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Triplet exciton losses in polymer: Fullerene-free acceptor blends

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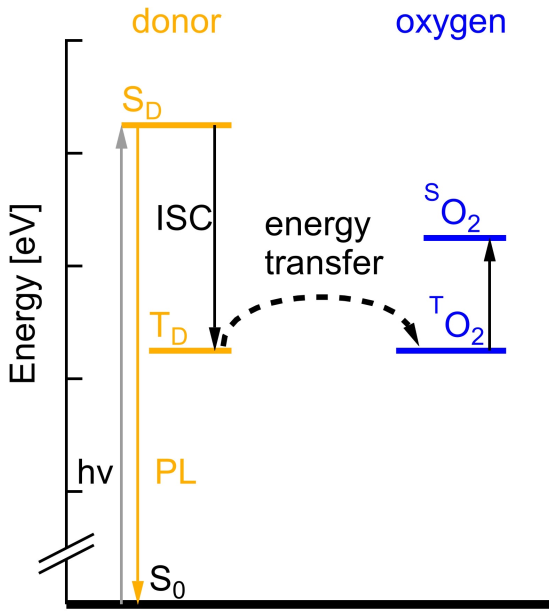
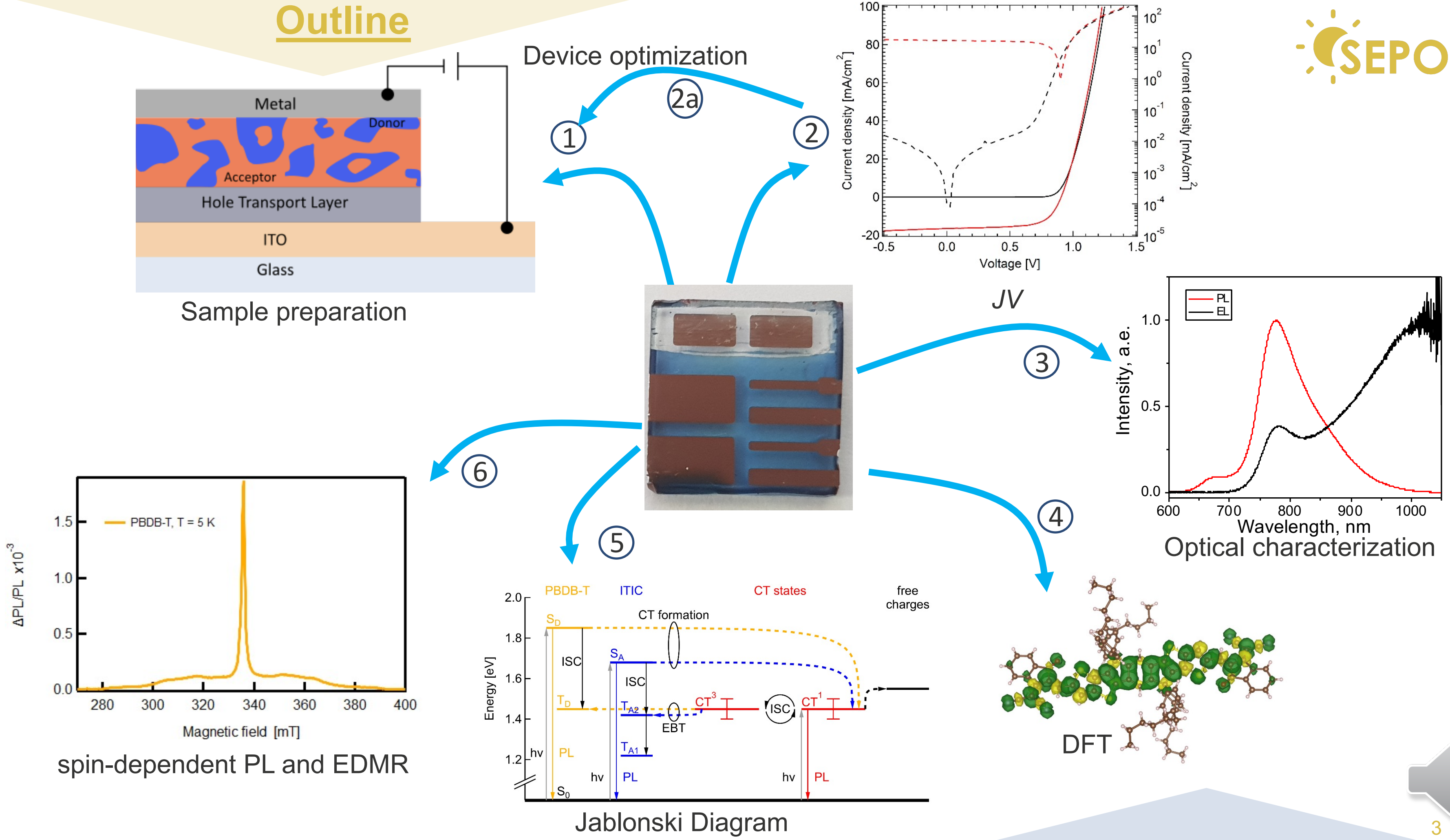


