BENZOFURAN END-CAPPED DIKETOPYRROLOPYRROLES AS A SEMICONDUCTIVE MATERIALS: SYNTHESIS, SPECTRAL AND ELECTROCHEMICAL PROPERTIES

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Abstract

A new key intermediate, 5-(1-benzofuran-2-yl)thiophene-2-carbonitrile, has been prepared and further been used for the synthesis of three DPP pigments by a base catalyzed condensation with succinic ester, 2-phenyl- and 2-(thiophene-2´-yl)-pyrrolinone esters. Their soluble N,N´ dialkyl derivatives were prepared either by direct alkylation with branched alkyl, alkyl ester and acetal, or by Pd catalyzed cross-coupling reactions starting from smaller dialkylated 3,6-dithiophene substituted DPP precursors. Both synthetic routes were critically compared. The second route is considerably more efficient for N,N´-alkylation with branched alkyls, while for an alkylation with branched alkyl esters the yields are comparable. Thermal properties of N-unsubstituted pigments were investigated by TGA which proved high thermal stability. The high sublimation temperature of this pigment (492 °C) exceeded other commercially available DPP pigments. Both absorption spectra as well as electrochemical measurements revealed that the tuning of opti-cap properties and the HOMO-LUMO gap can be carried out either by varying N-substituents or the number of peripheral benzofuran moieties. The experimental data were further supported by the DFT calculations and structure-property relationships were elucidated. Owing to the excellent electrical and optoelectronic properties, DPP derivatives have been attracting extensive attention in solution-processed organic electronics, such as field-effect transistors (OFETs) and photovoltaics (OPVs), which can offer large-area and flexible devices of next generation. In particular, OFETs are an important fundamental component for such devices.

Keywords: DPP derivatives, organic semiconductors, OLED, OPV

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