Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Unveiling the Phase Behavior of C_iE_j non-ionic surfactants in water through Coarse-Grain Molecular Dynamics Simulations

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1. CG Mapping

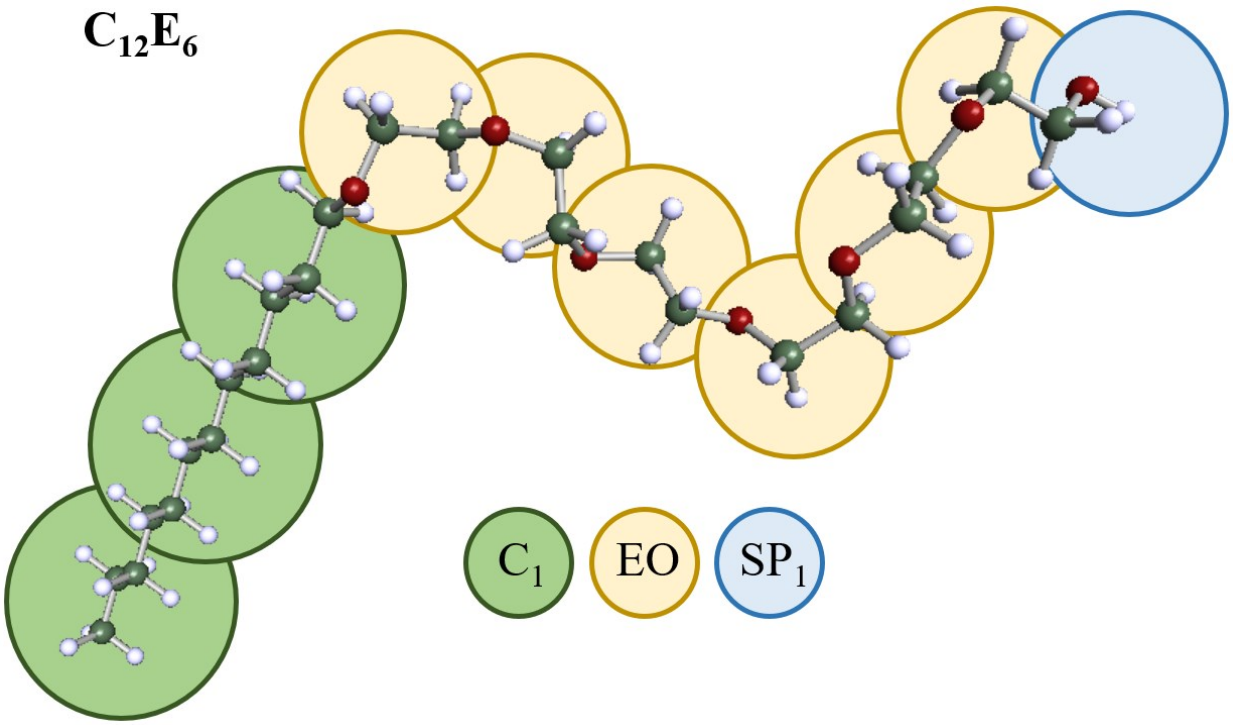

Figure S1. Schematic representation of the CG mapping considered for the $C_{12}E_6$ surfactant.

