Supplementary Information for

Computational Investigation of a Switchable Emulsion Stabilized by the Mixture of Surfactant and Tertiary Amine

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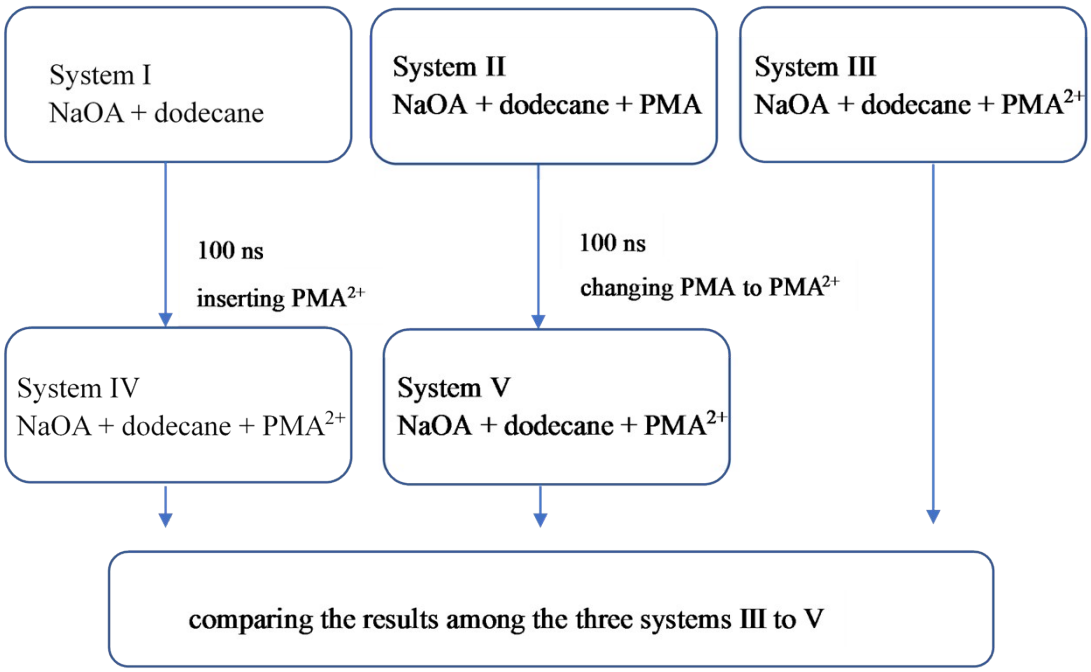
Table S1. Summary of the Simulated Systems

system	oil	OA^-	Na^+	PMA	PMA^{2+}	HCO_3^-	water	simulation time / ns	length of cubic box / nm
I	300	100	100				27243	100	9.936
II	300	100	100	100			26069	100	9.929
III	300	100	100		100	200	25418	50	9.888
IV	300	100	100		100	200	25028	20	9.840
V	300	100	100		100	200	25038	20	9.846

A flowchart showing the relationship of the above systems:



