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Microemulsions: a new model for organic phases involved in ion separation methods

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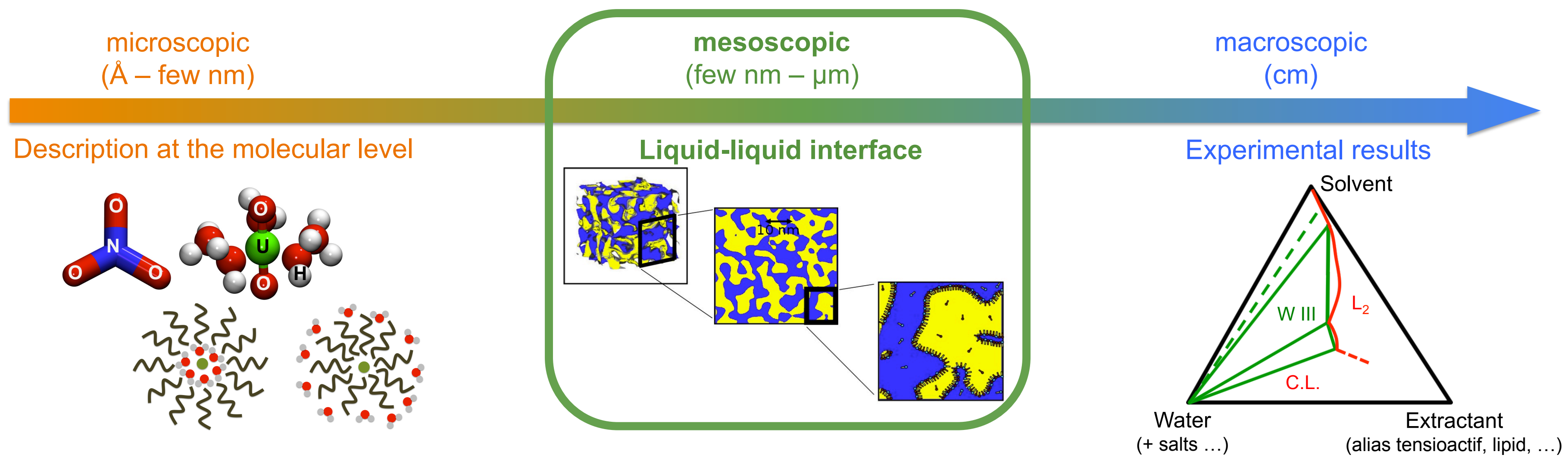
Introduction

Context

- ✓ Improvement of the reprocessing of spent nuclear fuel
- ✓ **Liquid-liquid extraction** equilibria
- ✓ **Microemulsion** model to describe the **organic phase**
- ✓ **Multi-scale** approach



Method

- ✓ The **physics** of a system composed of **soft interfaces** (low bending energy compared to the thermal one, negligible long-range electrostatic and steric interactions) is **dominated** by the **Helfrich Hamiltonian** of the surfactant interface (between oil and water) [1].
- ✓ In our model, the **surfactant interface** is **described** by appropriate **two level-cuts** of a **Gaussian random field** based on wavelets proposed by Arleth *et al.* [2].
- ✓ The **free energy density** of the Gaussian random field with level-cuts can be approximated by:

$$f_{\text{free}} = \frac{S}{V}\left[2\boldsymbol{\kappa}\langle(H-\boldsymbol{H_0})^2\rangle + \bar{\boldsymbol{\kappa}}\langle K\rangle\right] - \frac{1}{2\pi^2}\int_k \mathrm{d}k\; k^2 \ln \nu(k)$$

Rigidity controlled by κ and $\bar{\kappa}$

- ✓ Two constants:
  - → the bending elastic constant κ
  - → the Gaussian elastic constant $\bar{\kappa}$
- ✓ One unique constant:

