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

Molecular Dynamics Simulation of CO_2-switchable Surfactant Regulating Reversible Emulsification/Demulsification Processes of a Dodecane-Saline System†

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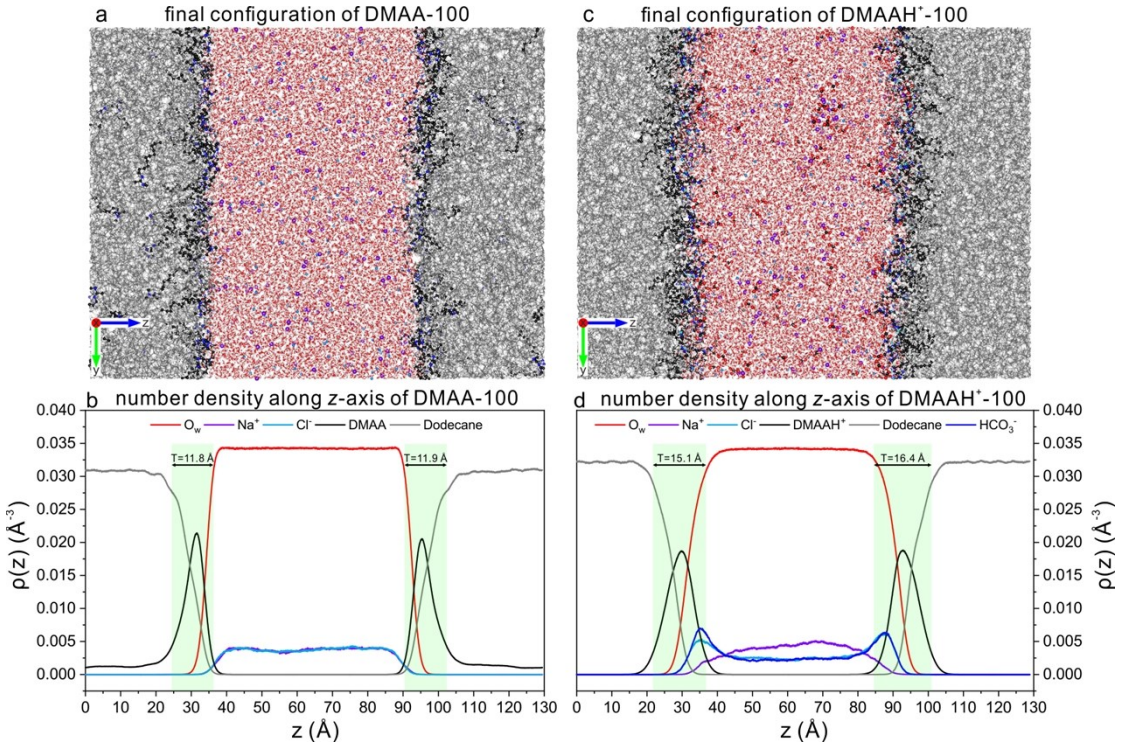

Figure S1. Equilibrated configurations (a and c) and number density profiles along *z*-axis (b and d) of model DMAA-100 and model $DMAAH^+$-100. O_w denotes the O atom of water molecule. The density profiles of DMAA, $DMAAH^+$ and dodecane are calculated by using all atoms except hydrogen atoms. The density profiles of Na^+ and Cl^- are magnified 10 times for the sake of clarity. The characterization of species in equilibrated configurations is same as that in Figure 1.