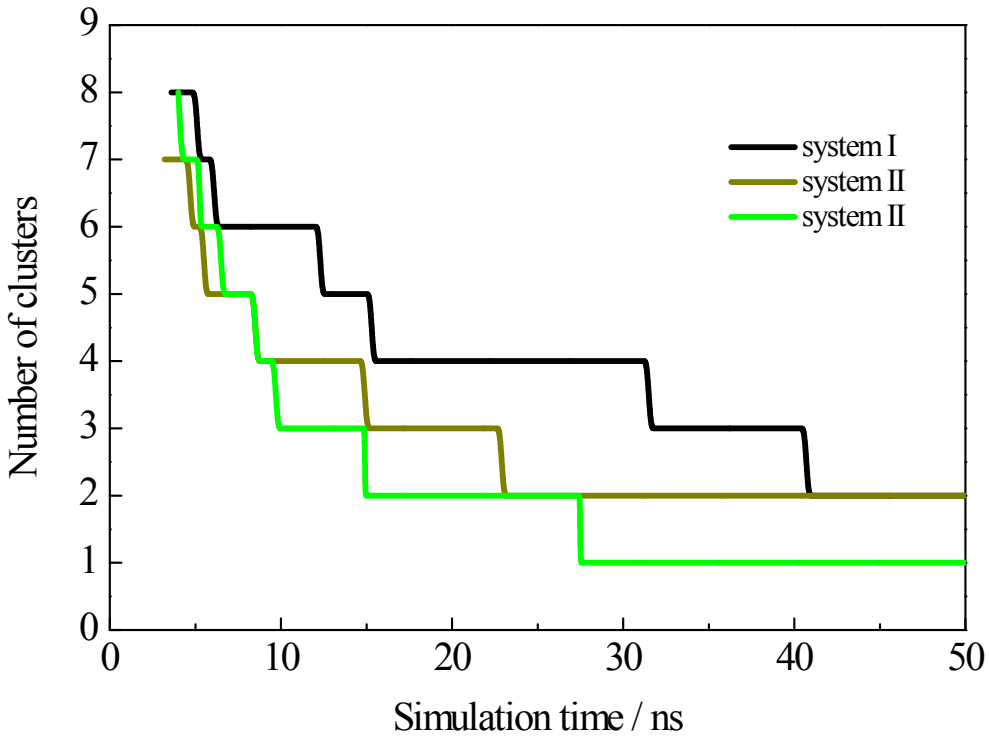


Fig. S1 Number of aggregated clusters with time evolution for the repeated systems.

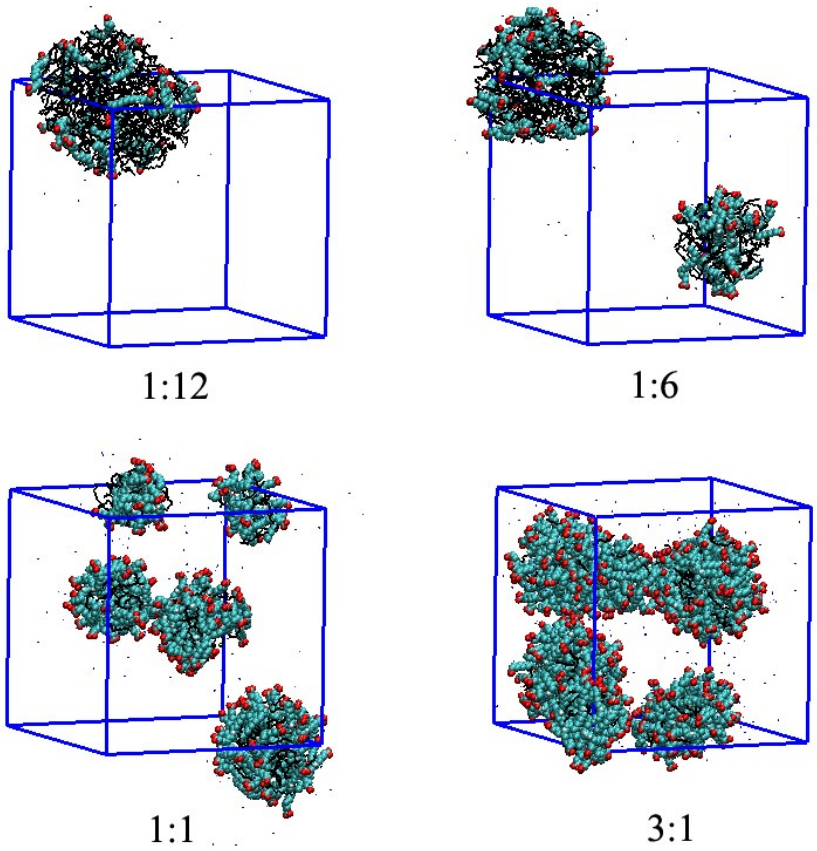


Fig. S2 Final configurations of the simulated systems with different surfactant-hexadecane proportion. The numbers of OA-: dodecane for these three systems are, in turn, 25:300, 50:300, 150:150, and 300:100.

