

# Molecular investigation of the coalescence dynamics of surfactant-laden droplets

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## Introduction

### Key concepts:

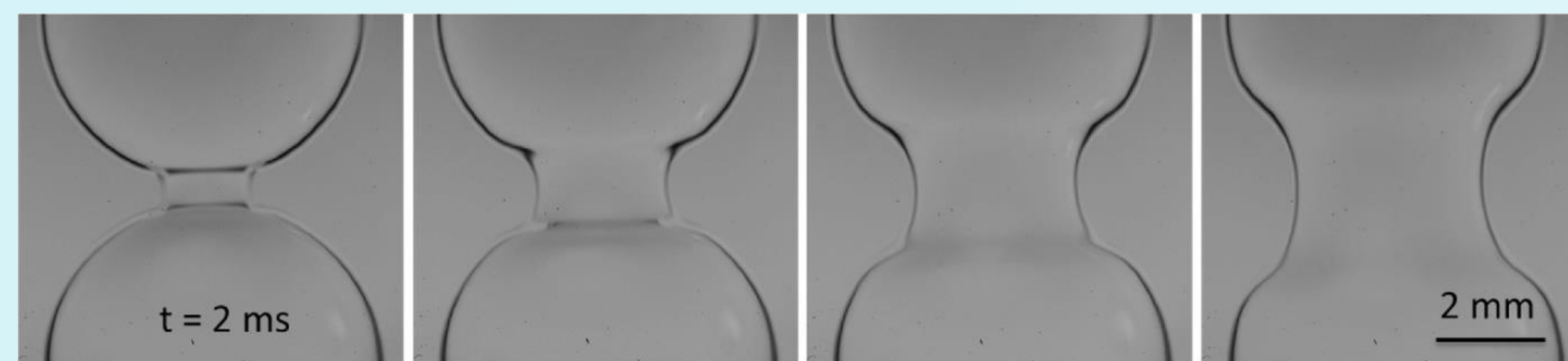
- Understand the coalescence dynamics of surfactant-laden droplets
- Optimize the coalescence process and inform surfactant design for relevant applications

### Aim:

- Reveal the mass transport mechanism and the role of key parameters in coalescence process

### Applications:

- Microfluidics, Inject printing, Spray cooling



Experimental image of droplets coalescence (aqueous solution SLES) [1]

## Model and Methodology

### Model:

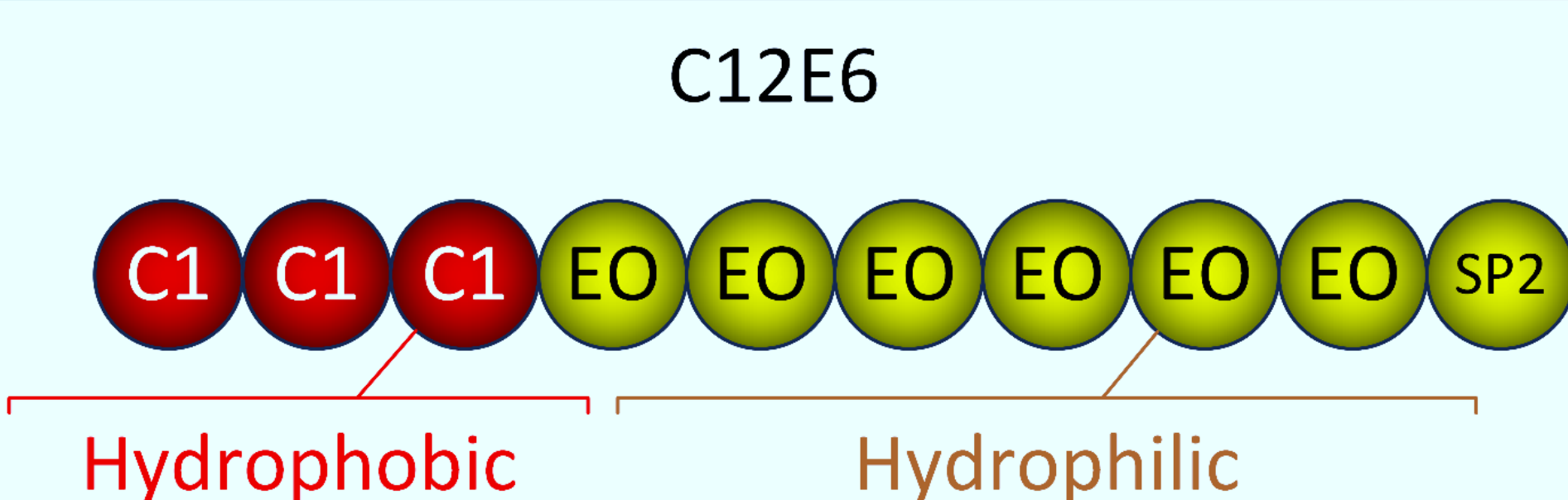
- Martini coarse grained force-field [2]

