Abstract

The thesis entitled "***Synthesis and Functionalization of Bay-Substituted Terrylenes for Optoelectronic Device and Sensing Applications***" presents the synthesis and application of terrylene-based conjugated small molecules and polymers as multifunctional materials for overcoming optoelectronic and environmental-related challenges. It begins with outlining terrylene and terrylene diimides (TDI)-based small molecules, including their novel synthetic strategies, positional functionalization, and applications in optoelectronic devices. It highlights existing gaps and defines the scope of this work in organic phototransistors, HTMs for PSCs, and toxic pollutant sensing. It describes the synthesis of 7,8-bis(alkyloxy)terrylenes using a novel synthesis route. Bay-substituted alkyloxy groups improved solubility, enabling the first solution-processed terrylene-based OFETs and OPTs, which showed p-type behaviour, and strong photoresponse with high detectivity. Later, the first terrylene homopolymers, polyterrylenes, were synthesized from 7,8-bis(hexadecyloxy)terrylene, demonstrating multi-fold higher mobility and enhanced photodetection than the monomer. It also reports the first terrylene-based sensing probe, a pyridine-substituted terrylene as a selective colourimetric and fluorometric sensor for mercuric ion and 2,4,6-trinitrophenol (TNP) with high sensitivity and selectivity. Furthermore, it explores terrylene-based small molecules as hole-transporting materials for perovskite solar cells. This study highlights terrylene as a promising building block for further functionalization in optoelectronic devices. The first peri-substituted terrylene-based A-D-A type near-infrared (NIR) small molecules, which exhibit ultra-narrow band gaps and emission in the NIR-II region, are also synthesized and the structure-property relationship is described. The synthesis of 7,15-bis(octyloxy)terrylene is described, and its photophysical properties and solid-state structure are analysed. The thesis ends with a conclusion and provides the scope for further research in these areas. Altogether, this body of work not only expands the functional scope of terrylene-based small molecules and polymers but also establishes a foundation for their future exploration in multiple optoelectronic application domains.

Keywords: Terrylene, Polyterrylene, Pollutant detection, OFET, OPT, Hole Transporting Materials, Perovskite solar cell, NIR active small molecules.