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

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► **To cite this version:**

Magali Duvail, Jean-François Dufrêche, Thomas Zemb. Microemulsions: a new model for organic phases involved in ion separation methods. Emulsification : Modélisation, Technologies et Applications, Nov 2012, Lyon, France. <hal-04693919>

HAL Id: hal-04693919

<https://hal.umontpellier.fr/hal-04693919v1>

Submitted on 11 Sep 2024

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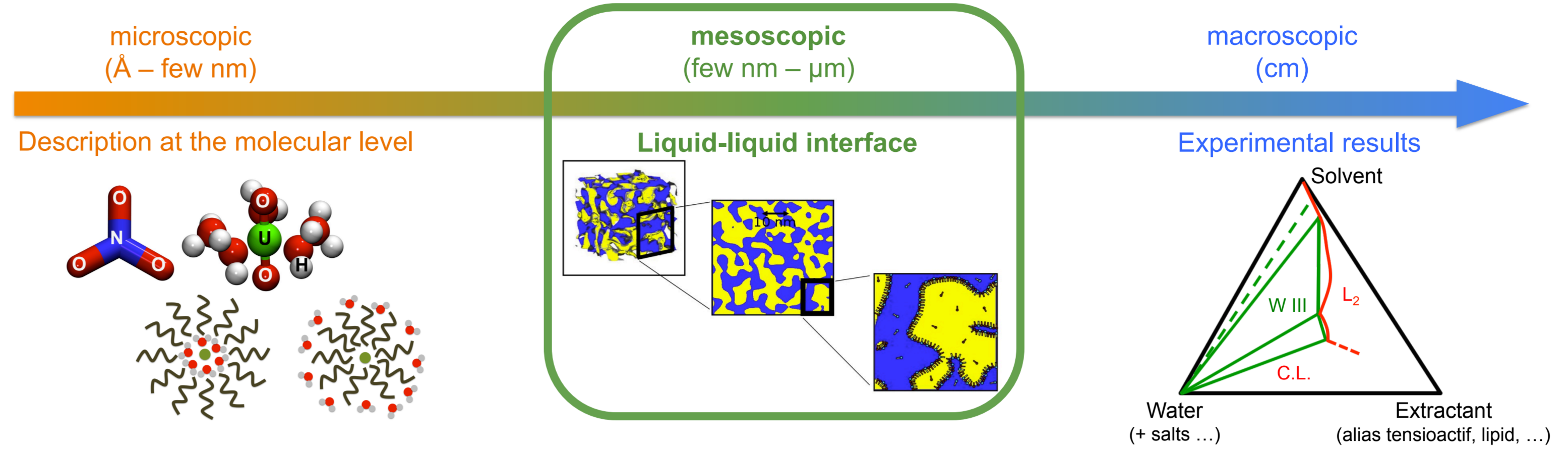


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Introduction

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:

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

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

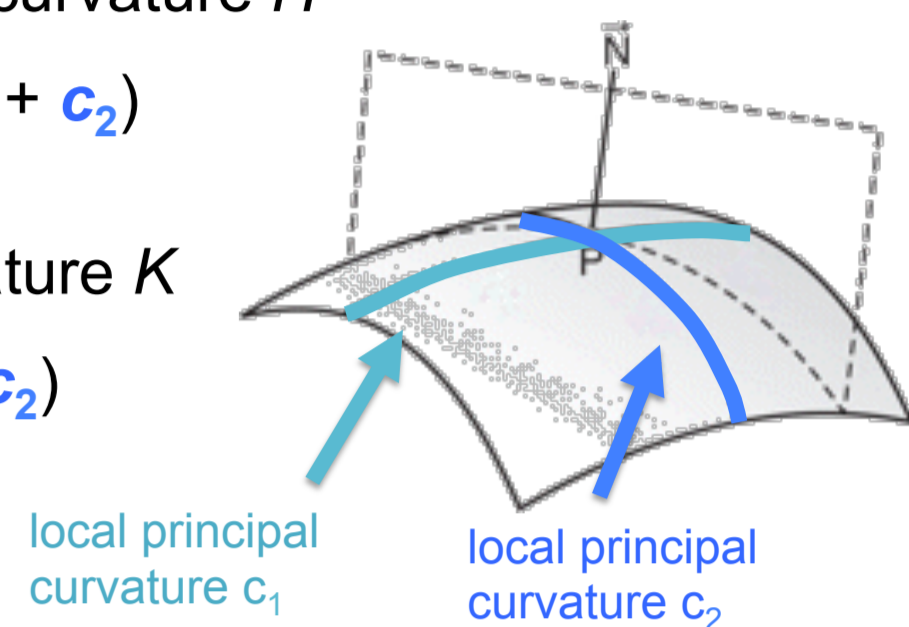
- ✓ Two constants:
 - the bending elastic constant κ
 - the Gaussian elastic constant $\bar{\kappa}$
 - ✓ One unique constant:
 - $\kappa^* = 2\kappa + \bar{\kappa}$
 - Analogy with the packing parameter p_0
- $$f_{\text{free}} = \frac{1}{2} \kappa^* (p - p_0)^2$$

