: A

Molecular Dynamics Simulation Study

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Table S1: Calculated values of the average area per lipid (APL) and bilayer thickness for the DMPC and Cer240 bilayers at 313.15 K and 350.15 K under a pressure of 1 bar from molecular dynamics (MD) simulations.

Properties	DMPC bilayer ^a		Cer240 bilayer ^b	
	313.15 K ^c	350.15 K ^c	313.15 K ^d	350.15 K ^d
APL (Å ²)	61.54	66.72	42.81	51.70
Thickness (Å) ^e	35.63	34.32	48.10	42.94

^a Composed of 200 DMPC lipids and 23000 water molecules.

^b Composed of 256 Cer240 lipids and 23000 water molecules

^c A total run time of 200 ns with a production run of last 50 ns.

^d A total run time of 300 ns with a production run of last 50 ns.

^e Defined as the average distance between P atoms (N atoms) at the upper and lower leaflets in the DMPC (Cer240) bilayer.

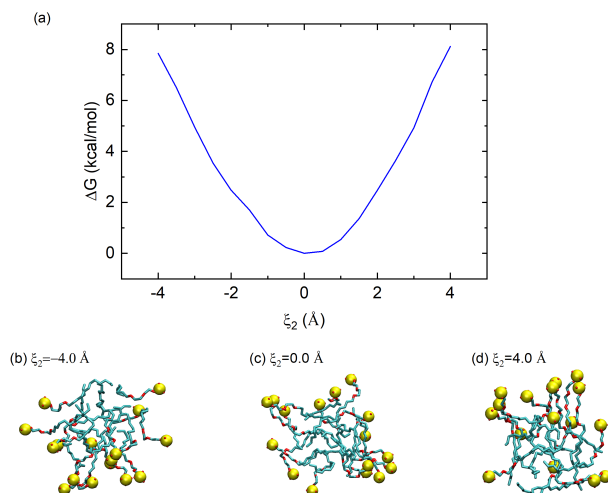


Figure S1: (a) A one-dimensional (1D) potential of mean force (PMF) profile for an SLE2S micelle in bulk water as a function of ξ_2 . (b)-(d) Representative micellar structures corresponding to $\xi_2 = -4.0, 0.0$, and 4.0 Å, illustrating lower hemispherical, spherical, and upper hemispherical shapes, respectively. A series of MD simulations for the PMF calculation were performed at 313.15 K and 1 bar using the US sampling method under the NPT ensemble. The system contained 13858 water molecules and a micelle composed of 16 SLE2S surfactants.

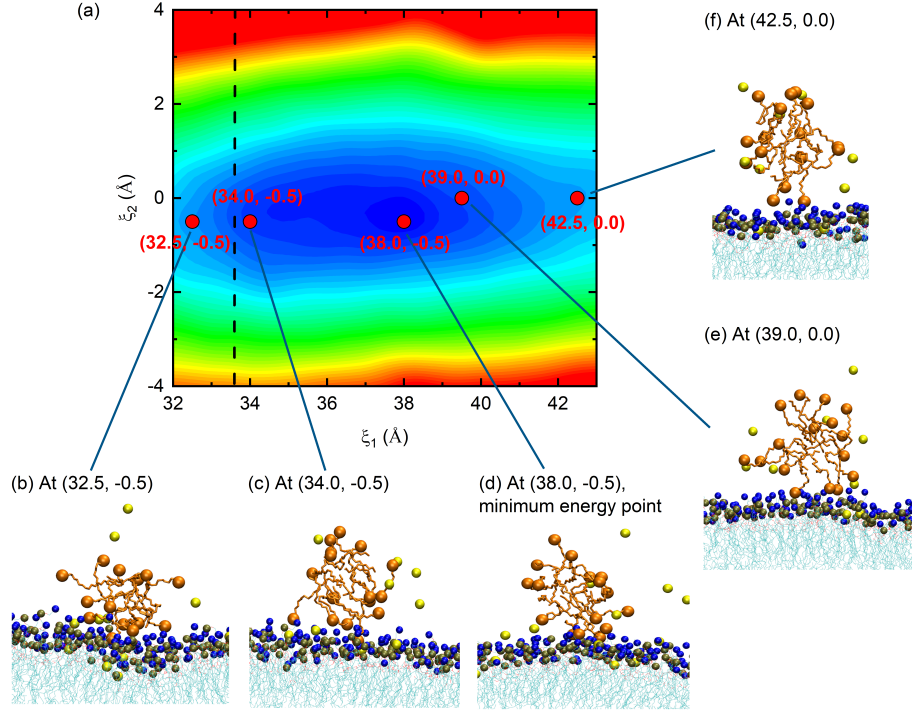


Figure S2: (a) A two-dimensional (2D) PMF profile for a micelle on the DMPC bilayer as a function of ξ_1 and ξ_2 and (b)-(f) snapshots for a typical micellar structure at a given ξ_1 and ξ_2 position. The vertical dashed line in (a) represents the bilayer-micelle contact distance, d_{bmc}^{DMPC} at $\xi_1 = 33.6$ Å for the micelle on the DMPC bilayer. For the definition of d_{bmc} , see the text.