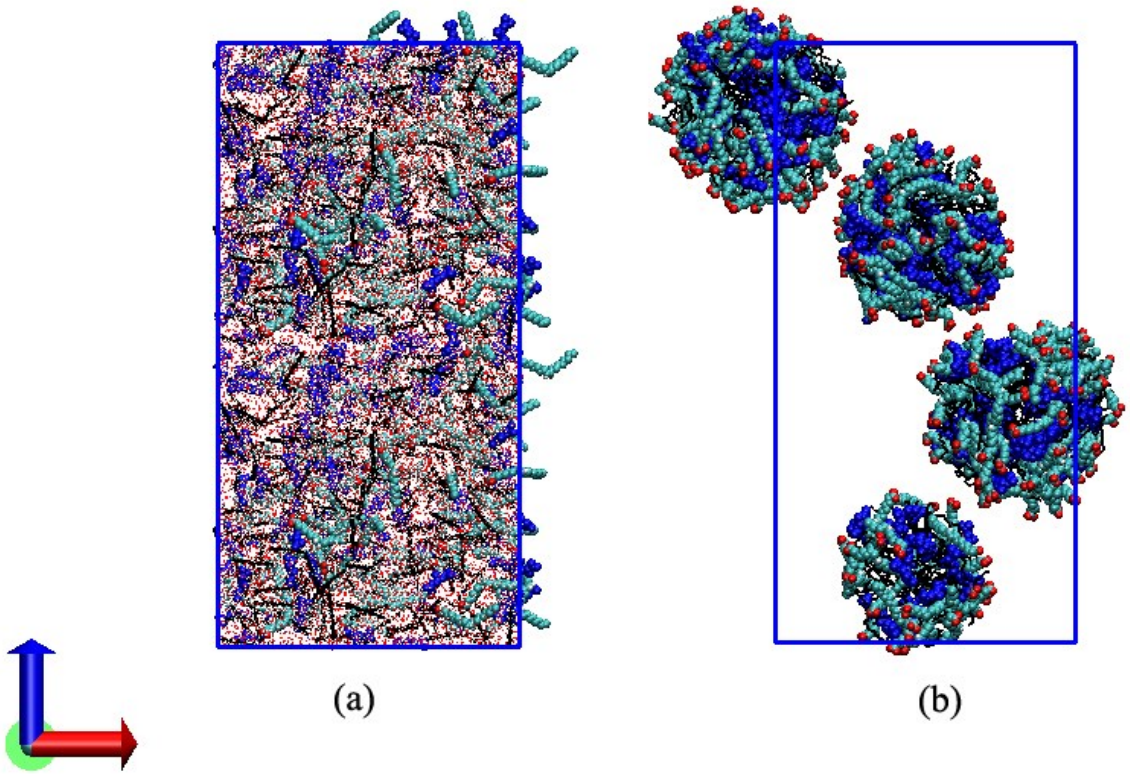


Fig. S3 Simulated results of system II whose dimension was doubled along z direction.