2. CG-MD Simulations for C_8 surfactants

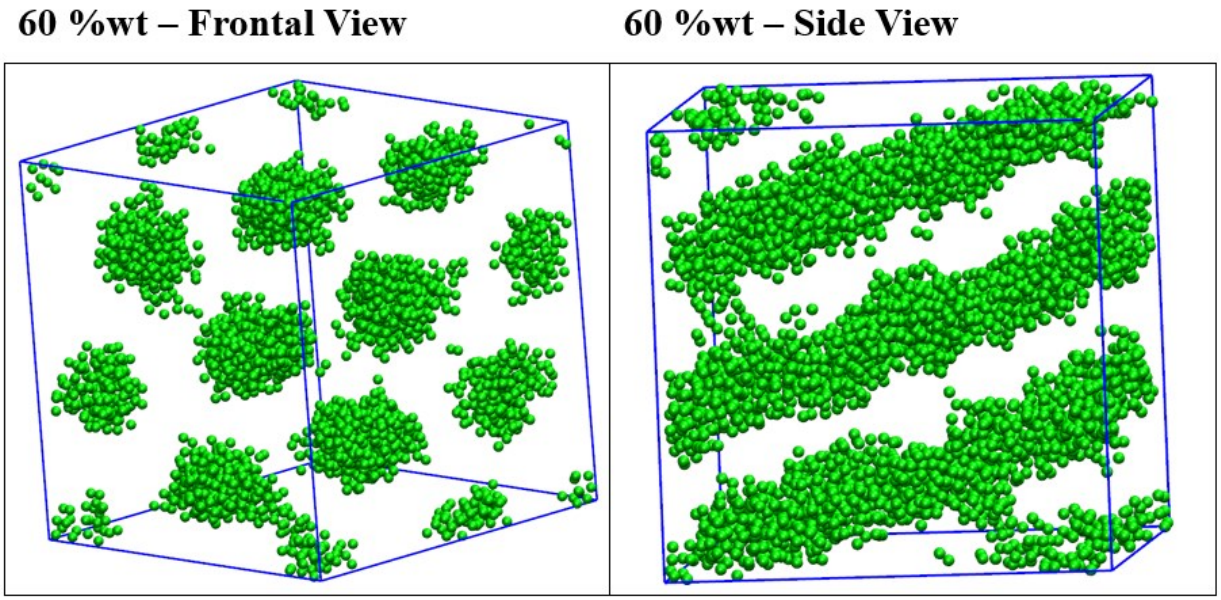

Figure S2. Final snapshot of the CG-MD simulation of C_8E_6/water at 60 %wt, showing the alkyl tails disposition in the H_1 phase observed.

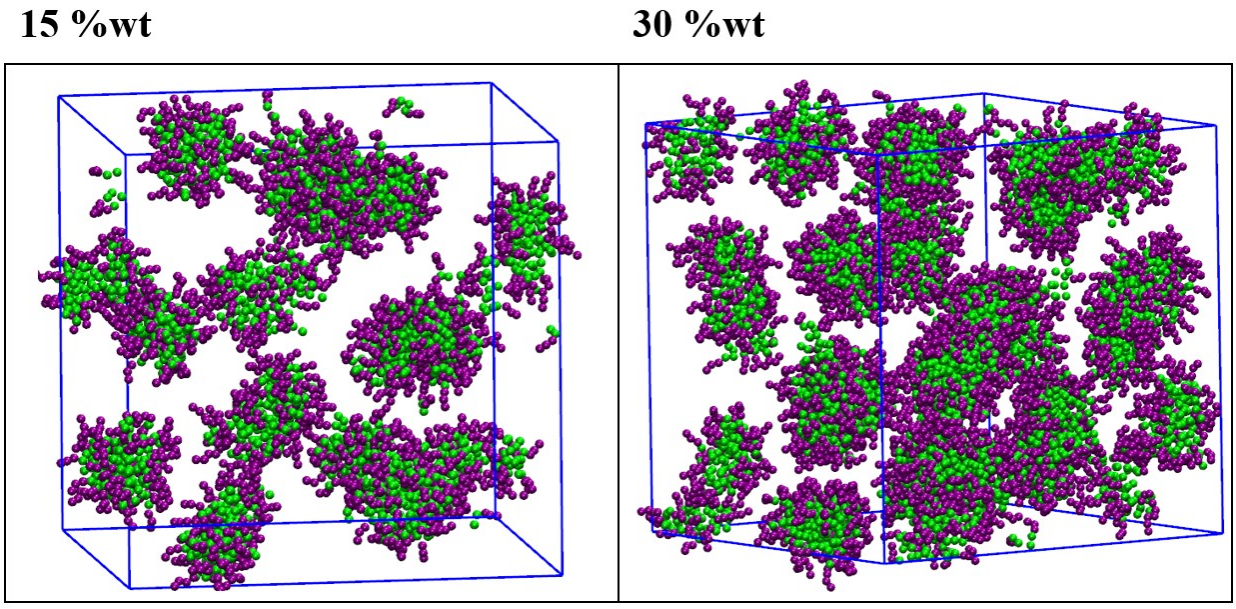

Figure S3. Final snapshots of the CG-MD simulations carried out for the system C_8E_6/water at 15 and 30%wt. Green is used to represent the alkyl tail beads, while purple represents the beads from the hydrophilic moiety. Water molecules are omitted to allow for an easier visualization.

