

Small Angle X-ray Scattering of Conjugated Polyelectrolytes Surfactant Complexes in Aqueous Solution

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Inspired by natural light harvesting systems that were fine-tuned by nature through billions of years of evolution, the focus of this research aims to mimic nature's approach of capturing solar energy by constructing a self-assembled, artificial light-harvesting antennae capable of efficient electronic energy transfer. The platform of our work focuses on a pair of oppositely charged conjugated polyelectrolytes (CPEs) as a donor-acceptor system – the energy donor, a cationic poly(fluorene-co-phenylene) (PFPI), and the acceptor, an anionic polythiophene (PTAK). This study focuses on the role that surfactants have on the solution structure and optical properties of CPE complexes, with the goal of controlling complex formation with ternary ionic surfactant agents. Small-angle X-ray scattering (SAXS) was used to gain insight in the structural self-assembly of CPE(+)/CPE(-)-Surfactant complexes with surfactants of oppositely charged head groups above and below their cmc concentrations. The scattering data is converted into a real space via the pair-distance distribution function (PDDF) using the indirect Fourier transform (IFT). By using the IFT method, no model assumption is needed to convert the scattering data to the PDDF. This method represents one of the few means to obtaining statistical structural information on largely disordered, macromolecular aqueous complexes. We find that the ionic self-assembly of CPEs is highly dependent on the charge of the head group as well on the surfactant concentration. Our results show that proper choice of surfactant can either largely shut off energy transfer, or tune the photophysics and structure in a way that shifts electronic resonances while allowing energy transfer to persist. Our results indicate that we can alter the solution structure of CPEs-surfactant complexes from extended locally ordered structures to compressed disordered structures, which can be used to control of their electronic energy transfer efficiencies.