$$\kappa^* = 2\kappa + \bar{\kappa}$$

→ Analogy with the packing parameter p_0

$$f_{\text{free}} = \frac{1}{2}\boldsymbol{\kappa}^*(p - \boldsymbol{p_0})^2$$

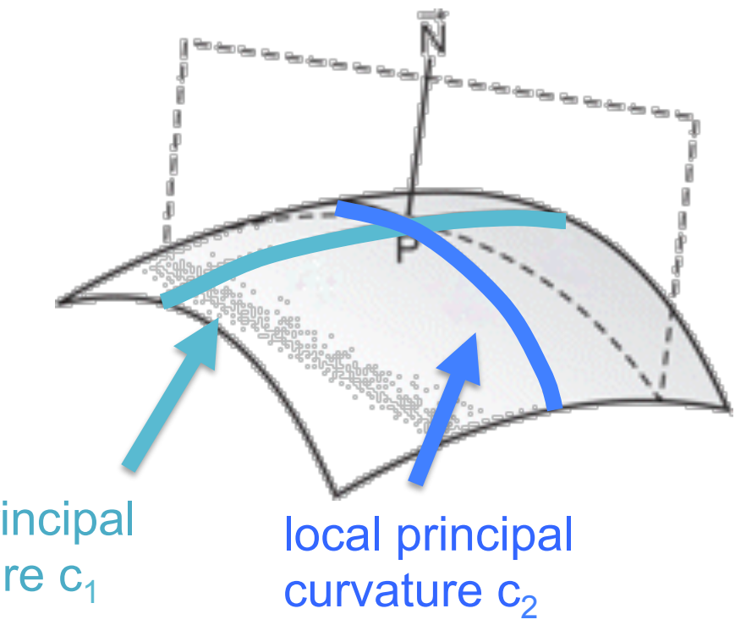
Curvatures:

- ✓ Spontaneous curvature H_0 imposed
- ✓ Mean average curvature H

$H = ½ (c_1 + c_2)$

- ✓ Gaussian curvature K

$K = (c_1 \times c_2)$



Results

Microemulsion swelling (case of zero spontaneous curvature)

