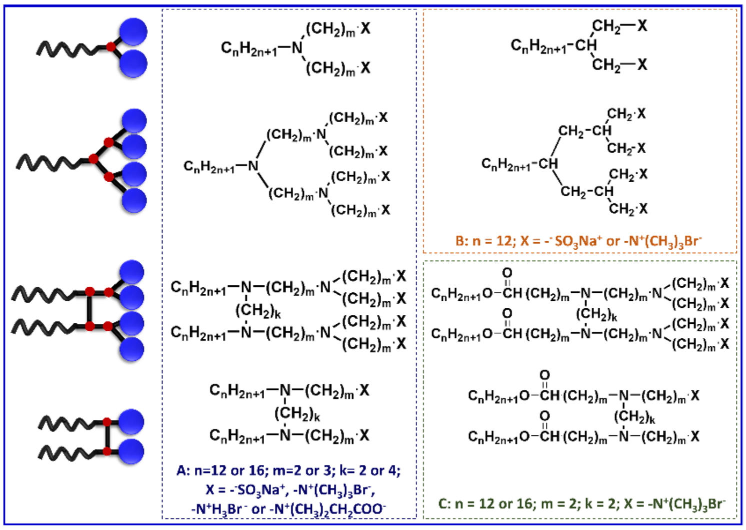
DESCRIPTION FOR THE GENERAL PUBLIC

New generation of multi-charge surfactants of dedicated functionality

Contemporary research in surfactant science and technology comprises a variety of requirements for designing surfactant structures with widely varying architectures to achieve unique physicochemical properties and dedicated functionality. Such approaches are necessary to make them applicable in modern technologies such as nanostructures engineering or surface restructurization, or as fine chemicals (e.g., as magnetic surfactants, capping and stabilizing reagents or reactive agents at interfaces). Properties and performance of the present-day surface-active compounds, so-called specialty or added value surfactants, may be controlled by certain slight structural modifications: functionalizing the engineered surfactant structure by incorporation of an additional alkyl chain (double-tail single-head structures) or headgroup (multicharge or multiheaded structures) as well as by varying the linker, exemplary such as the ester-type moiety, connecting the hydrophobic and hydrophilic parts. Such modifications may enable to fabricate a wide range of unique functional structures containing multiple ionic head groups of different architecture and purposes.

In this project, several groups of new multi-charge surfactants will be synthesized and characterized, i.e., both bifunctional (dicephalic) and gemini (dimeric) – type, containing dendronium hydrophilic moieties (G1 references and new G2 structures; as shown in the picture). Generally, to synthesize the designed series of multicharge surfactants in the most effective manner - in most cases - the modular synthesis will be performed based on step-by-step reactions with suitable building blocks. Such an approach comprises a group of synthetic routes involving the initiator (e.g. hydrophobic tail source or hydrophilic entity) and appropriate building reagents enabling reproduction of the previous endgroup in the multiplied manner. In the case of a hydrophilic initiator, the coupling reaction of hydrophobic grouping will be performed with the modularly-formed dendronium-based hydrophile. The syntheses will be followed by extensive experimental research to establish the adsorption and aggregation properties of synthesized surfactants and the possibility of using them to form nanostructures or functional specialty products. Those tasks will be accompanied by the theoretical effort to provide description of observed phenomena with advanced models through physically well-defined parameters.



Therefore, we aim to fabricate and evaluate new custom-designed multicharge structures based on the premise that their unique relationships: chemical structure - self-organization properties at interfaces and in solution could provide a variety of valuable products having new functionalities, e.g., surface active polyelectrolyte-surfactant complexes (PESCs) as new drug vehicles, surfactants with magnetic property, biologically active capped-metal nanoparticles and antimicrobial agents. It is planned to apply both dynamic light scattering (DLS) and diffusion-ordered nuclear magnetic resonance (DOSY NMR) to monitor the formation of the PESCs in different media (pure water, basic or acidic solutions). To deduce the required correlations between the surfactants' structures and their aggregation behavior toward their potential application, the following features will be varied in the surfactant structures: the alkyl chain length, the dendrimeric generations number (i.e. number of hyperbranched units: G0, G1 and G2), the type of charged hydrophilic group. The application of molecular dynamics methods combined with the approach based on the thermodynamic models of multicharged surfactant adsorption can explain some experimentally observed phenomena. It can provide the basis for developing novel materials designated for a variety of applications. That type of integrated approach is rather scarce in the literature. The obtained results may broaden our knowledge and enhance the ability to design functional materials for various applications in industrial and academic fields.