Contribution ID: 13 Type: not specified

## Static and Dynamics of Aggregation in Surfactant-Free Ternary Mixtures

Wednesday, 17 December 2025 11:00 (20 minutes)

Presumably simple solutions can show a variety of nanoscale aggregation structures. Ternary mixtures of three liquids, in which two show only partial mutual solubility, resemble different types of microemulsions even in the absence of classical surfactants. We present fully atomistic molecular dynamics simulations of octanol/ethanol/water mixtures, a typical representative of these "surfactant-free microemulsions". We compare MD simulations results with different scattering experiments: SAXS/WAXS and neutron scattering reveal the structures present. Neutron Spin-Echo and NMR experiments gives insight into their dynamic behaviour.

## References

- 1) Schöttl, S.; Marcus, J.; Diat, O.; Touraud, D.; Kunz, W.; Zemb, T.; Horinek, D. Emergence of Surfactant-Free Micelles from Ternary Solutions Chem. Sci. 2014, 5, 2949-2954.
- 2) Schöttl,S.; Lopian, T.; Prévost, S.; Touraud, D.; Grillo, I.; Diat, O.; Zemb, T.; Horinek, D.

Combined MD/SAS analysis of organization on a nanometer-scale in ternary solvent solutions containing a hydrotrope. J. Coll. Inter. Sci. 2019, 540, 623-633.

3) Malayil Kalathil, F.; Plazanet, M..; Koza, M.M.; Falus, P.; Czakkel, O.; Fouquet, P.; Horinek, D.; Alba-Simionesco, C.; Hoffmann I.

How the formation of ultra-soft microemulsions affects dynamical properties at different length scales J. Mol. Liquids 2025, 432. 127684.

## **Abstract Title**

Static and Dynamics of Aggregation in Surfactant-Free Ternary Mixtures

Primary author: HORINEK, Dominik (University of Regensburg)

**Presenter:** HORINEK, Dominik (University of Regensburg)

**Session Classification:** Talks