Triplet driven OSC degradation:

- Long living triplet states in OSCs
- Energy transfer from D triplet state to oxygen triplet ground state
- Excitation to reactive singlet oxygen state
- Oxidation of double bonds
- Polymer destruction

Triplet energy loss channel

Outline

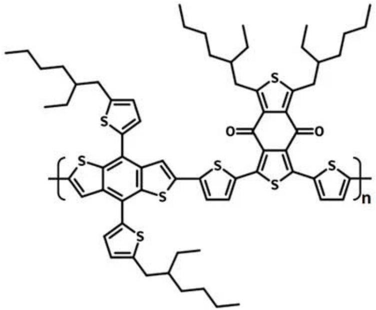


Metal
Donor
Acceptor
Hole Transport Layer
ITO
Glass
Sample preparation
Device optimization
1
2a
2
Current density [mA/cm^2]
Current density [mA/cm^2]
Voltage [V]
JV
3
PL
EL
Intensity, a.e.
Wavelength, nm
Optical characterization
4
DFT
5
PBDB-T
ITIC
CT states
free charges
CT formation
Energy [eV]
ISC
EBT
hv
PL
Jablonski Diagram
6
PBDB-T, T = 5 K
ΔPL/PL x10^{-3}
Magnetic field [mT]
spin-dependent PL and EDMR

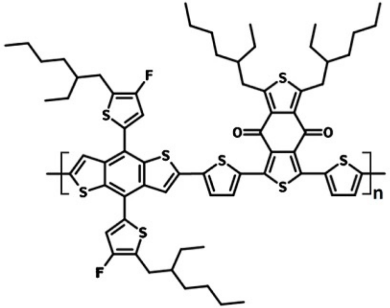
Material Systems

SEPOMO

Donors

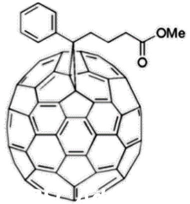


PBDB-T

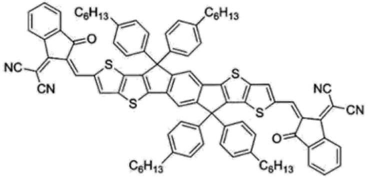


PBDB-T-2F(PM6)

