Surfactants, or surface-active agents (SAAs), play a central role in daily life — from shampoos and soaps to household cleaners — thanks to their ability to reduce surface tension and form micelles. While spherical micelles are well known, surfactants can also self-assemble into elongated structures called wormlike micelles (WLMs). These “living polymers” give many everyday products their smooth, gel-like consistency. We encounter WLMs more often than we might think. For example, the pleasant texture and easy spreadability of a shampoo or shower gel are often due to the presence of these flexible micelles. Like polymers, WLMs give fluids viscoelastic properties — they behave partly like liquids, partly like solids. But unlike polymers made of covalently bonded chains, WLMs are held together by reversible physical forces, meaning they constantly break and reform. This dynamic behavior makes them both fascinating from a scientific perspective.

One of the key parameters in describing WLMs is the scission energy, which characterizes the energy required to break a micelle into two fragments. Traditional characterization techniques for WLMs - such as cryogenic electron microscopy (Cryo-EM) and small-angle neutron scattering (SANS) - are time-consuming, costly, and require highly specialized equipment. Even rheological methods, though more accessible, demand careful optimization of parameters such as concentration, molar ratios, and salt content to induce micellar self-assembly. In this context, computational modeling and molecular thermodynamic theory (MTT) offer promising tools to better understand micellar association and overcome current experimental limitations.

Self-assembly is a fundamental mechanism in soft matter physics. A deeper understanding of this process is essential for developing predictive models of micelle formation and transformation. **This project aims** to quantitatively describe micellar association processes using MTT and to validate its predictions through rheological measurements, establishing a predictive framework applicable to complex surfactant systems. The study will include both classical systems (e.g., SDS/NaBr, TTAB/NaBr) and novel nonionic/anionic surfactant mixtures with added.

Scission energy will be determined through both oscillatory rheological measurements and interfacial tension data utilized using MTT. In addition, computer simulations will be employed to test the predictive capability of the MTT when extended to new systems. This model will use basic parameters, such as interfacial tension and component concentrations, to estimate the scission energy of micelle formation and then number of micelle aggregation. Subsequently, these results will be integrated with rheological Cates model to predict the viscoelastic properties of these fluids. Using these parameters, the model will explore how well theoretical predictions reflect experimentally observed micellar behavior and viscoelasticity. The project introduces **two innovations:**

(1) Applying MTT to mixed nonionic/anionic surfactant systems: MTT has so far been applied mainly to ionic systems with added salts or to nonionic surfactant mixtures. This project will be the first to adapt and apply MTT to mixed nonionic/anionic surfactant systems, enabling theoretical analysis of formulations not previously described in the literature. Supported by interfacial tension measurements, this will enhance understanding of micellar behavior in more complex systems.

(2) Comparative analysis of rheological data and molecular thermodynamic predictions: This project will, for the first time, directly compare MTT outputs with rheological data to evaluate model accuracy and develop a predictive, simulation-based framework for WLMs characterization.

Together, these innovations provide a coherent framework for the fundamental characterization of WLMs by linking rheological behaviour with interfacial thermodynamics through molecular-level theory. This integrated approach contributes to the development of theoretical models in soft matter physics and surfactant science. By focusing on model systems, it aims to reveal universal structure–property relationships governing self-assembly, thus expanding our fundamental understanding of micellar association processes.