Curvatures:

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

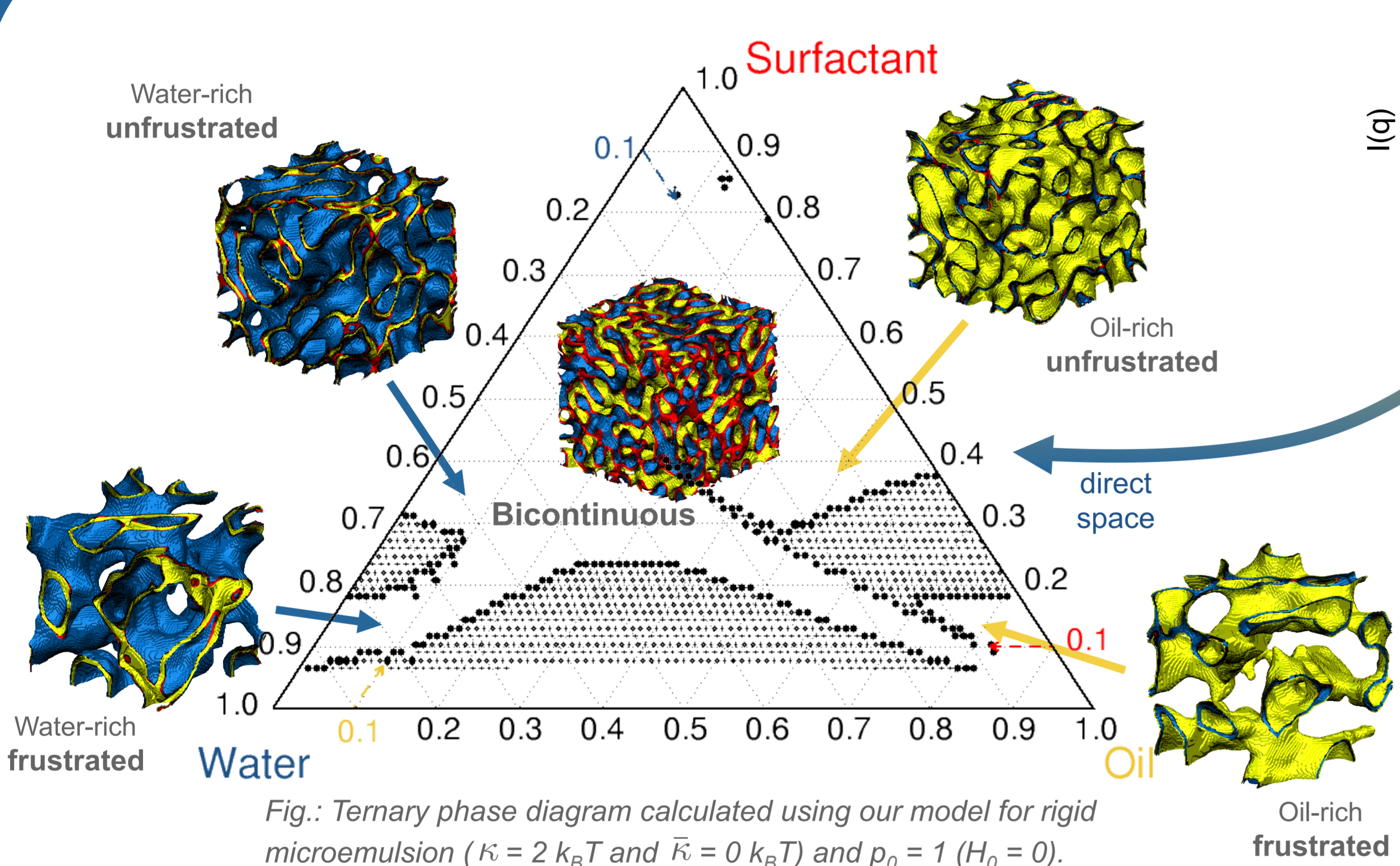
$$H = \frac{1}{2} (c_1 + c_2)$$
- ✓ Gaussian curvature K