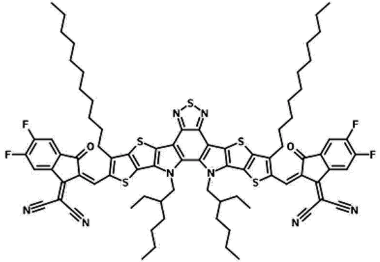
Acceptors



$PC_{71}MB$

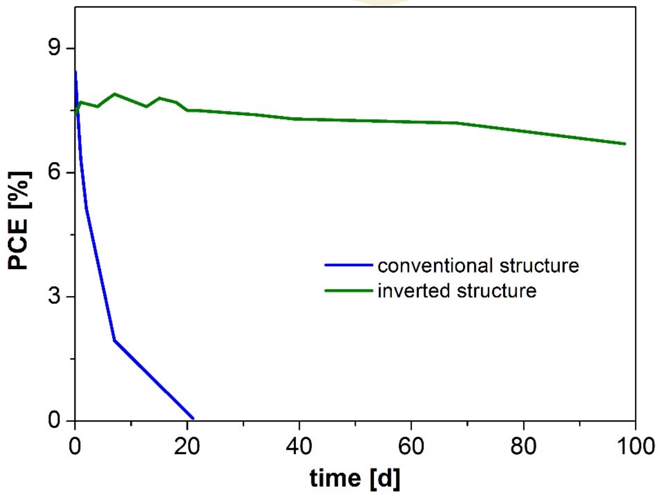


ITIC

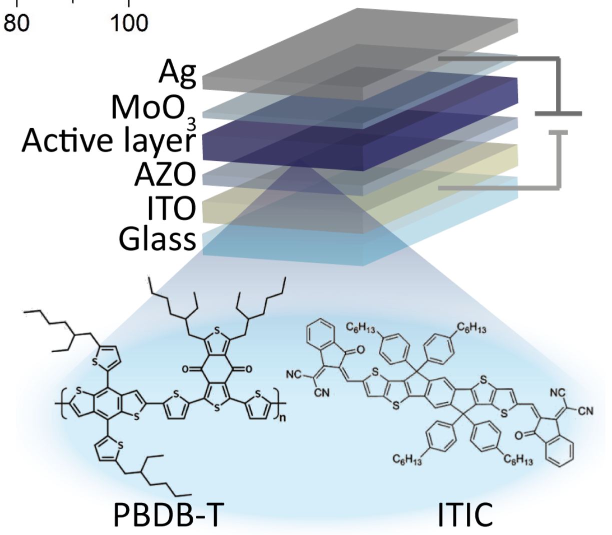


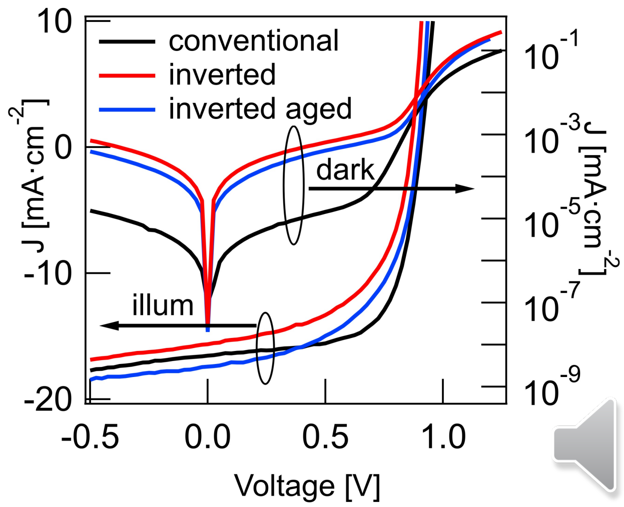
Y6

Organic Photovoltaics – inverted vs conventional

