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Self-Assembly of Diblock Polythiophene Polyelectrolytes for Organic Photovoltaic Devices

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The performance of organic photovoltaic devices (OPVs) depends critically on simultaneous control of the optoelectronic properties and nanoscale morphology of conjugated polyelectrolytes (CPEs).[1] Recently, self-assembly strategies have emerged as an elegant approach for the design and fabrication of reproducible nanoscale aggregates from CPE building blocks.[2] The challenge, however, is to determine the key structure-property relationships in these novel materials and demonstrate how structural order tailoring can be harnessed to deliver highly efficient OPVs.

Here we will demonstrate the solvent-mediated[3] (methanol, water and methanol/water mixtures), surfactant-mediated[4] (SDS, d25-SDS and PFOS) self-assembly of a series of amphiphilic diblock copolymers each containing a hydrophobic poly(3-hexylthiophene) (P3HT) block and a hydrophilic cationic P3HT block bearing different terminal ionic groups. Their optical properties and aggregate structures were studied in solution, and in subsequently prepared thin films, using photoluminescence, scattering and microscopic techniques. In particular, small-angle neutron scattering (SANS) was used to elucidate the nanoscale morphology and solvent content of the CPE and CPE-surfactant structures in solution. A variety of well-defined, solution-phase structures (e.g. rods, lamellar sheets) can be generated through careful modulation of the solvent polarity and surfactant charge ratio. In addition, direct comparison between the diblock copolymers and their analogous homopolymers has revealed the significance of the hydrophobic P3HT block in controlling aggregate morphology. Solvent- and surfactant-mediated self-assembly of all-conjugated block CPEs may therefore provide a simple inexpensive route for obtaining nanostructured active interfaces suitable for OPV devices.

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