### Method:

- Molecular dynamics simulation (NVT and NPT ensembles)

### Materials:

- Water
- Non-ionic surfactant C12E6

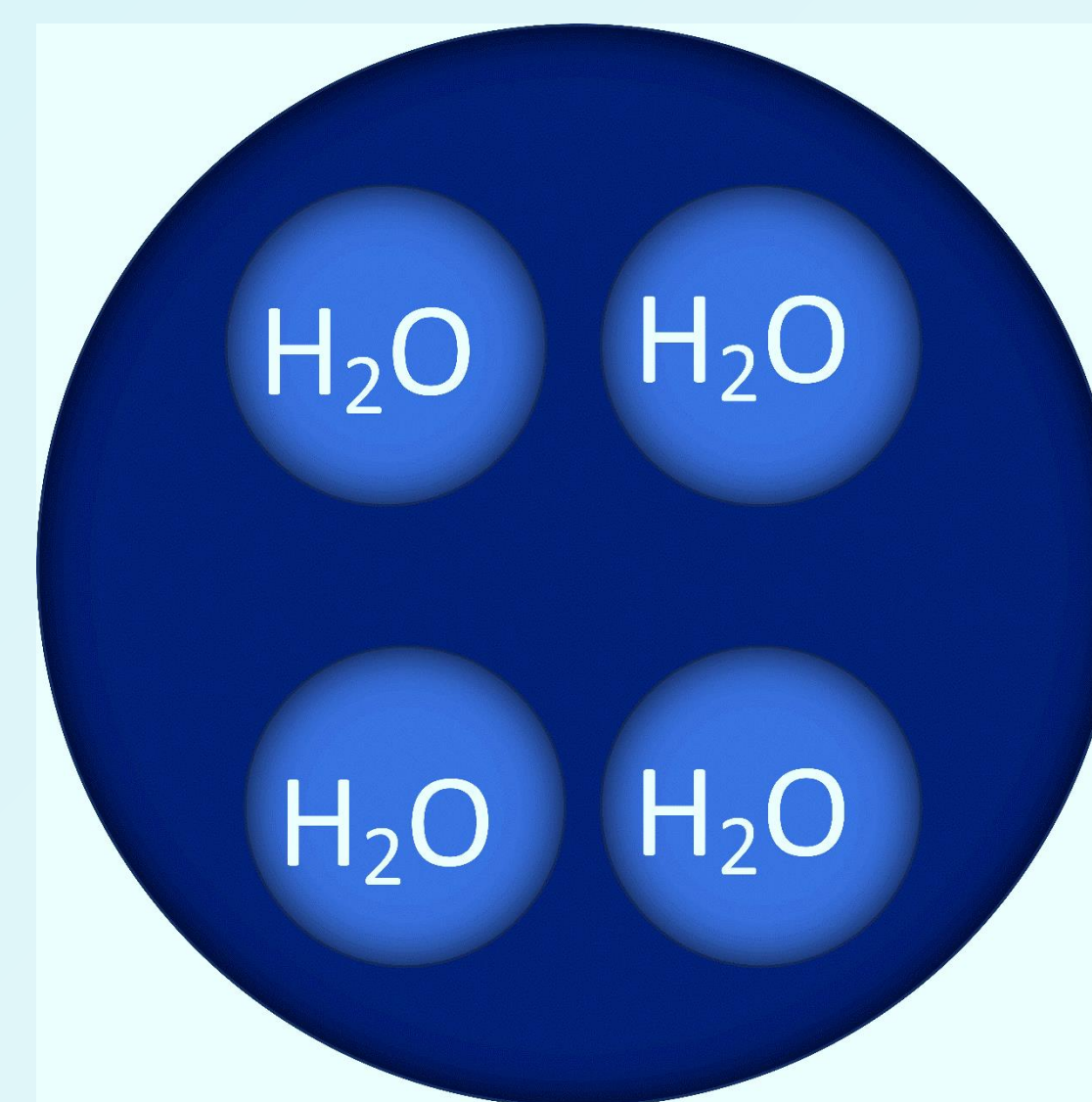


Martini representation of C12E6 surfactant