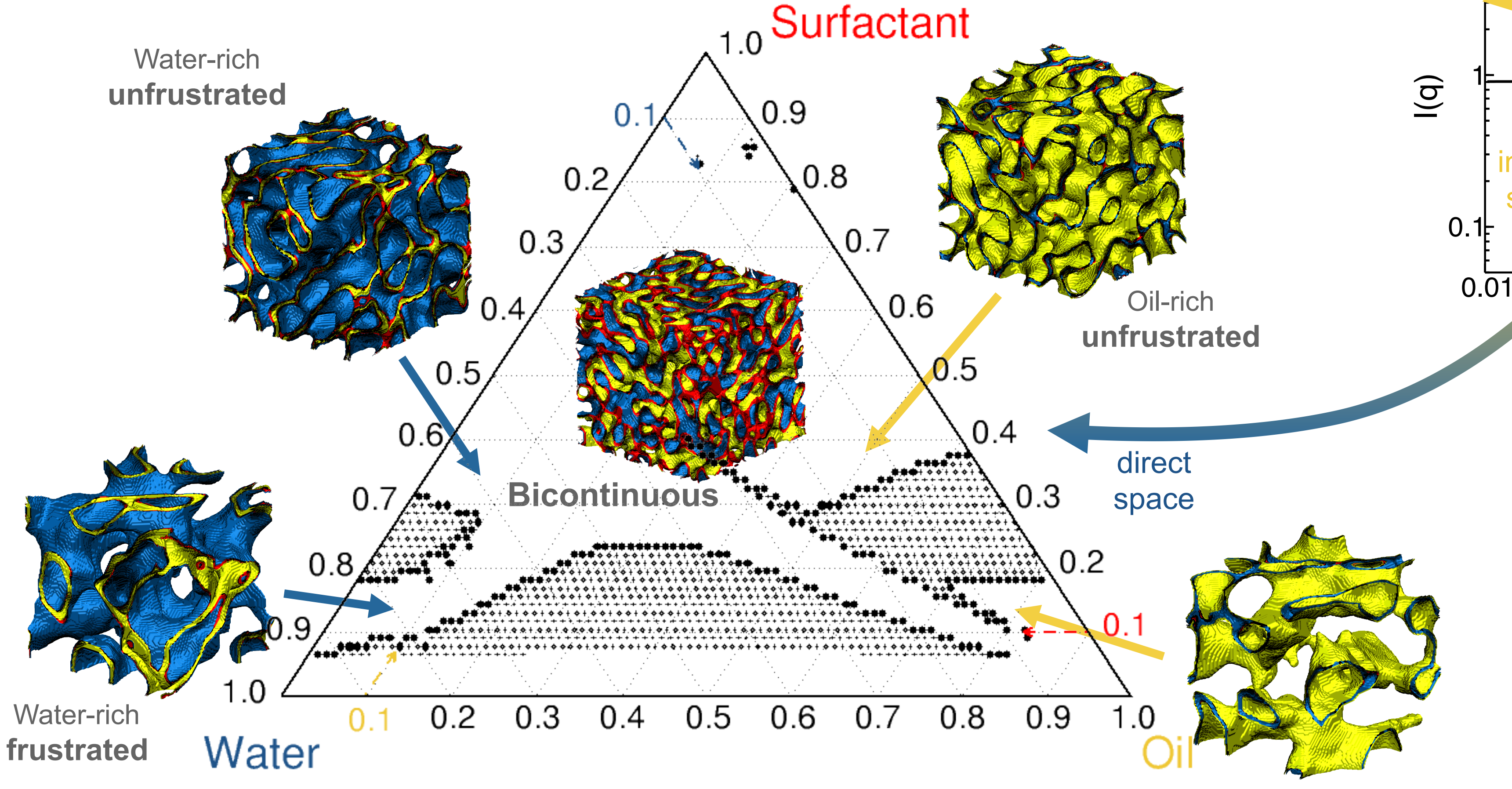
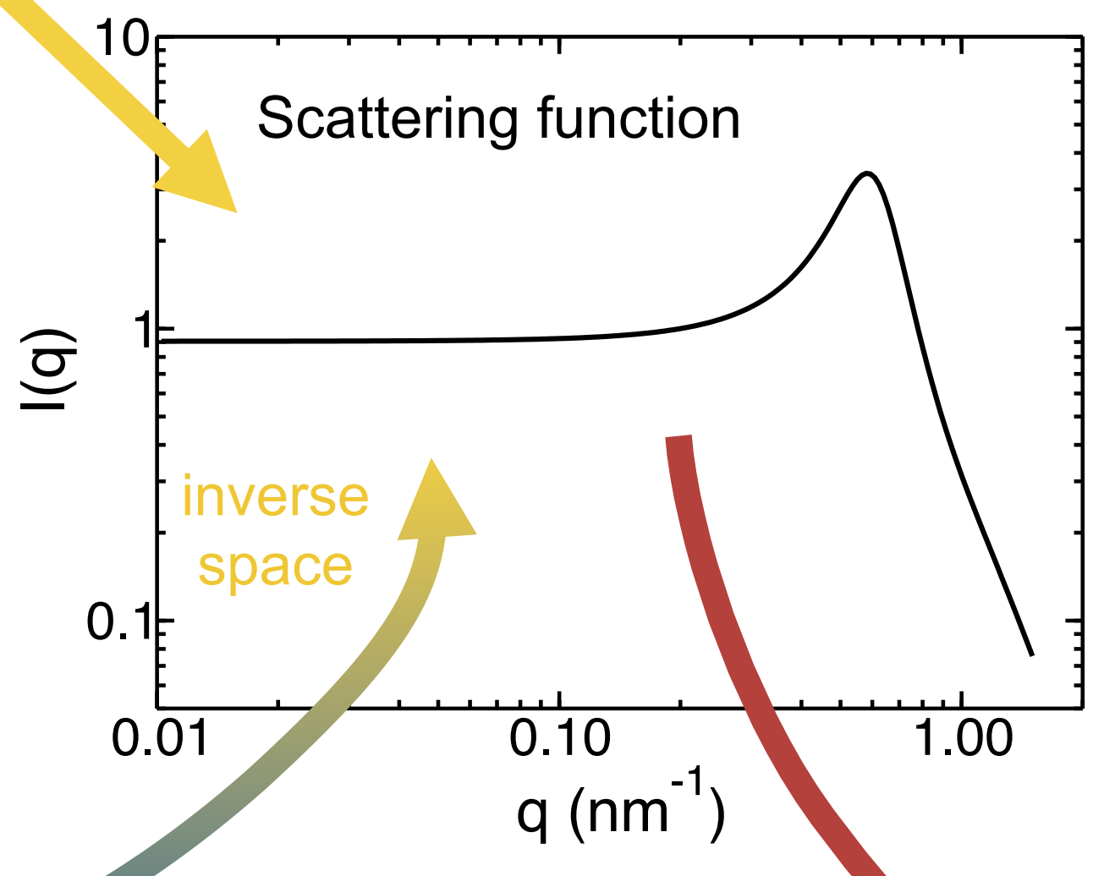


Fig.: Ternary phase diagram calculated using our model for rigid microemulsion (κ = 2 k_BT and $\bar{\kappa}$ = 0 k_BT) and p_0 = 1 (H_0 = 0).