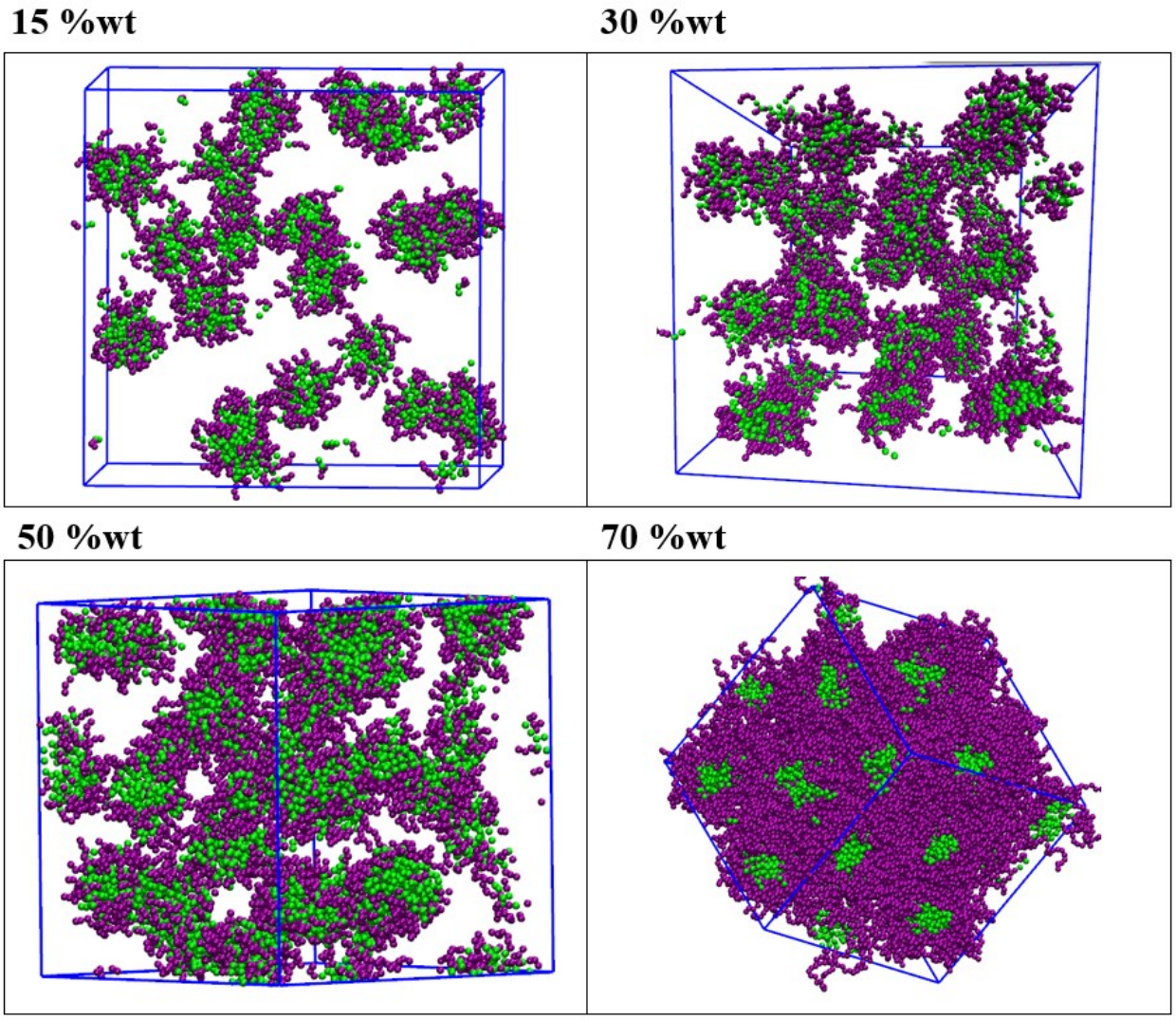

Figure S4. Final snapshots of the CG-MD simulations carried out for the system C_8E_{12}/water at different concentrations. Colors as in Figure S2.

