EXPLORING THE AGGREGATION BEHAVIOURS OF SURFACE-ACTIVE MATERIALS

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ABSTRACT

This comprehensive research explores the molecular interactions between diverse dyes and amphiphilic systems—comprising conventional surfactants and surface-active ionic liquids (SAILs)—in aqueous media, emphasising how variations in head group charge, hydrophobic tail structure, counterion size, and micellar polarity govern solubilization, aggregation, and spectroscopic properties. A multi-technique approach, including UV–visible and fluorescence spectroscopy, time-correlated single-photon counting (TCSPC), dynamic light scattering (DLS), zeta potential analysis, and conductometric titration, supplemented by Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) calculations, provides molecular-level insights. For the cationic dye Acridine Red (AR), the hydrophobic SAIL BMImOS exhibits superior solubilization compared to SDS and BMImBr, driven by reduced head-group repulsion and hydrophobic tail–mediated encapsulation, as supported by spectral shifts, fluorescence lifetime enhancement, and HOMO–LUMO overlap. The anionic dyes Eosin Y (EY) and Phloxine B (PhB) show maximum stabilisation and micellar incorporation with the zwitterionic surfactant C12DmCB, surpassing cationic and anionic analogues through balanced charge distribution and minimised electrostatic repulsion. In contrast, Methylene Blue (MB) interactions with CTAB, CTAT, and BMImOS reveal counterion-controlled binding, with CTAT forming the most stable ion-pair complex due to its bulky tosylate counterion. Across all systems, zwitterionic surfactants and hydrophobically tailored SAILs outperform conventional surfactants by enhancing solubilization, thermodynamic stability, and micellar efficiency while reducing toxicity. The strong agreement between experimental observations and DFT-derived electronic parameters establishes a predictive framework for rational amphiphile design. Collectively, the findings advance a generalizable strategy for tuning dye–micelle interactions through charge modulation, hydrophobic integration, and counterion engineering, with broad implications for drug delivery, photosensitization, bioimaging, solar energy harvesting, and wastewater treatment using sustainable amphiphilic materials.

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