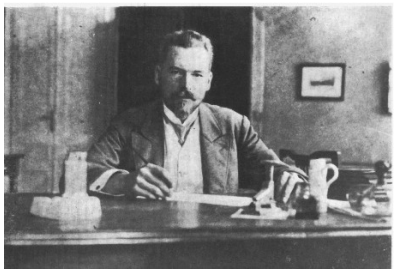

Contribution ID: **21** Type: **Poster**

Study of micelle formation in water by molecular dynamic simulations and thermodynamic approach

Monday, September 16, 2024 4:32 PM (1 minute)

Surfactant molecules, above a critical concentration in solution, are able to spontaneously self-assemble to form aggregates. One of these aggregates are micelles, which are used in many field of sciences and industry. In an aqueous environment, due to the amphiphilic nature of the surfactants, the micelles in the core have a hydrophobic part. Micelles comes into contact with the aqueous environment through the hydrophilic parts of the surfactants that constitute them. In hydrophobic core of micelles, it is possible to dissolve some molecules that usually dissolve very poorly in an aqueous environment. This property of micelles is crucial in the action of detergents and also in the process of drug delivery or solubilization of membrane proteins. In the context of application, the study of micelle formation is of great interest to better control their use in many applications fields.

In this work, I will use a molecular dynamics approach to simulate micelle formation for various aqueous environmental conditions and surfactant concentrations. Simulations of this process make it possible to analyze the structure of self-assembled structures and their stability, and finally to link them with thermodynamic and statistical properties.

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Session Classification: Poster Session and Coffee