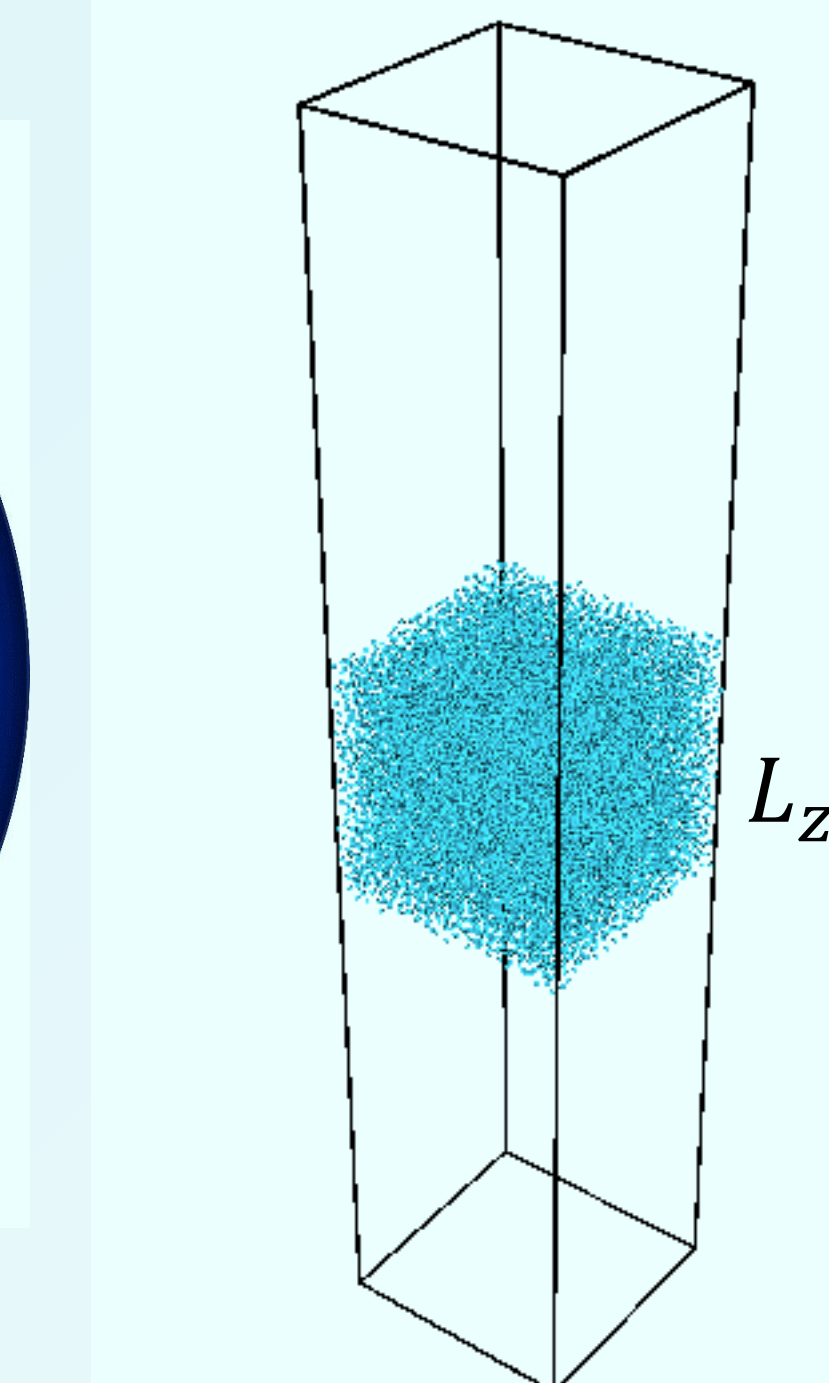
## Model and Methodology

Particle type (Martini)	Name
C1	Butane
EO	Ethylene oxide
SP2	Acetic acid

C12E6 beads definition in Martini force field [2]



