New Perylene Diimide-Based Materials for Photovoltaic Applications

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Considering the current state of the natural environment, the photoconversion of sunlight into electricity has become a significant area of research. Although inorganic photovoltaic cells are well established in the consumer market, they still suffer from several disadvantages and limitations, such as high production costs, considerable weight, and panels rigidity. This doctoral dissertation addresses the development of next-generation solar cells that have the potential to overcome the drawbacks of existing photovoltaic technologies.

The literature section presents the history and classification of photovoltaic devices, with particular emphasis on organic solar cells (OSCs) as a technology with high potential for large-scale commercialization. One of the key advantages of using organic materials is among other the ability to deposit thin layers via solution-based methods, which significantly reduces production costs compared to conventional silicon-based solar cells. Moreover, it is possible to fabricate semi-transparent, lightweight, and flexible devices, which greatly broadens their potential applications—including decorative functions.

However, it should be emphasized that OSCs, composed of multiple layers serving specific functions, still struggle with unsatisfactory photoconversion efficiency. Therefore, their architecture requires further improvements and optimizations. In view of the above, the aim of the present research was to develop new materials for use as cathode interlayers (CILs), enhancing electron transport and device stability, as well as acceptor-type additives in the active layer of bulk heterojunction (BHJ) solar cells.

In this work, 34 perylene diimide (PDI) derivatives bearing various polar anchoring groups were synthesized for application as CILs, along with 4 new acceptor derivatives featuring unique three-dimensional structures. Throughout the study, highly effective procedures for the synthesis and purification of the products were developed, and their structures were confirmed using NMR, IR and HRMS techniques. In addition, TGA, UV-Vis, and CV analyses were conducted, providing key insights into the properties of the synthesized materials.

Selected compounds were evaluated in photovoltaic devices as CILs, and the obtained results are presented in this dissertation as well as in a scientific article. One of the most notable outcomes was the construction of a device incorporating the PDI-4C-pyrol compound, which achieved a power conversion efficiency (PCE) exceeding 18%, representing an increase of approximately 3% compared to the reference cell without a cathode interlayer. Meanwhile, the results published in the journal *Small* enabled the formulation of conclusions regarding the relationship between the structures of PDI derivatives containing sulfobetaine moieties and the performance parameters of the devices fabricated from them. The results obtained constitute a significant contribution to the development of OSC technology as well as other areas of organic electronics.