3. CG-MD Simulations for C_{12} surfactants

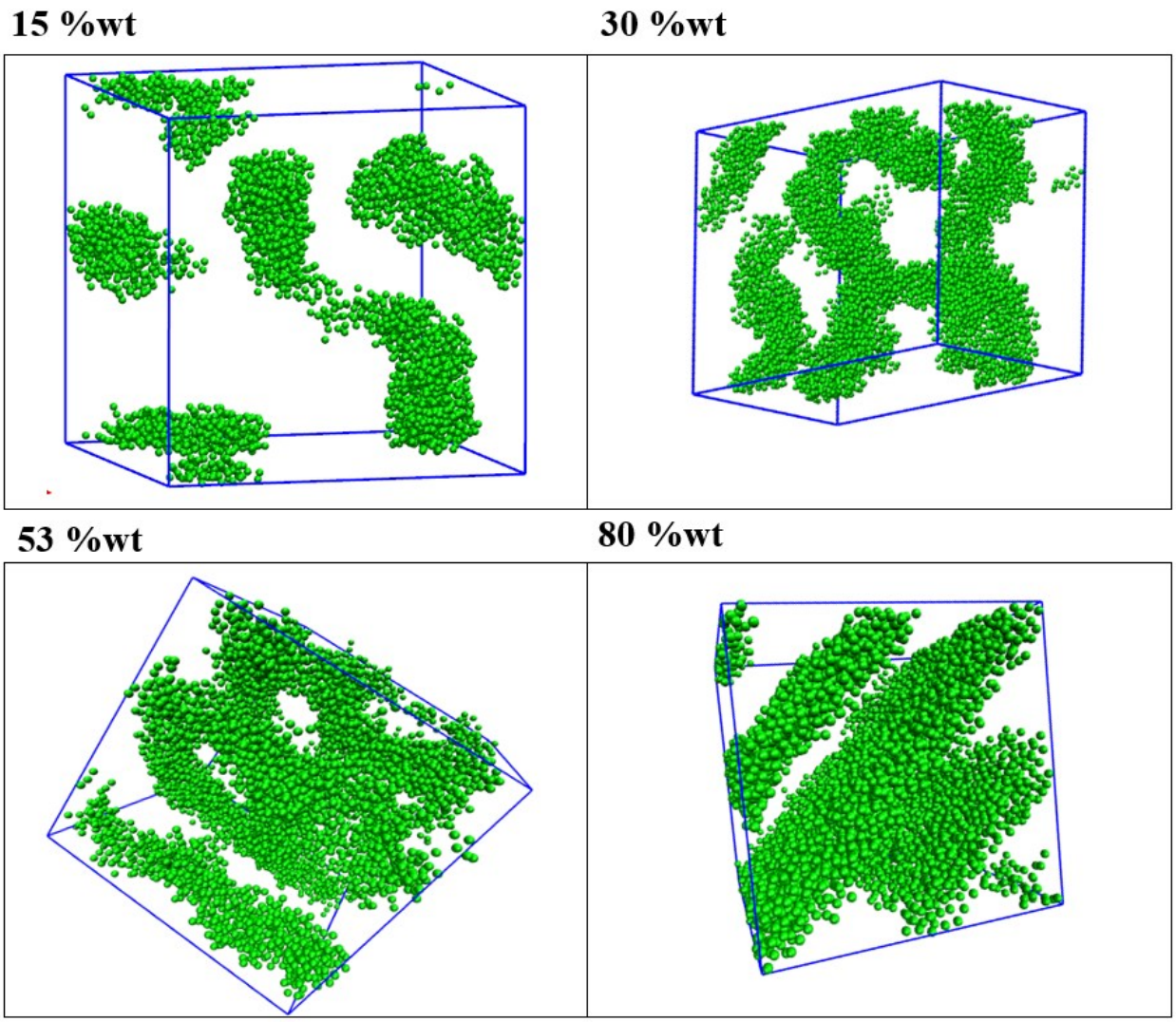

Figure S5. Final snapshots of the CG-MD simulations carried out for the system $C_{12}E_4$/water at different concentrations. For an easier visualization of the liquid structural organization only the alkyl chains are represented.