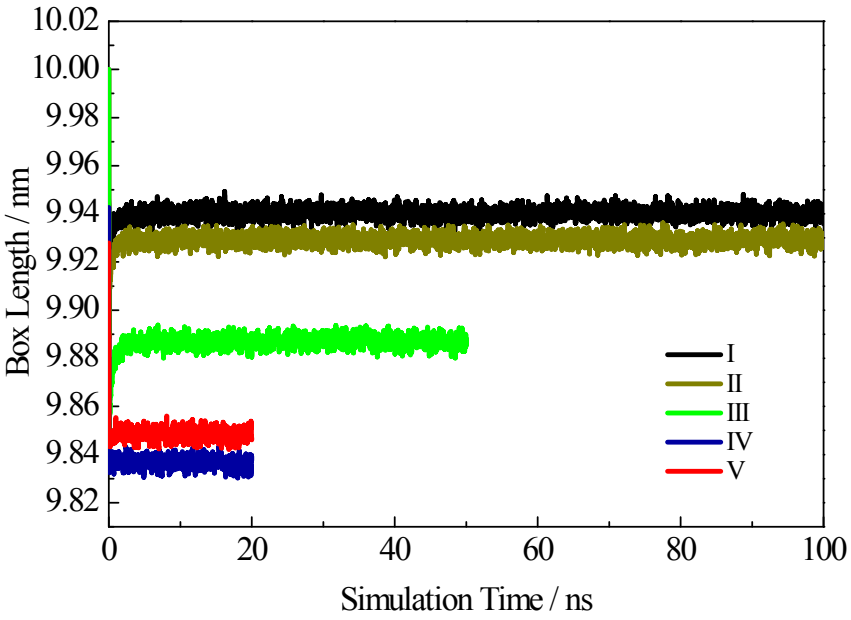


Fig. S4 Time variation of the simulation box in each system.

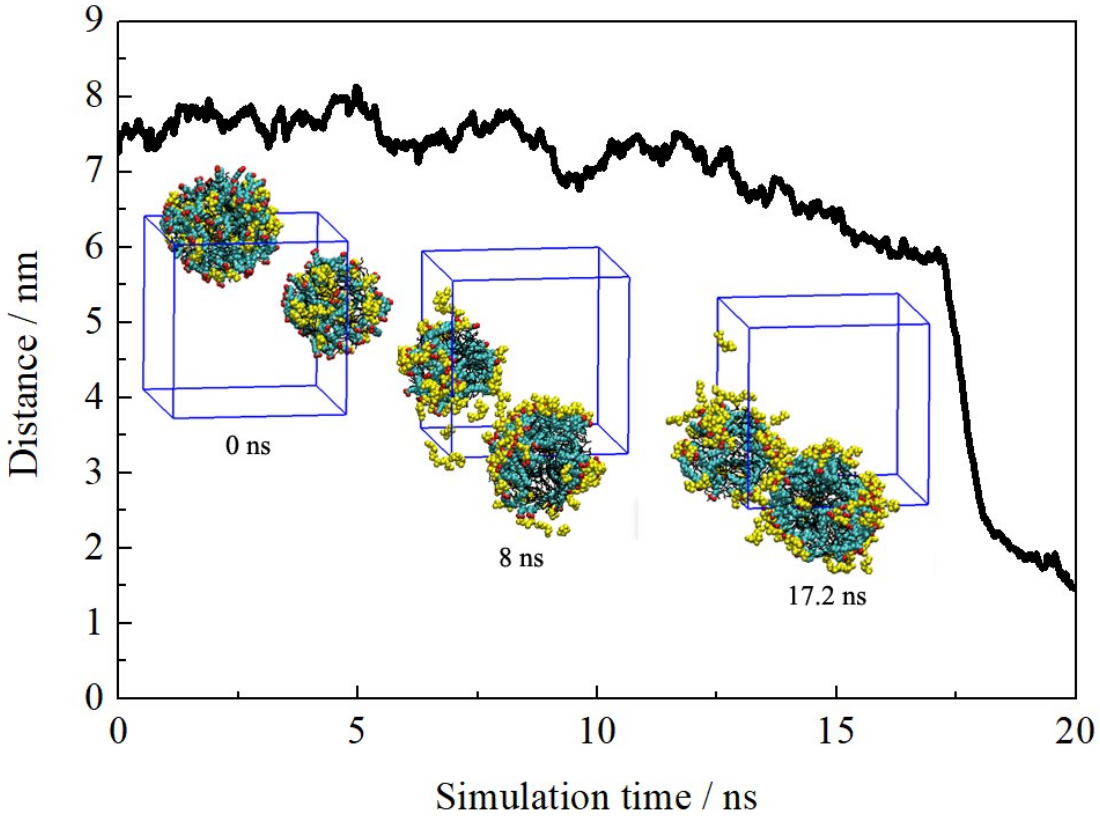


Fig. S5 Simulated results of system V.