Water bead in Martini force field



Water slab geometry for surface tension calculation

## Results

Evaluation of water surface tension (mechanical way), based on the relation:

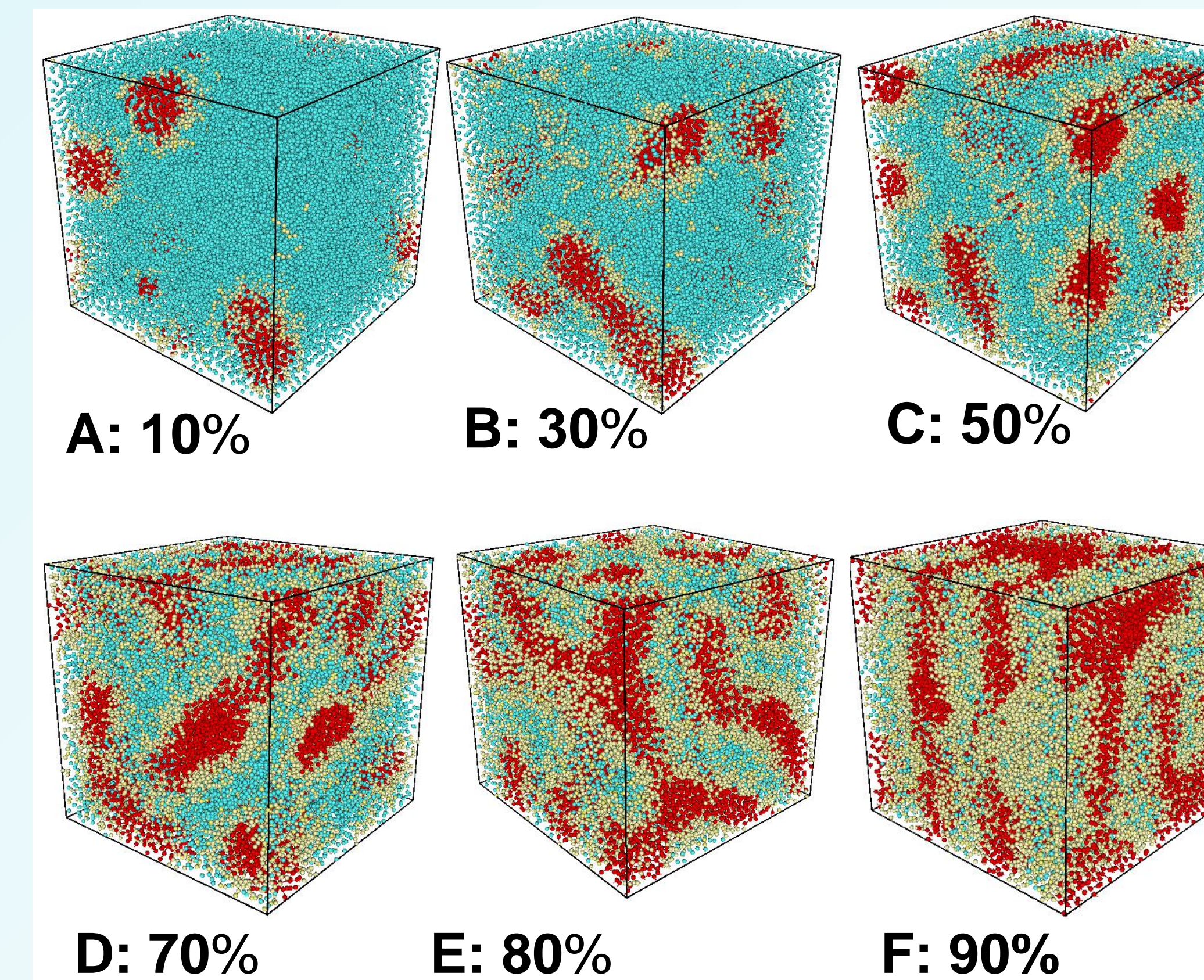
$$\gamma = \frac{L_z}{2} [P_{zz} - \frac{P_{xx} + P_{yy}}{2}]$$