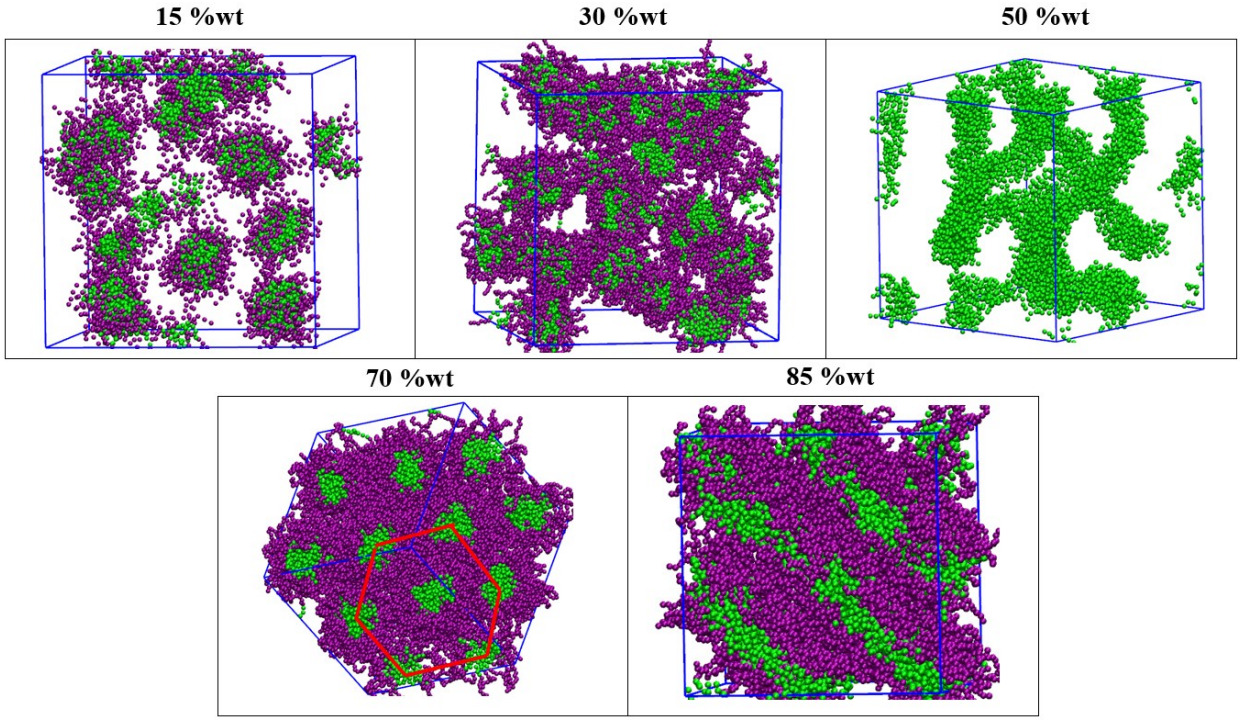

Figure S6. Final snapshots of the CG-MD simulations carried out for the system $C_{12}E_{10}$/water at different concentrations. Colors as in Figure S2.