Oil-rich
frustrated



$$D^*\Sigma = \frac{2\pi}{\boldsymbol{q_{\max}}}\frac{\phi_s}{l_s}$$

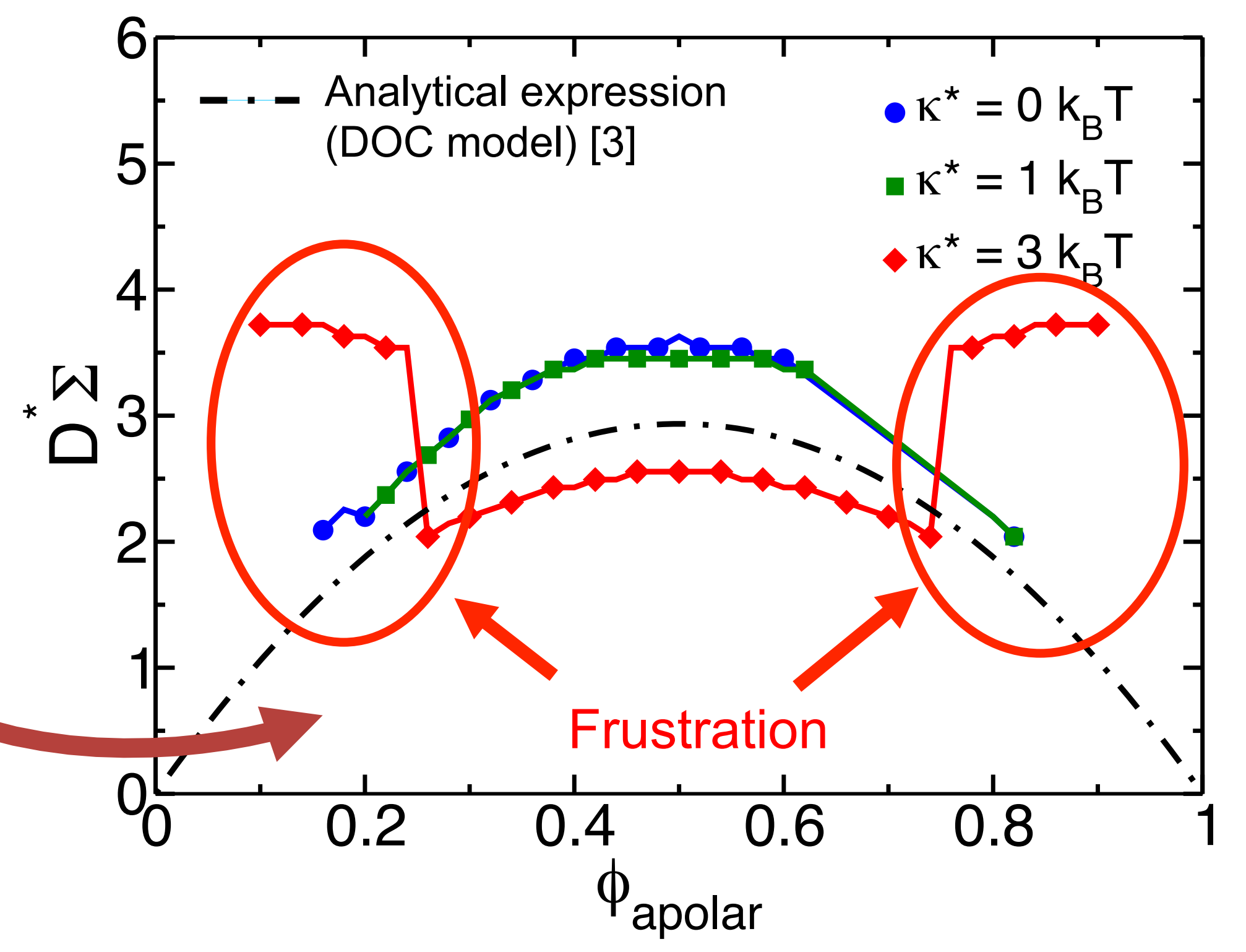


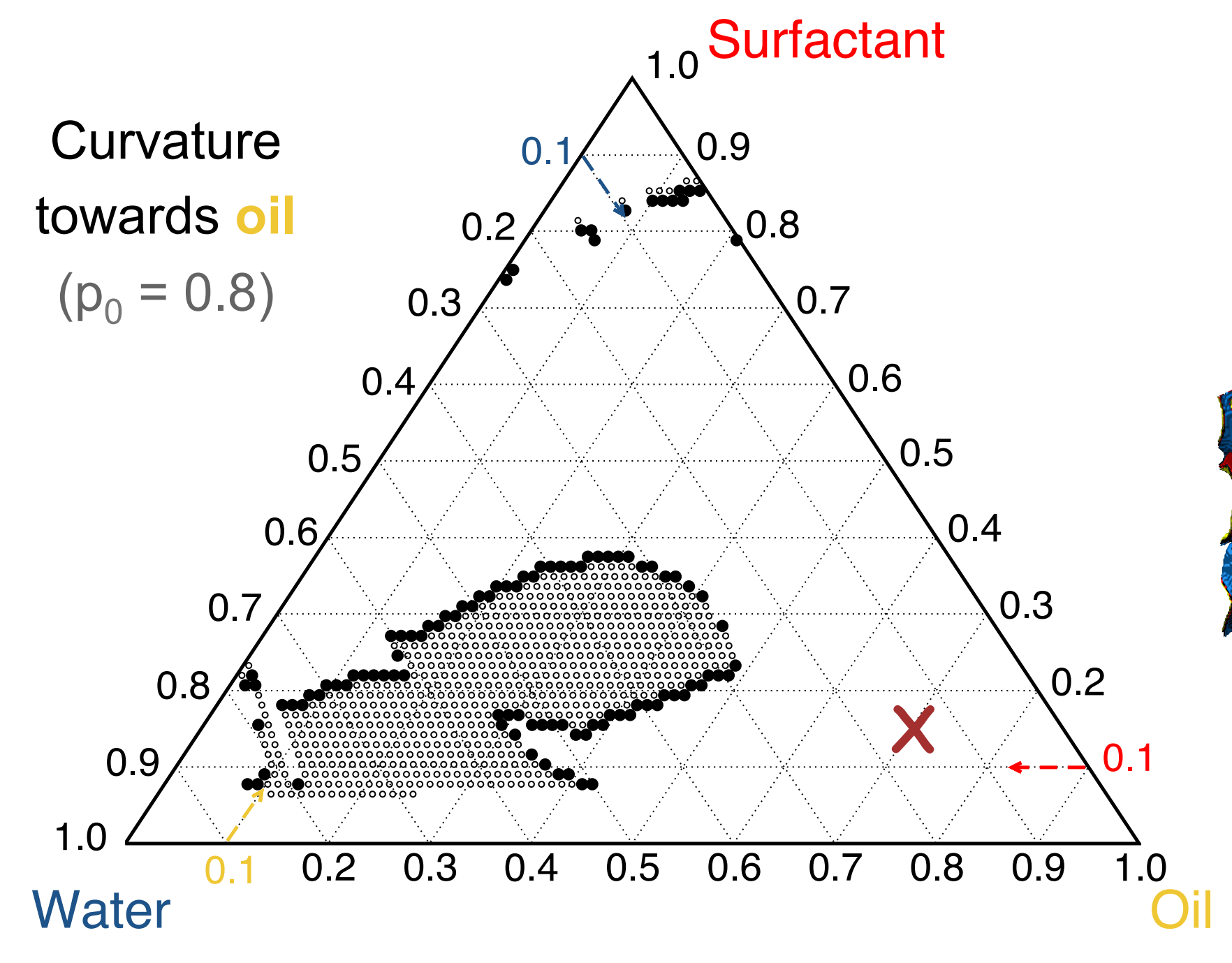
Fig.: Scaled peak position for flexible (blue and green) and rigid (red) microemulsion plotted as a function of the volume fraction of the apolar phase for a volume fraction of surfactant Φ_s = 0.15.

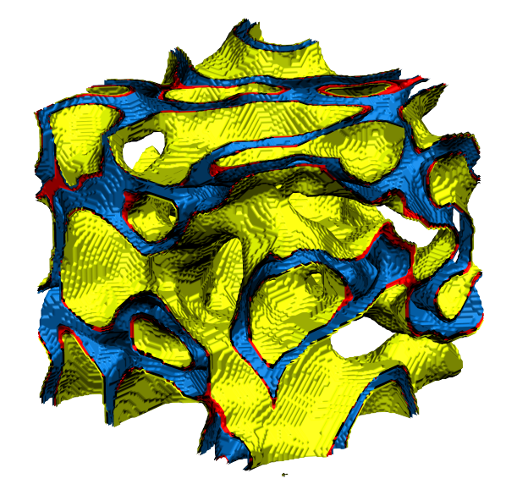
- ✓ **Spinodal instablities** calculations (case of rigid surfactant film)
- ✓ Thermalized **unfrustrated**, **frustrated** and **bicontinuous** microemulsions

- ✓ **Frustration** appears only in the case of **rigid microemulsions**
- ✓ **Unfrustrated bicontinuous microemulsions** for 0.2 < Φ_{apolar} < 0.8

Influence of the spontaneous curvature (case of rigid microemulsions)

Curvature towards **oil**
(p_0 = 0.8)