Martini version	cut-off [Å]	Surface tension [mN/m]
3	11	27.11
3	25	50.21
3	35	50.50
2	11	31.02
2	25	56.05
2	35	85.80

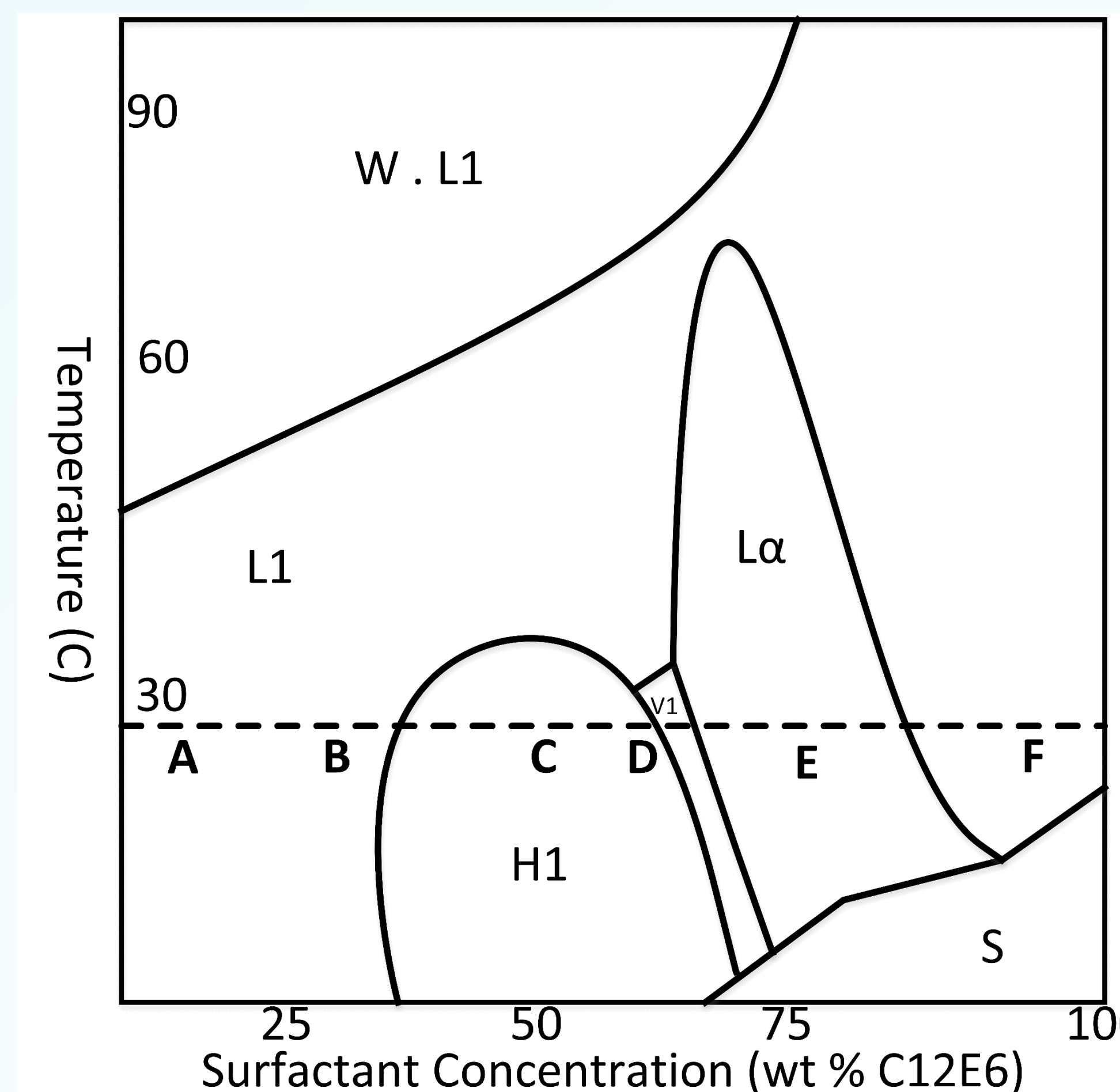
Surface tension of Water-air ( 25 °C): ~72 mN/m

## Results

Morphologies of water-surfactant system at different concentrations of surfactant (wt%)



