Investigation of dye-surfactant-mixtures in solution

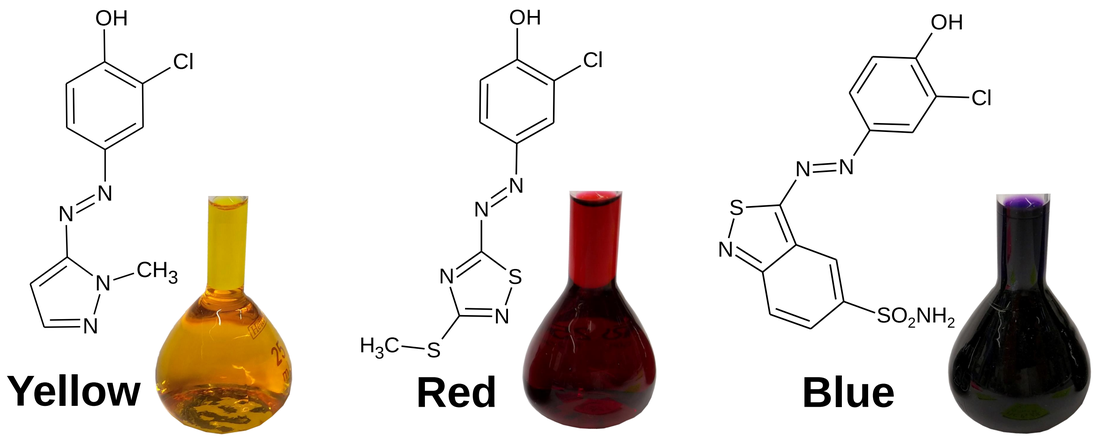
Micellar solubilization of organic molecules

The solubilization of hydrophobic substances into surfactant micelles is a commonly used technique for applications such as detergence, wastewater treatment, or drug transport in pharmaceutical applications. Another important field where these interactions play a vital role is the dyeing process.

In the context of hair dyes, dye-surfactant interactions come into play during hair-dyeing as well as hair-washing. Up until now developments in this field largely rely on empirical optimization of the dyeing conditions. Understanding the underlying principles of dye-solubilization and the morphology of dye-surfactant aggregates would help to find a more systematic approach towards the design of hair-dye-formulations.

Dissociative direct dyes for hair-dyeing

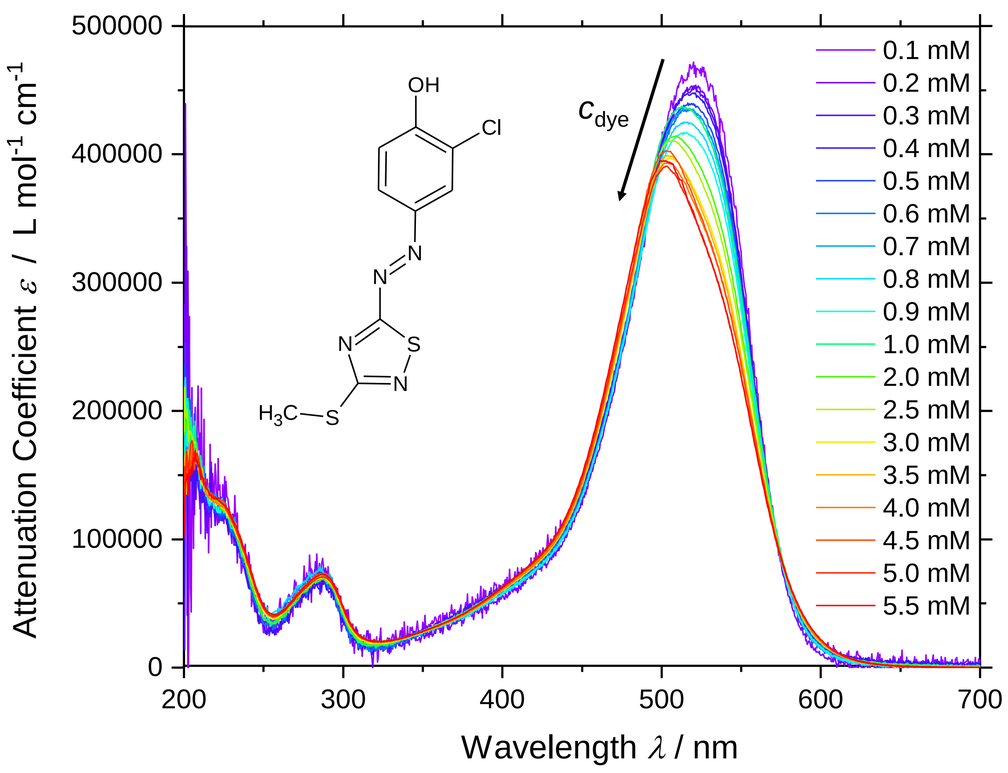
Three dissociative direct dyes are studied. Their water-solubility increases with increasing pH due to the dissociation of H^+ from the phenolic OH-group.