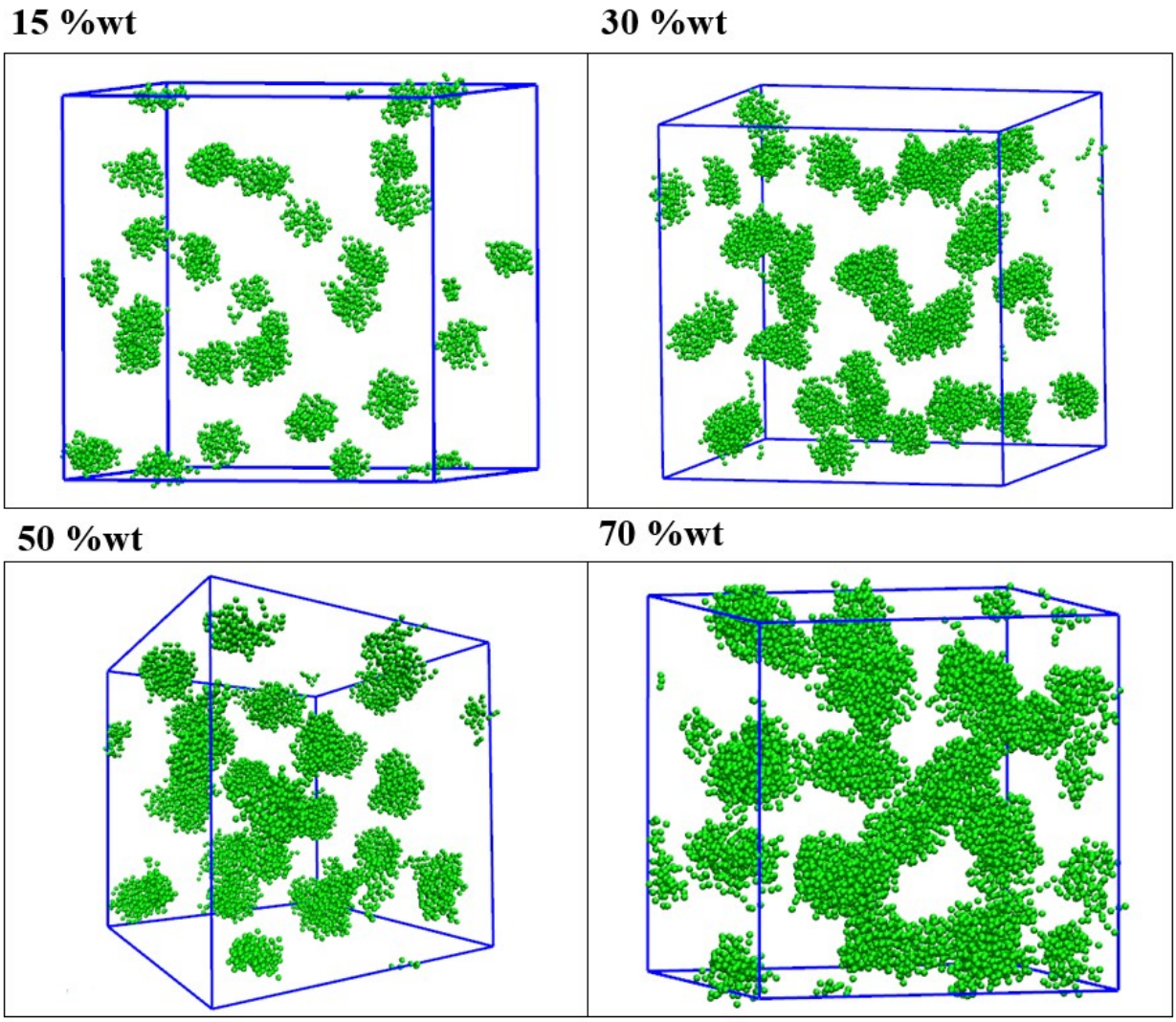

Figure S7. Final snapshots of the CG-MD simulations carried out for the system $C_{12}E_{23}$/water at different concentrations. For an easier visualization only the alkyl chains are represented.