$$K = (c_1 \times c_2)$$



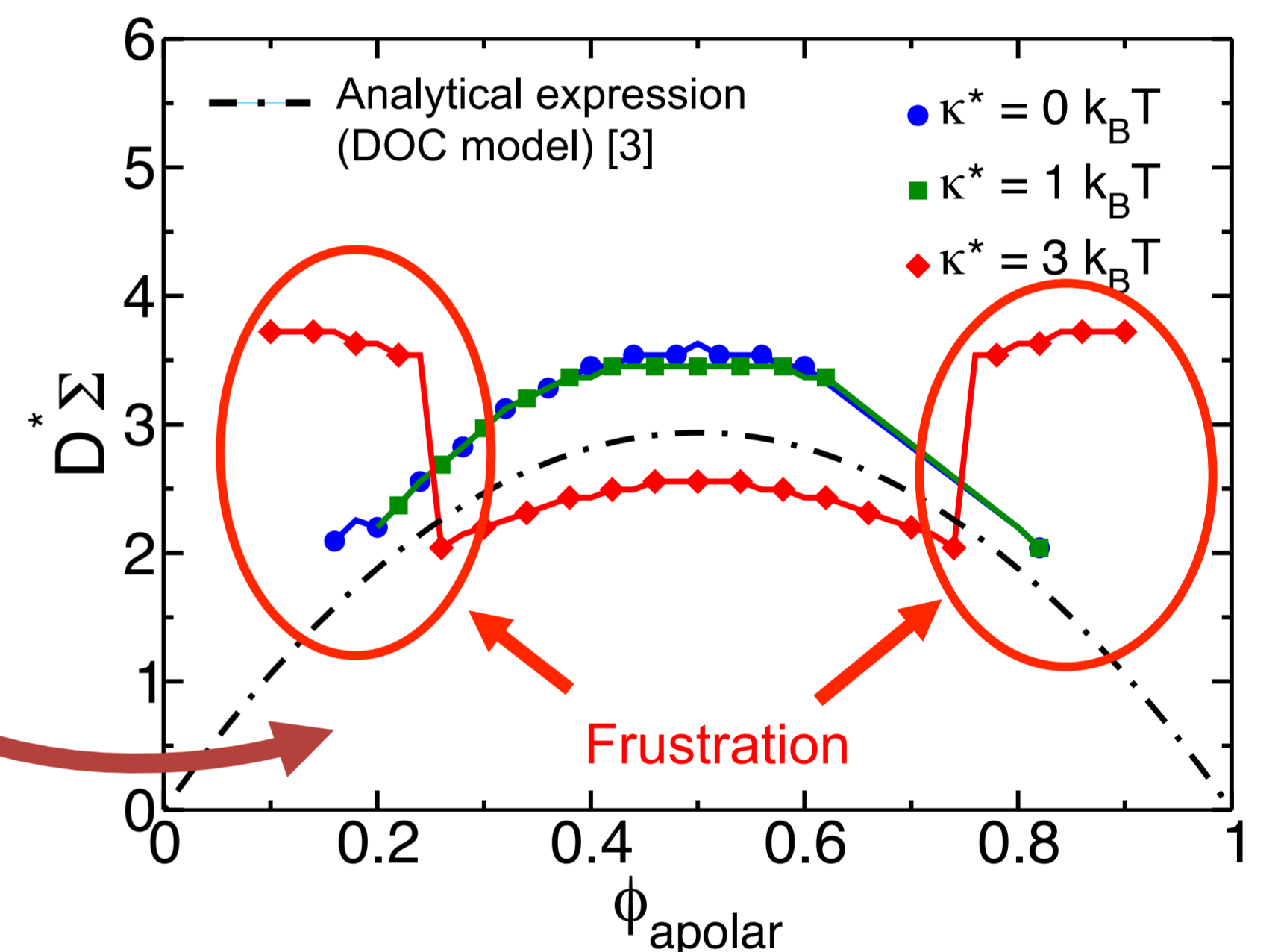
Results

Microemulsion swelling (case of zero spontaneous curvature)