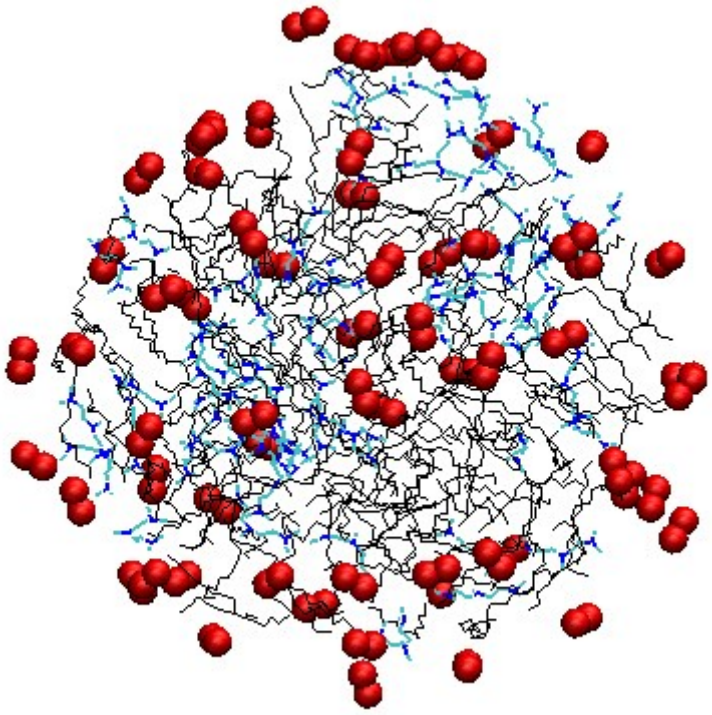


Fig. S6 Structure of the droplet formed by OA^-, PMA and dodecane molecules (derived from system III). The headgroup O atoms of OA^- are highlighted to give a clear view, and PMA molecules are shown by blue lines.

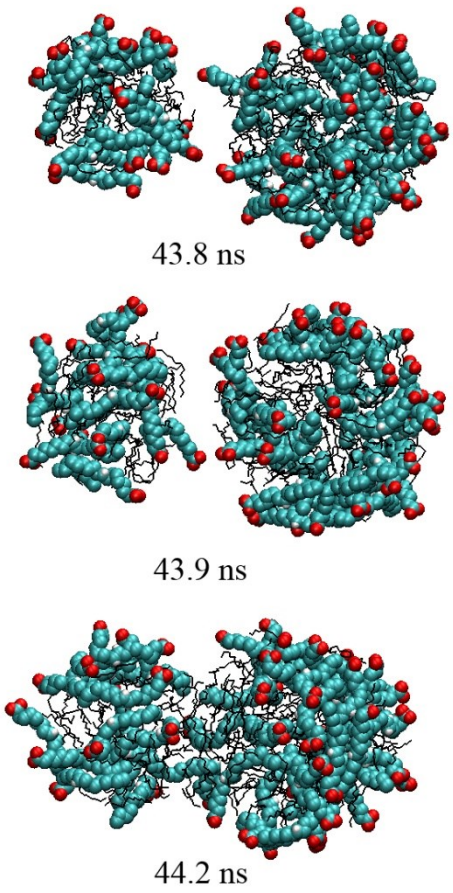


Fig. S7 Instantaneous configurations derived from MD trajectories of system I to show the dynamical process of the droplets' coalescence.