Locally lamellar

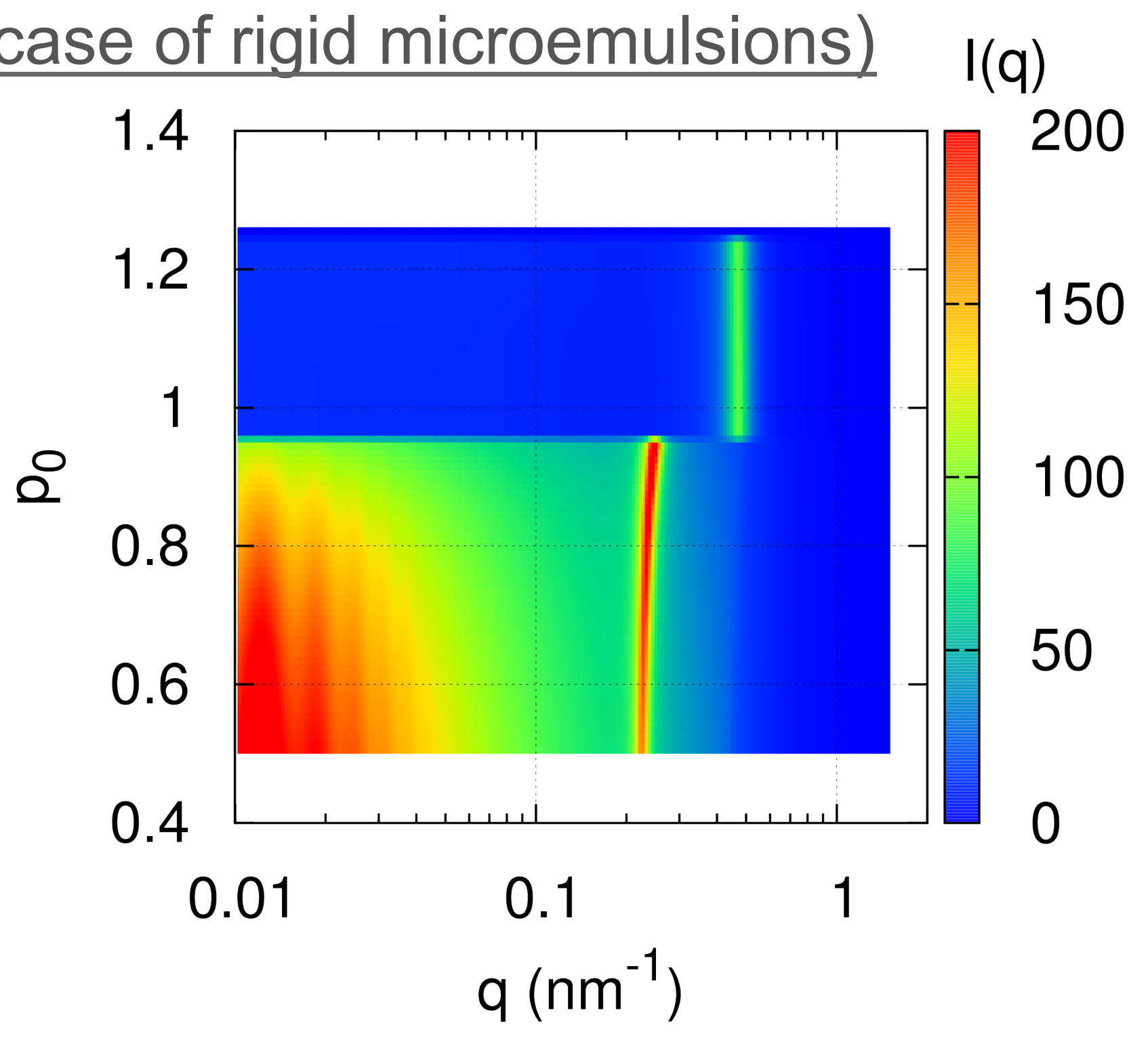
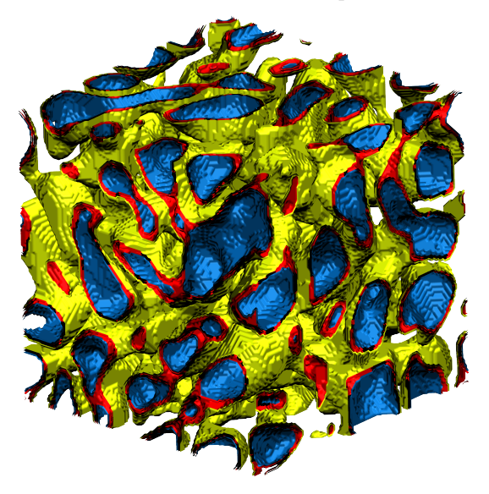
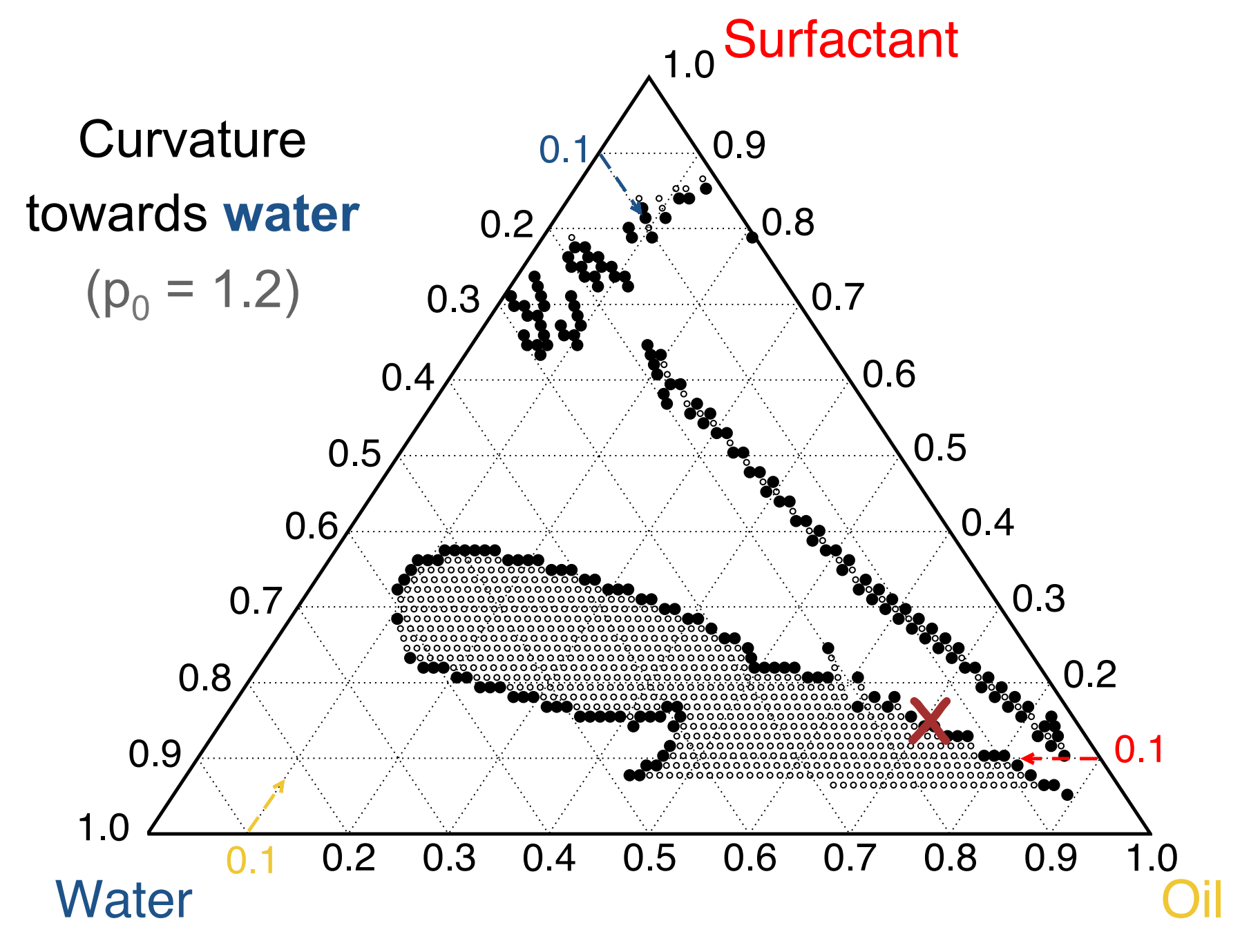


