



A Novel Series of Organic Semiconductors for OPV and OFET applications

Submitted by:

Diego Cortizo Lacalle

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A meu Pai, mi Madre y mi Hermana.

Eta zuri.

ABSTRACT

In the last three decades, the search for alternative energy for common fuel sources has been greatly developed. Among the already well-established and developing technologies (wind energy, hydrogen, geothermal energy or hydropower), solar cells have attracted enormous interest. This interest is due to the potentially vast solar energy that can be harvested on the Earth's surface. Currently, solar cells based on inorganic materials are widespread due to their high efficiency, whereas the power conversion efficiency of organic photovoltaics (OPVs), being new technology, is continuously increasing towards that of their inorganic counterparts.

The improvement of this promising field is strongly linked to the development of new materials to increase the harvesting properties of the organic solar cell, as well as a better understanding of the physics and the behaviour of every component within the device.

In that sense, this thesis presents the synthesis and characterisation of three novel series of organic materials and their performance in organic photovoltaics. Chapter 2 describes the incorporation of a well-known dye (BODIPY) into conjugated polymers. A BODIPY core was co-polymerised with bis-EDOT and bis-EDTT units and their performance in OPVs was studied. Chapter 3 shows the effective fusion of TTF units *via* a thiophene unit to the main conjugated polymer chain. A fused thieno-TTF moiety was copolymerised with a soluble derivative of DPP and tested in organic photovoltaics and OFETs showing excellent results. Finally, the synthesis and characterisation of two new "small molecules" based on BODIPY-DPP-BODIPY triads are described in Chapter 4. The performance of these two novel compounds in OPVs is currently under study.

ABBREVIATIONS

AFM	Atomic Force Microscopy
AM1.5	Air Mass 1.5 spectrum
a.u.	arbitrary units
BEDT-TTF	Bis-(ethylenedithio)-tetrathiafulvalene
BHJ	Bulk Heterojunction
BLA	Bond Length Alternation
BODIPY	Boron-dipyrromethene
CIGS	Chalcogenide Copper Indium Gallium Diselenide
cod	Cyclooctadiene
CuPc	Copper Phthalocyanine
CV	Cyclic voltammetry
D-A	Donor-Acceptor
DCM	Dichloromethane
DDQ	2,3-Dichloro-5,6-dicyano-1,4-benzoquinone
DFT	Density Functional Theory
DMF	<i>N,N</i> -Dimethylformamide
DMSO	Dimethyl Sulfoxide
DSC	Differential Scanning Calorimetry
DPP	Diketopyrrolopyrrole
ECD	Electrochromic Devices
EDOT	Ethylenedioxythiophene
EDTT	Ethylenedithiathiophene
E_g	Band gap
EPR	Electron paramagnetic resonance

EQE	External Quantum Efficiency
eV	Electron-volt
Fc/Fc ⁺	Ferrocene/Ferrocenium
FF	Fill factor
GPC	Gel Permeation Chromatography
HPLC	High Pressure Liquid Chromatography
HOMO	Highest Occupied Molecular Orbital
HT	Head-to-Tail
ICT	Internal Charge Transfer
IPCE	Incident Photon to Current Efficiencies
IR	Infrared
ir	Irreversible
I _{sc}	Short Circuit Current
ISC	Intersystem Crossing
ITO	Indium Tin Oxide
LDA	Lithium Diisopropylamide
LUMO	Lowest Unoccupied Molecular Orbital
M	Molar
MALDI	Matrix-Assisted Laser Desorption Ionisation
MO	Molecular Orbital
MS	Mass Spectrometry
NCS	<i>N</i> -Chlorosuccinimide
n-doped	Negatively-Doped
NBS	<i>N</i> -Bromosuccinimide
NMR	Nuclear Magnetic Resonance
OFET	Organic Field-Effect Transistor

OLED	Organic Light Emitting Diode
ONSH	Oxidative Nucleophilic Substitution of Hydrogen
OPV	Organic Photovoltaic
OSC	Organic Solar Cell
OTS	Octadecyltrichlorosilane
p-doped	Positively-Doped
P3HT	Poly(3-hexylthiophene)
PCBM	Phenyl-C ₆₀ -butyric acid methyl ester
PCE	Power Conversion Efficiency
PDI	Polydispersity index
PEDOT	Poly(ethylenedioxythiophene)
PITN	poly(isothianaphthene)
ppm	Parts Per Million
PPV	Poly(<i>p</i> -phenylene vinylene)
PSS	Polystyrene Sulfonate
qr	Quasi-reversible
r	Reversible
TBAPF ₆	Tetrabutylammonium hexafluorophosphate
TCNQ	7,7',8,8'-Tetracyano- <i>p</i> -quinodimethane
TFA	Trifluoroacetic acid
TGA	Thermal Gravimetric Analysis
THF	tetrahydrofuran
TMTSF	Tetramethyl tetraselenafulvalene
TOF	Time of Flight
TTF	Tetrathiafulvalene
UV	Ultraviolet

V_{OC}

Open Circuit Voltage

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