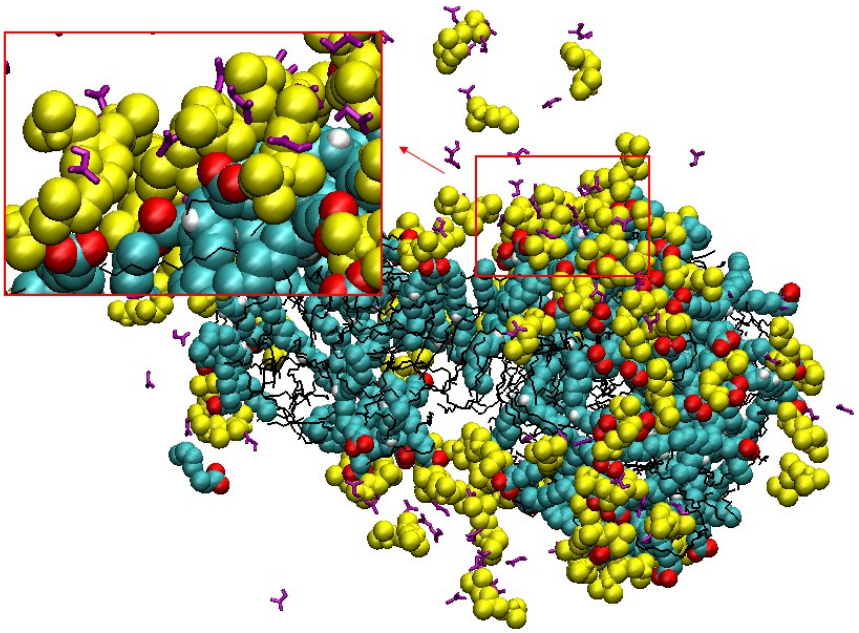


Fig. S8 Configurations of HCO_3^- in the dynamical process of droplets' coalescence (at 6.6 ns shown in Fig. 7).

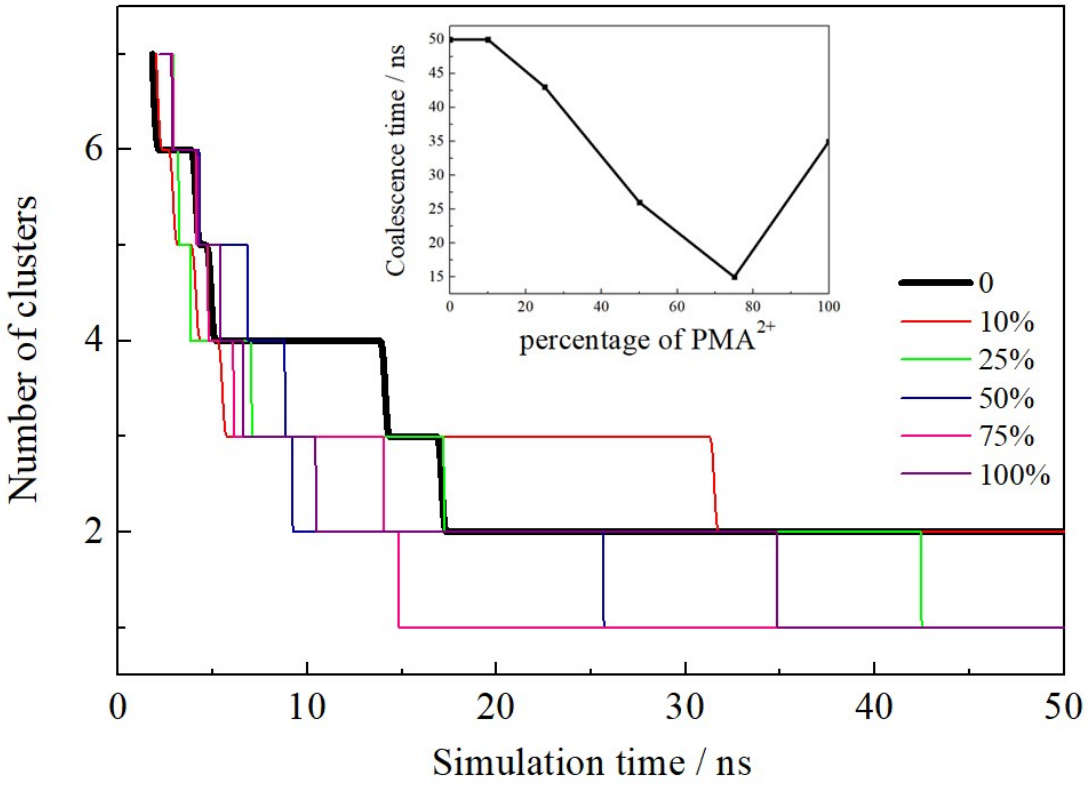


Fig. S9 Number of aggregated clusters with time evolution for the systems with different percentages of PMA^{2+}. The inset profile shows the simulation time of one droplet formed plotted against the percentage of PMA^{2+}.