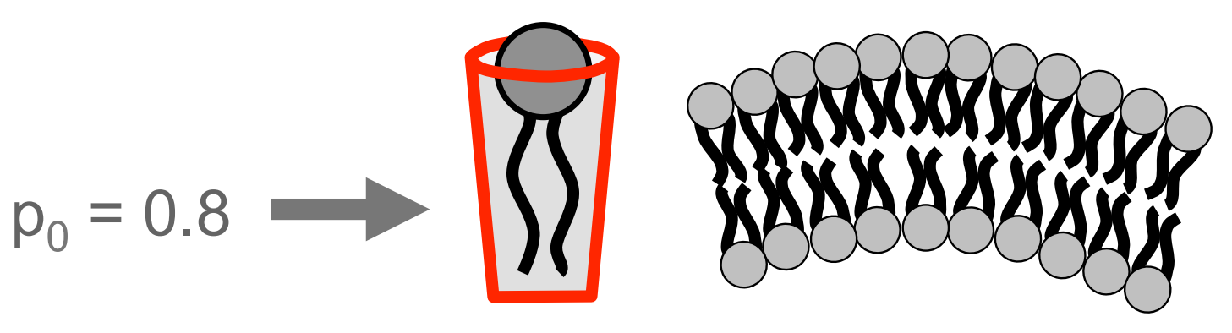
Fig.: 2D map of the scattering functions as a function of the spontaneous packing parameter p_0 calculated for x_{water} ≈ 0.15, x_{oil} ≈ 0.70 and $x_{surfactant}$ ≈ 0.15.