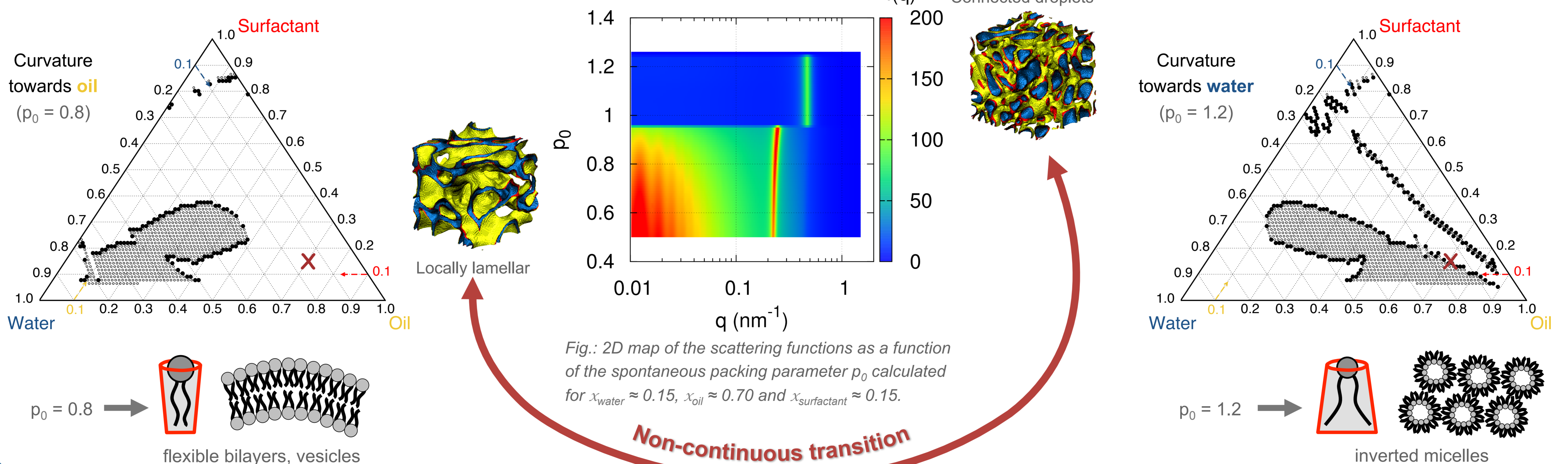
- ✓ **Spinodal instabilities** calculations (case of rigid surfactant film)
- ✓ Thermalized **unfrustrated**, **frustrated** and **bicontinuous** microemulsions

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



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

Influence of the spontaneous curvature (case of rigid microemulsions)



Non-continuous transition

Acknowledgments

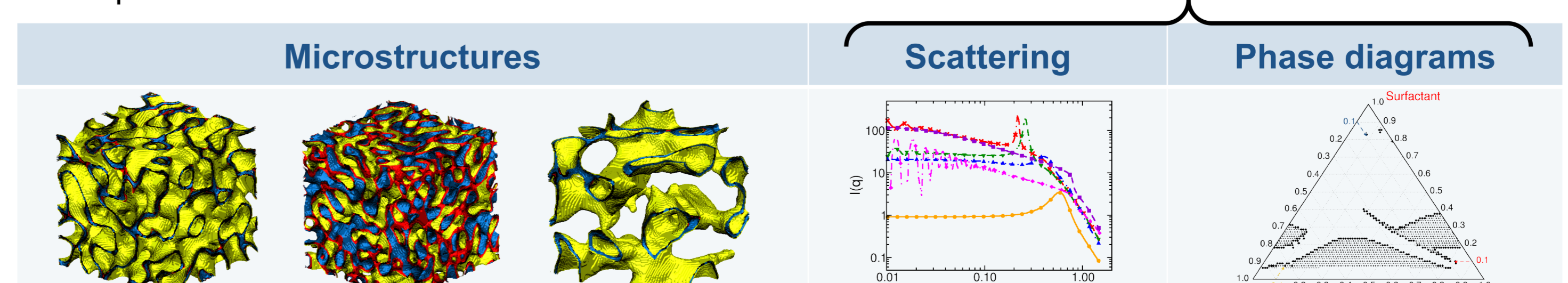
The authors are grateful to Pr. L. Arleth (University of Copenhagen, Niels Bohr Institute) and Dr. S. Marčelja (Australian National University – Canberra, Department of Applied Mathematics) for helpful discussions and suggestions.

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.