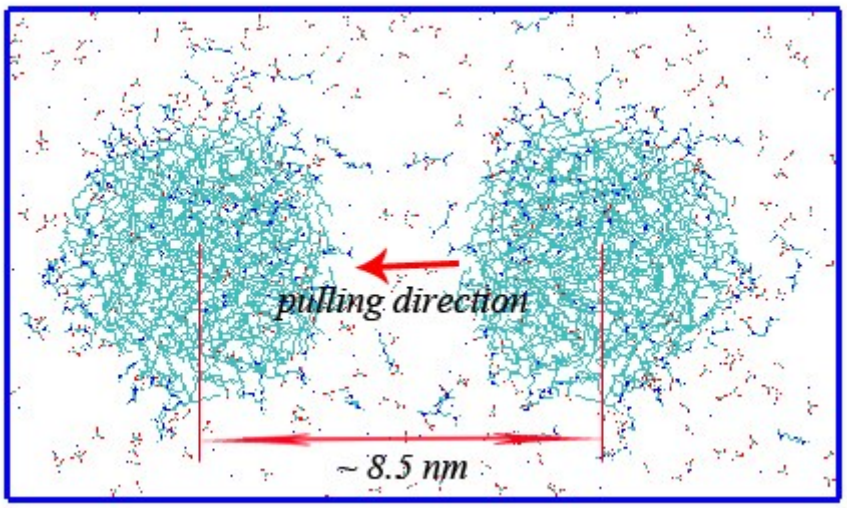


Fig. S10 An illustration of the initial setup for the pulling simulation of the two droplets' coalescence. The solid blue rectangle represents the periodic boundaries.

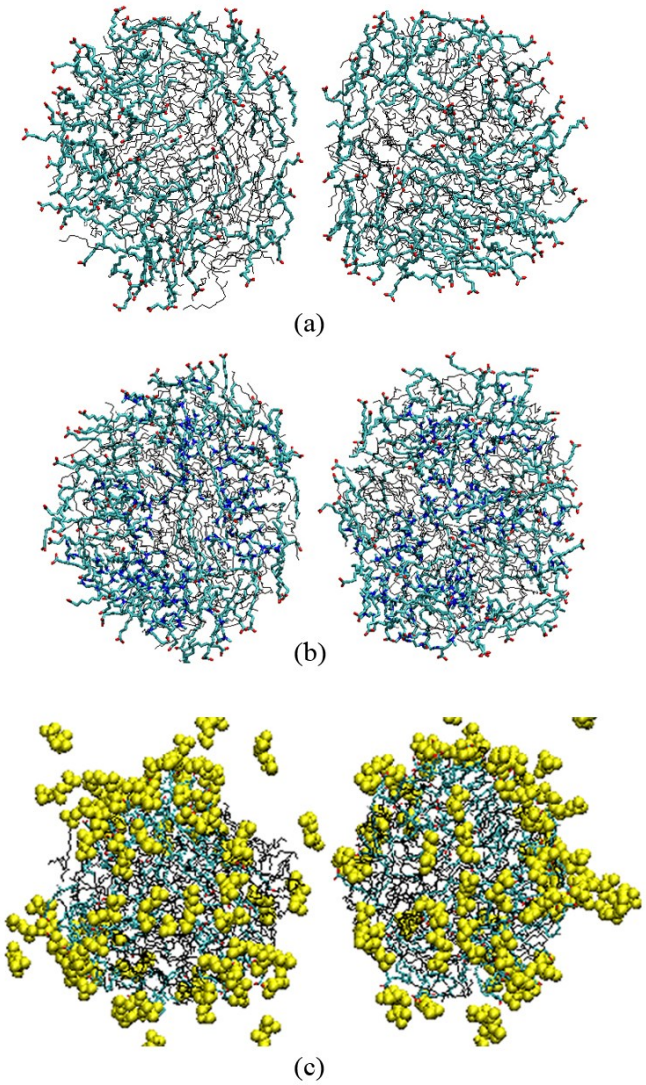


Fig. S11 Configurations corresponding to the maximum of the PMF curves.