Solubility of pure dye

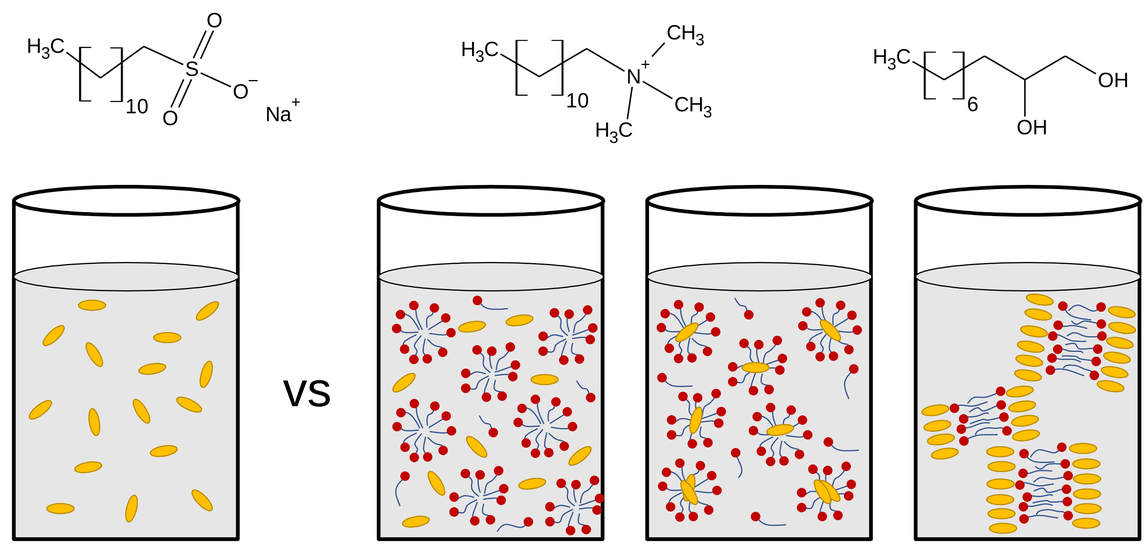
Two different buffer systems with pH-values of either 10.5 or 9.8 ± 0.5 are developed to dissolve the dye and to establish a suitable reference system.

The UV/vis-absorption maximum of the red dye in a buffer solution of pH = 9.8 ± 0.5 shows a blue-shift with increasing dye-concentration. This could be an indication of dye-aggregation, which has yet to be confirmed via light-scattering.

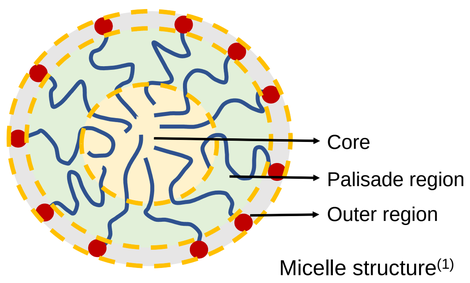


Solubilization of dye with surfactant

Dye solutions will be prepared with surfactants in selected buffer systems. The resulting solutions of dye and surfactant will be compared to the solutions with pure dye serving as the reference.

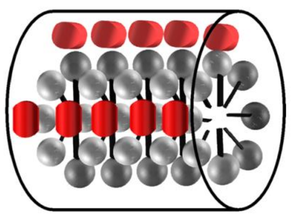


Aggregation of the dye and surfactant is expected. This could happen due to the incorporation of the dye into different parts of the surfactant micelles:(1)



Micelle structure(1)

In a study by Kutz et al. dye-surfactant aggregates with cylindrical shape were reported:(2)

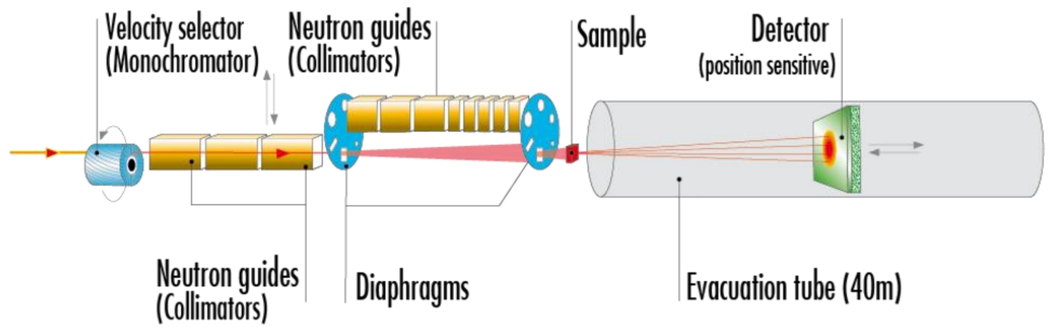


Cylindrical aggregate(2)

During this project, the morphology of the dye-surfactant aggregates will be studied in detail.

Techniques for studying aggregate morphology

Light scattering will be used to analyse the aggregate size of yellow and red dye. Absorption of light prohibits corresponding analysis of the blue dye. Thus, **small-angle neutron scattering** will be the method of choice to find out about aggregate size and shape. In addition, contrast variation could reveal the position of dye molecules within the surfactant micelle. **Contrast variation** experiments will be done with the blue dyestuff, which is available in a completely hydrogenated as well as partly deuterated form.



Layout ILL SANS-Instrument D11(3)

References

(1) Tehrani-Bagha, A. R.; Holmberg, K. Solubilization of Hydrophobic Dyes in Surfactant Solutions. *Materials* **2013**, *6* (2), 580–608. https://doi.org/10.3390/ma6020580.

(2) Kutz, A.; Mariani, G.; Gröhn, F. Ionic Dye–Surfactant Nanoassemblies: Interplay of Electrostatics, Hydrophobic Effect, and π–π Stacking. *Colloid Polym Sci* **2016**, *294* (3), 591–606. https://doi.org/10.1007/s00396-015-3814-2.

(3) ILL. D11 - Lowest momentum transfer & lowest background small-angle neutron scattering instrument https://www.ill.eu/users/instruments/instruments-list/d11/description/instrument-layout (accessed Jan 5, 2021).

Wenke MUELLER
muellerw@ill.fr

Innovaxn.eu
innovaxn-contact@innovaxn.eu

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 847439.