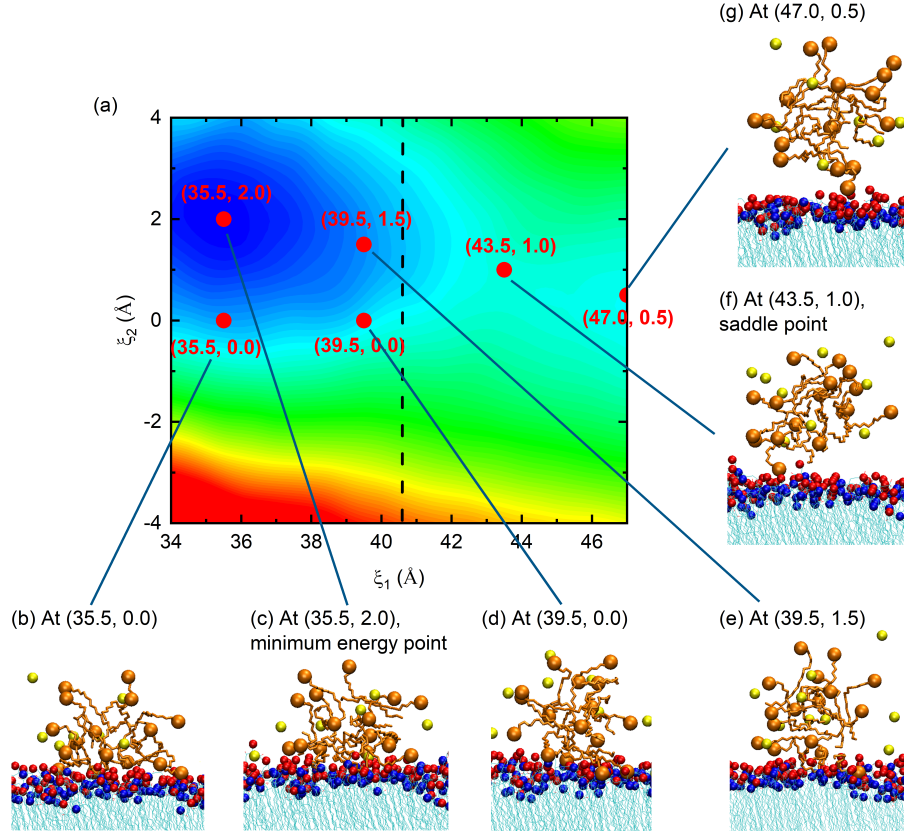


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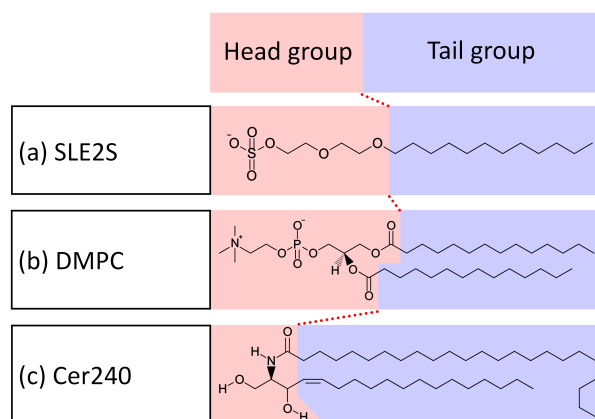


Figure S4: Definitions of the head and tail groups for (a) the SLE2S surfactant, (b) DMPC and (c) Cer240 lipid molecules.

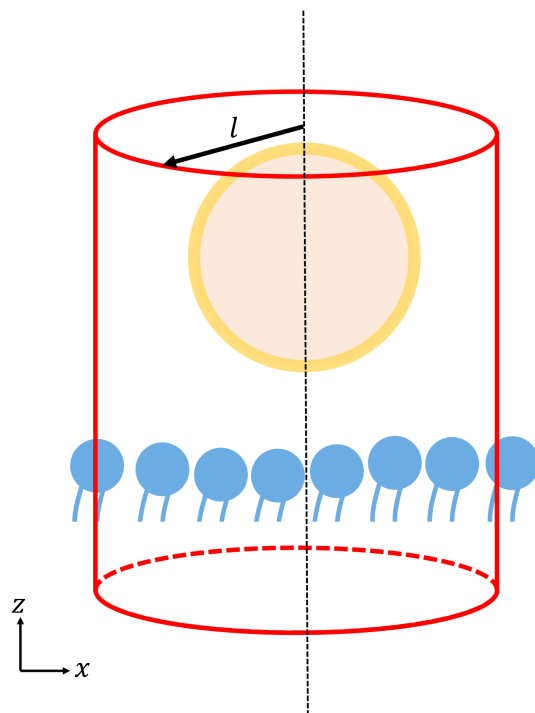


Figure S5: Definition of a cylinder that is centered at the CoM of the SLE2S micelle and aligned along the z axis with a radius of l in the lateral direction.