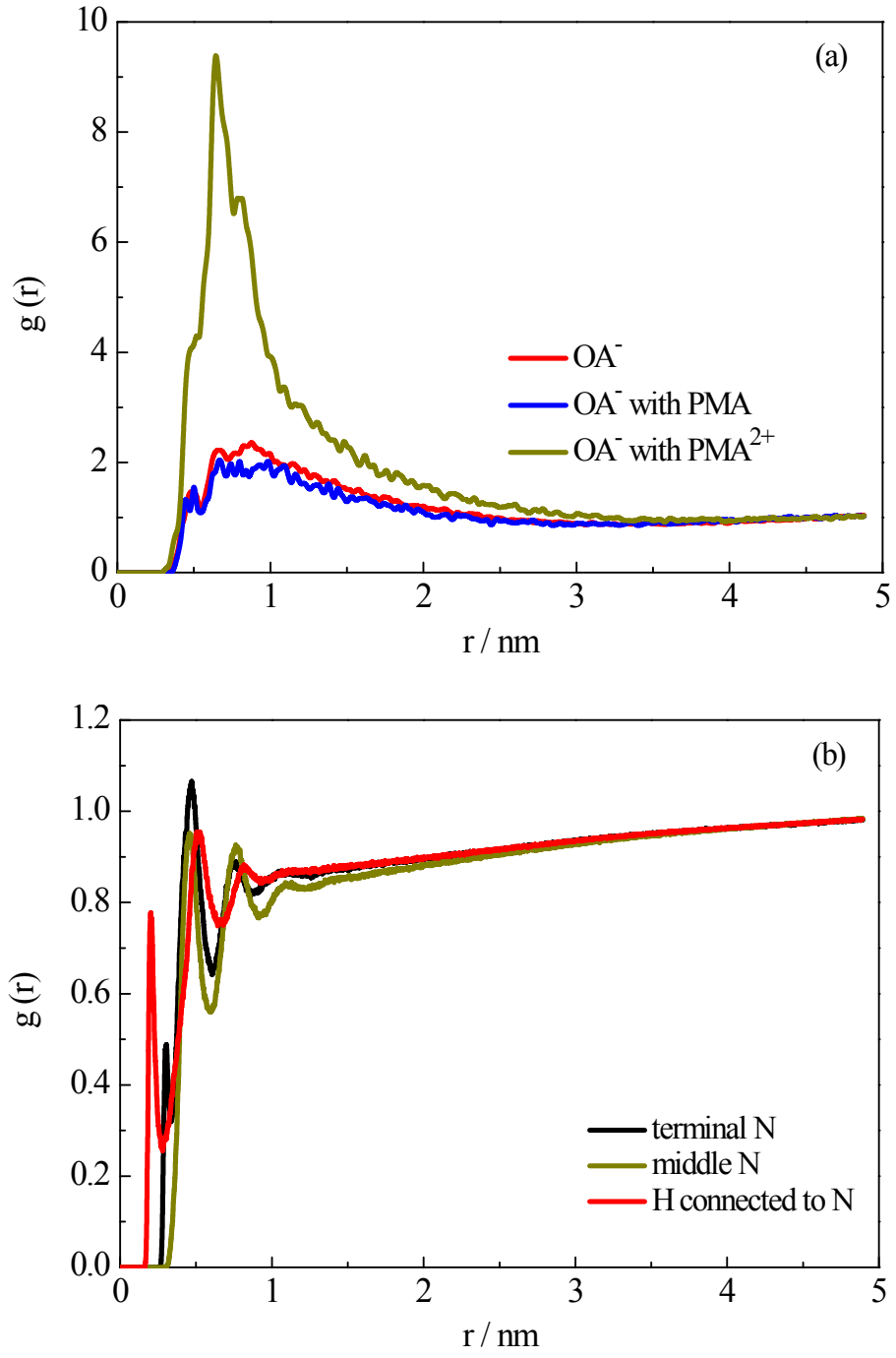


Fig. S12 (a) RDFs between headgroup oxygen atoms of surfactant OA^-. (b) RDFs of water molecules around the selected atoms in PMA^{2+}.