Connected droplets

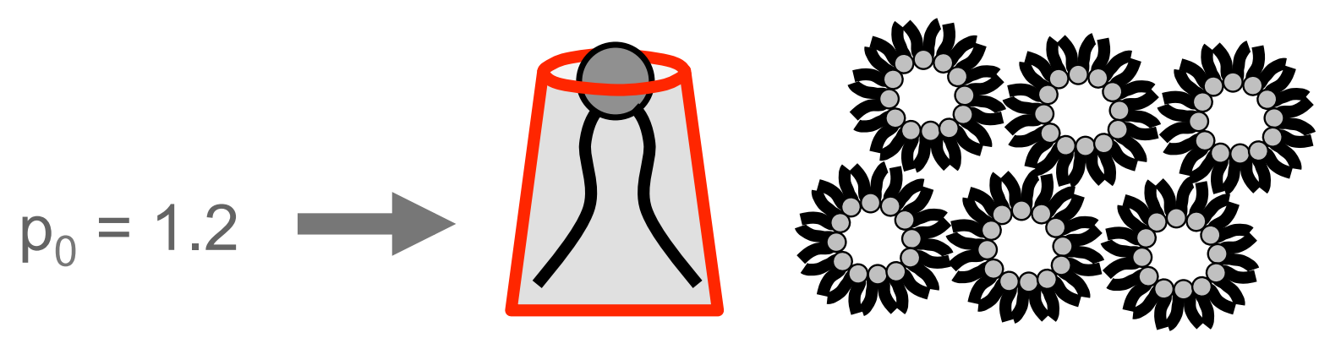


Curvature towards **water**
(p_0 = 1.2)





flexible bilayers, vesicles



inverted micelles

Acknowledgments

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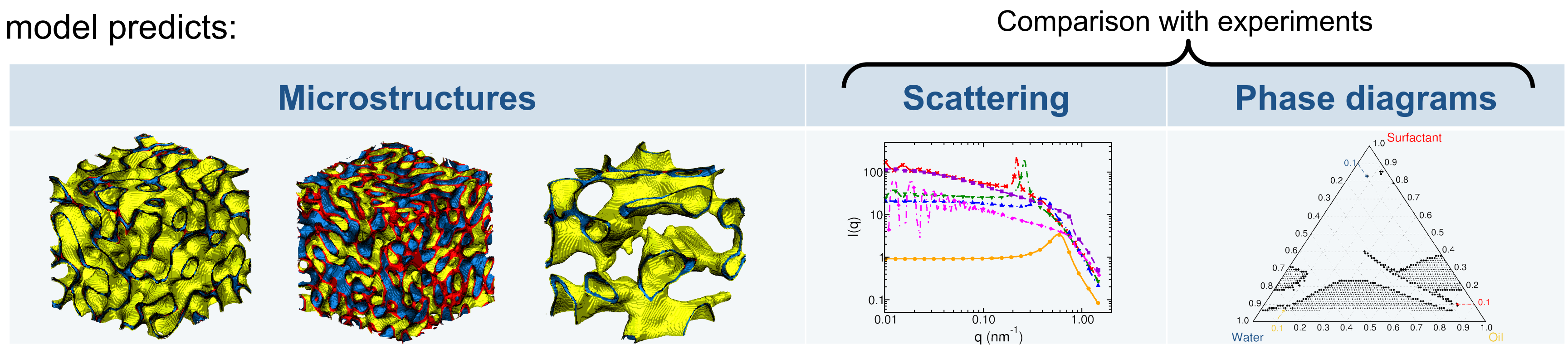
References

[1] W. Helfrich, *Z. Naturforsch. C* **28**, 693 (1973)
[2] L. Arleth *et al.*, *J. Chem. Phys.* **115**, 3923 (2001)
[3] J. Jouffroy *et al.*, *J. Phys.* **43**, 1241 (1982)

Conclusions and outlooks

Our model predicts:



Improvement of our model to take into account:

- ✓ the **presence** of **charged species** (ions and ionic surfactant),
- ✓ the **aggregation** of surfactant molecules.