

ABSTRACT

The aim of this doctoral thesis is the design, synthesis and measurement of the optical and electronic properties of non-fullerene acceptor molecules used in bulk heterojunction photovoltaic devices.

At this time, the most widely used acceptor materials are fullerene derivatives such as PC₆₁BM and PC₇₁BM, since they have a number of advantages such as high electron mobility and good electrochemical properties. However, they also have disadvantages such as morphological instability, high synthesis costs or limitations in their light-harvesting capacity. Because of this, in recent years, non-fullerene acceptors have become interesting, since they can overcome these drawbacks.

In this doctoral thesis, non-fullerene acceptors with A- π -A- π -A structure have been studied, which have as a central base a unit of DPP or DPP-Se unit attached to different terminal electron acceptor fragments, as set out in *Chapter I*. Moreover, *Chapter I.III* also includes the results obtained from the synthesis and characterization of new non-fullerene acceptors based on BT as a central core, CPDT as a π -bridge and terminal electron acceptor groups.

On the other hand, another line of research has focused on the synthesis and analysis of the electronic properties of quinoidal compounds derived from CPDT. Quinoidal structures have an efficient delocalization along the backbone, which allows a reduction in the band gap compared to aromatic analogues, shifting the absorption towards the NIR spectral region. In addition, these structures have a very low LUMO level, which favors the electronic transport in the active layer. These structures can be used in OSCs and NIR-OPDs (*Chapter II*).