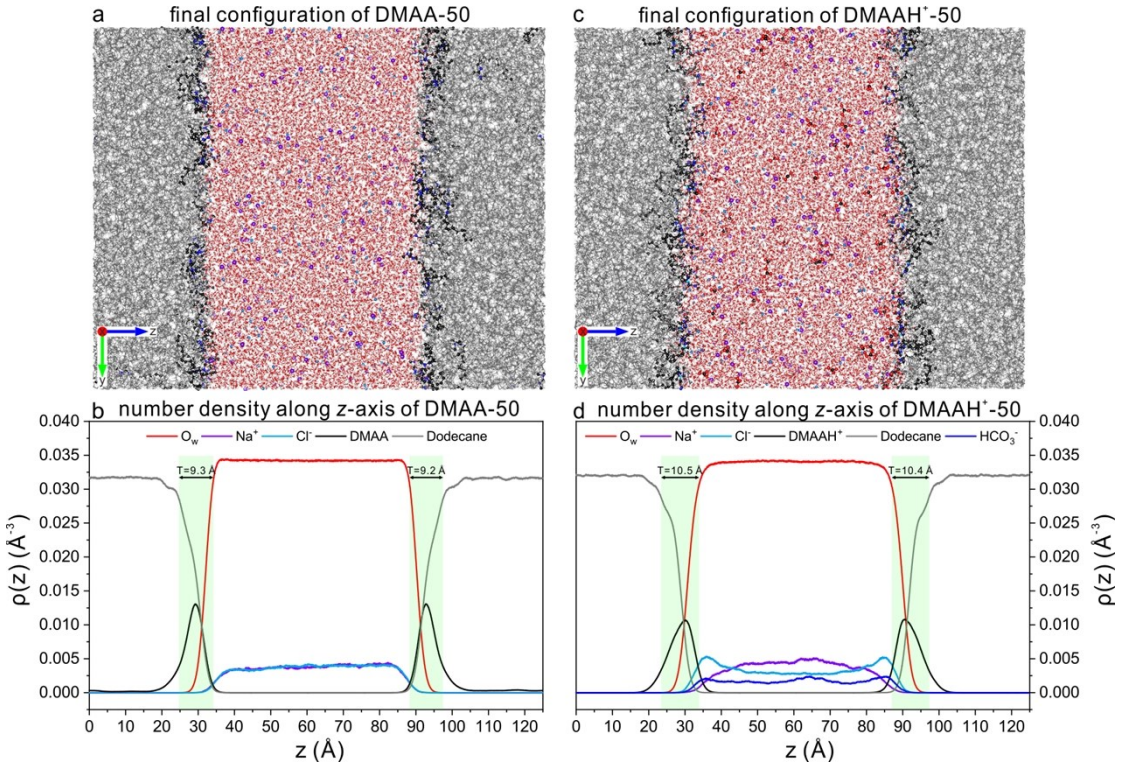

Figure S2. Equilibrated configurations (a and c) and number density profiles along *z*-axis (b and d) of model DMAA-50 and model $DMAAH^+$-50. O_w denotes the O atom of water molecule. The density profiles of DMAA, $DMAAH^+$ and dodecane are calculated by using all atoms except hydrogen atoms. The density profiles of Na^+ and Cl^- are magnified 10 times for the sake of clarity. The characterization of species in equilibrated configurations is same as that in Figure 1.

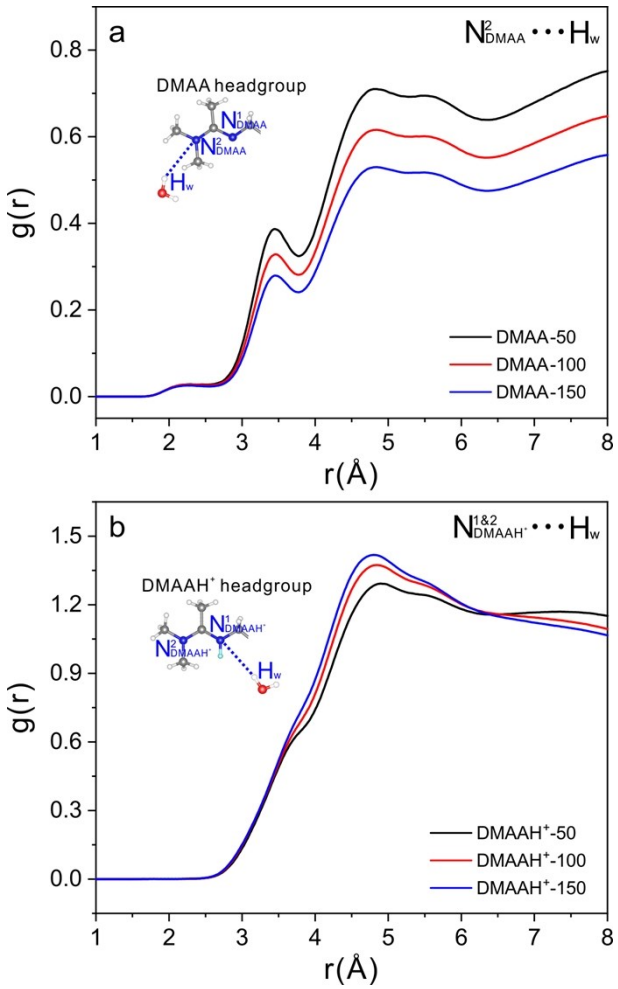

Figure S3. RDFs between the polar headgroup of DMAA/DMAAH$^+$ and water molecules. For DMAA, N1 DMAA and N2 DMAA denote the nitrogen atom connected with alkyl tail and dimethyl, respectively. N1 DMAAH$^+$ and N2 DMAAH$^+$ denote the corresponding nitrogen atoms in DMAAH$^+$. H_w represents the hydrogen atom in water molecule.