4. CG-MD Simulations for C_{16} surfactants

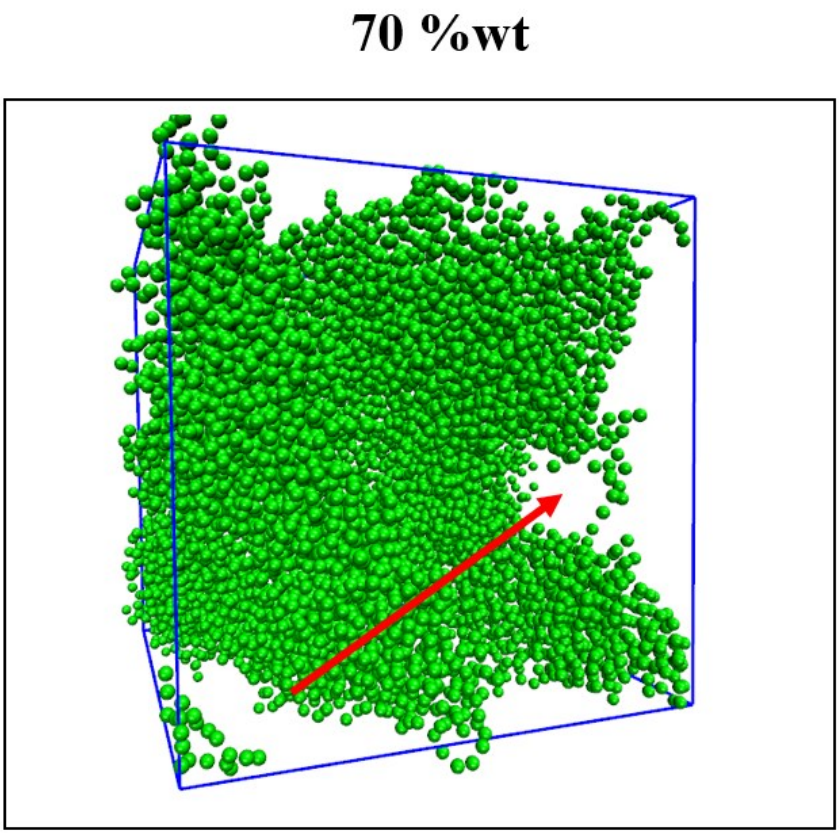

Figure S8. Pore defect in the $C_{16}E_6$/water system at 70%wt.

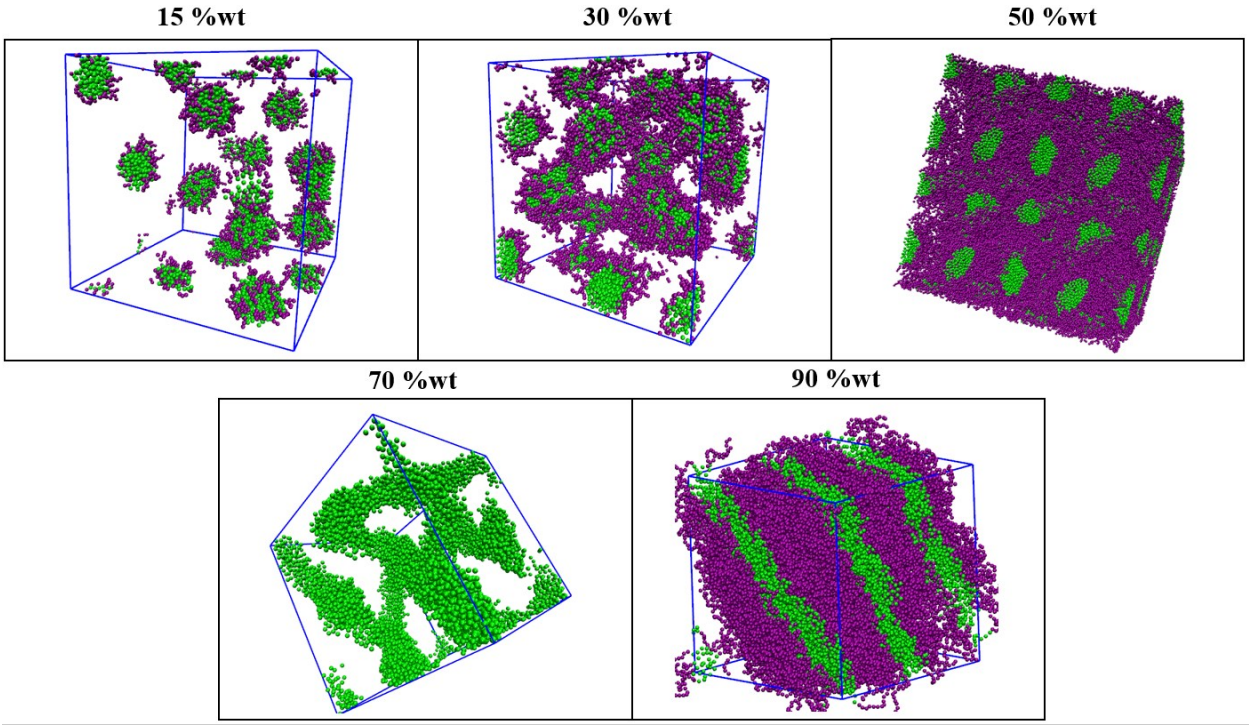

Figure S9. Final snapshots of the CG-MD simulations for the $C_{16}E_{12}$/water system at different concentrations. Colors as in Figure S2