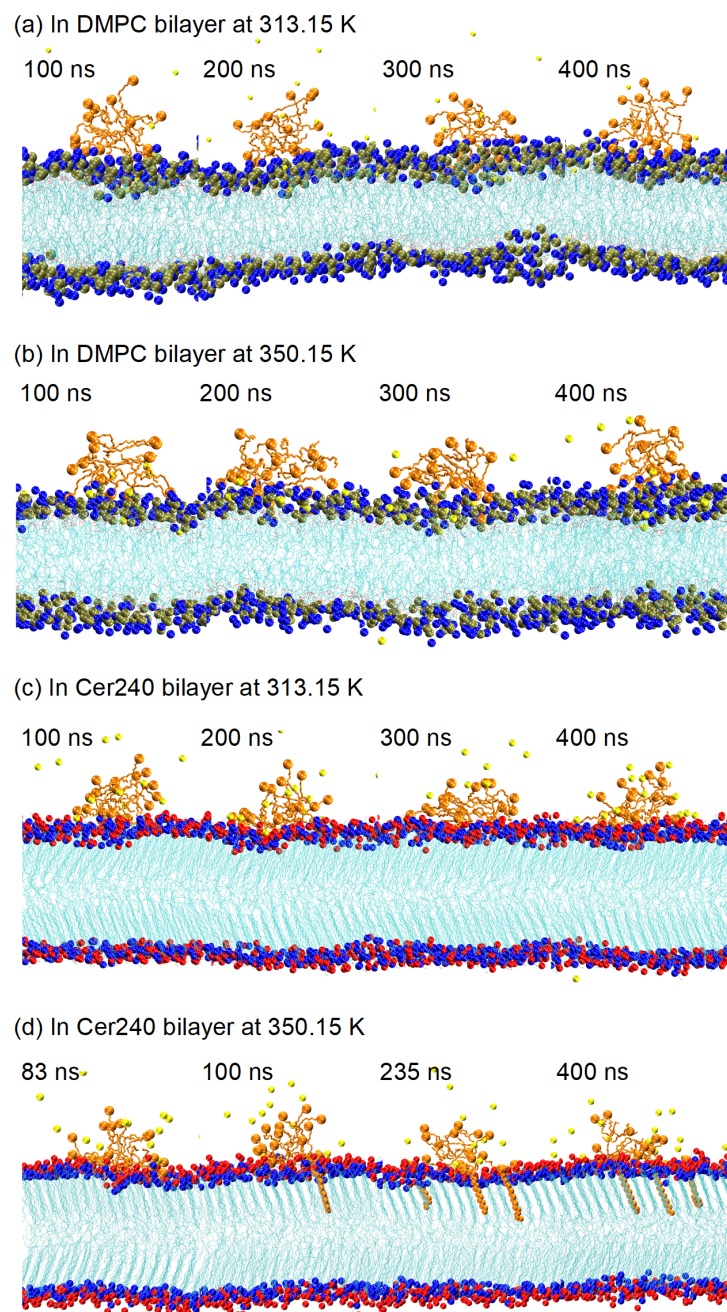


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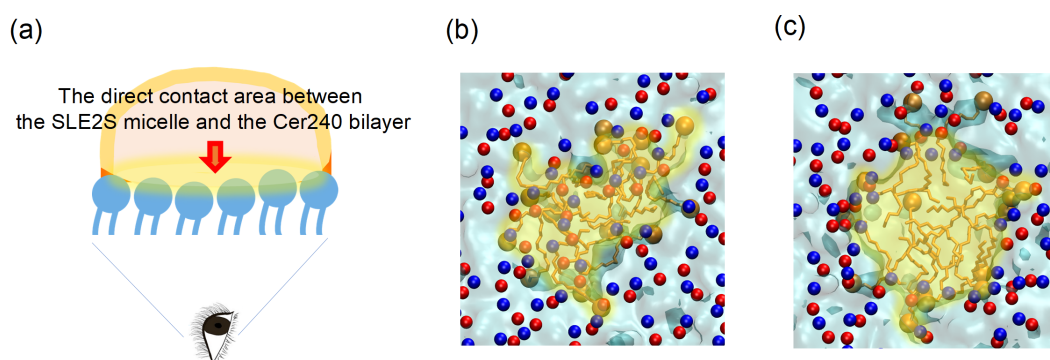


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