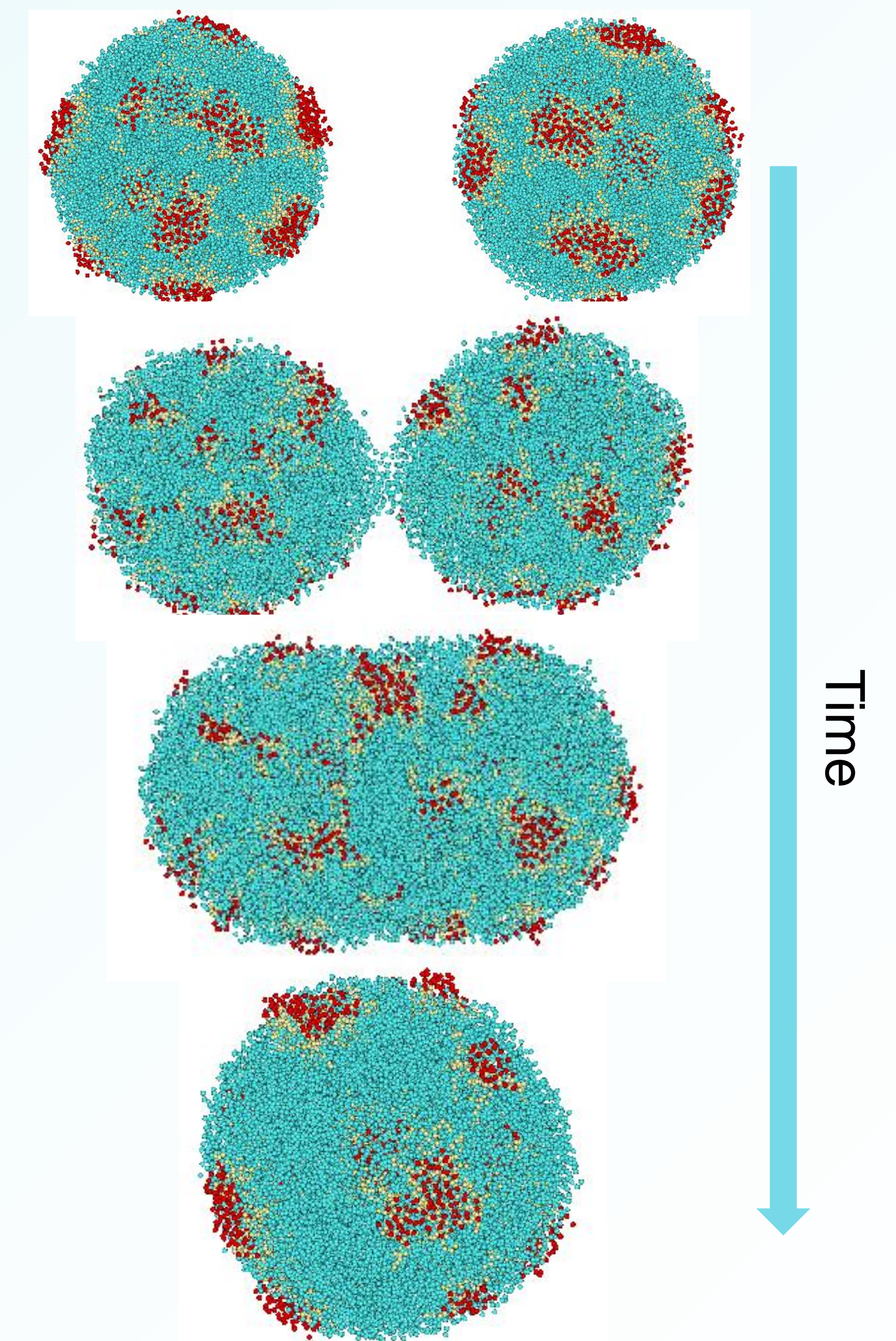
Experimental phase diagram of C12E6/water system [3]



Further simulations are needed to validate the phase behavior of the surfactant-water solution

## Results

Coalescence of surfactant-laden droplets



## Conclusion

- The Martini2.2 force-field with a cut-off of 25 Å indicates a close match with experimental results. Further model validation is required.
- We have presented early examples of droplet coalescence, which will enable us to carry out the full investigation of this phenomenon.

### References:

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