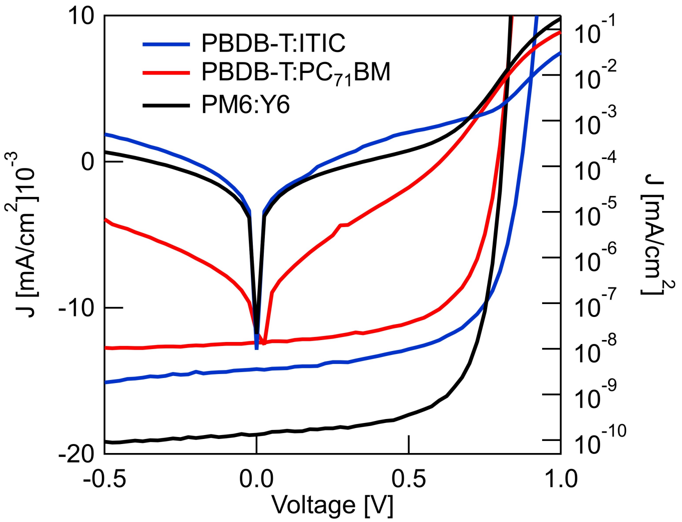


structure	V_{oc} [mV]	FF [%]	J_{sc} [mA cm^{-2}]	PCE [%]
conventional	905	66	16.5	9.8
inverted	868	56	16.4	7.5
aged inverted	895	54	17.4	8.5





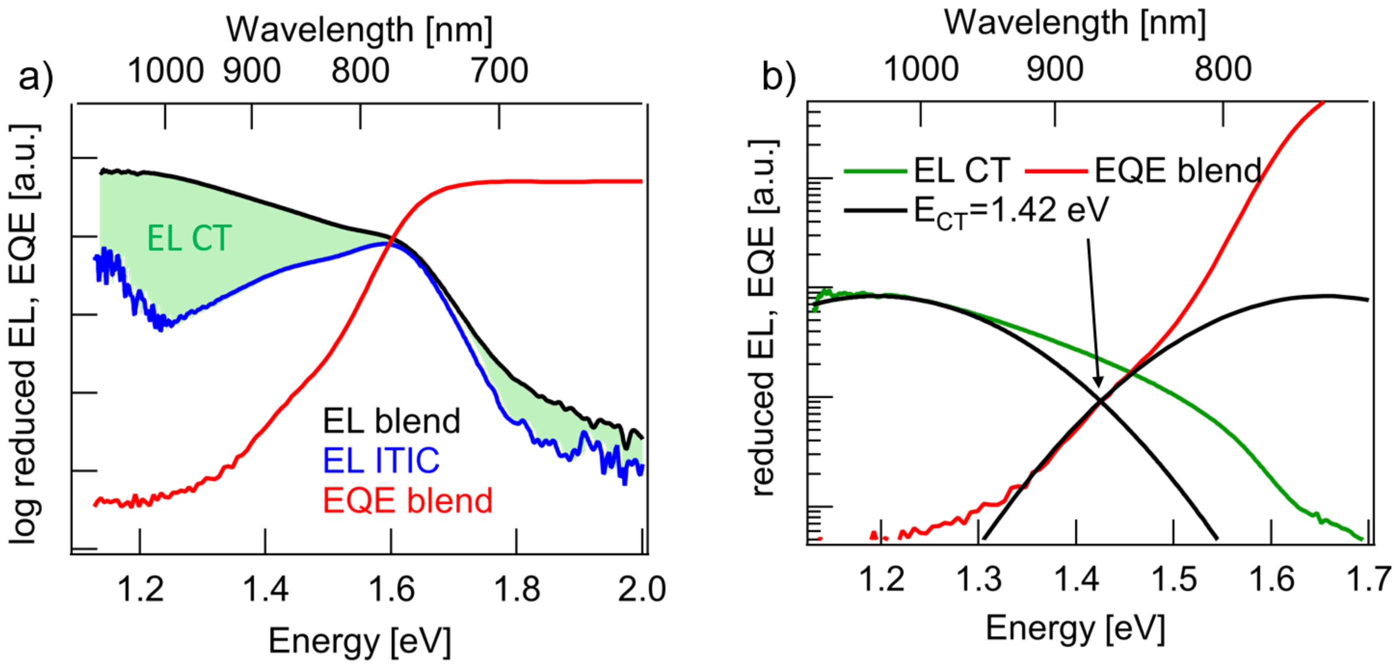
Solar cell performance



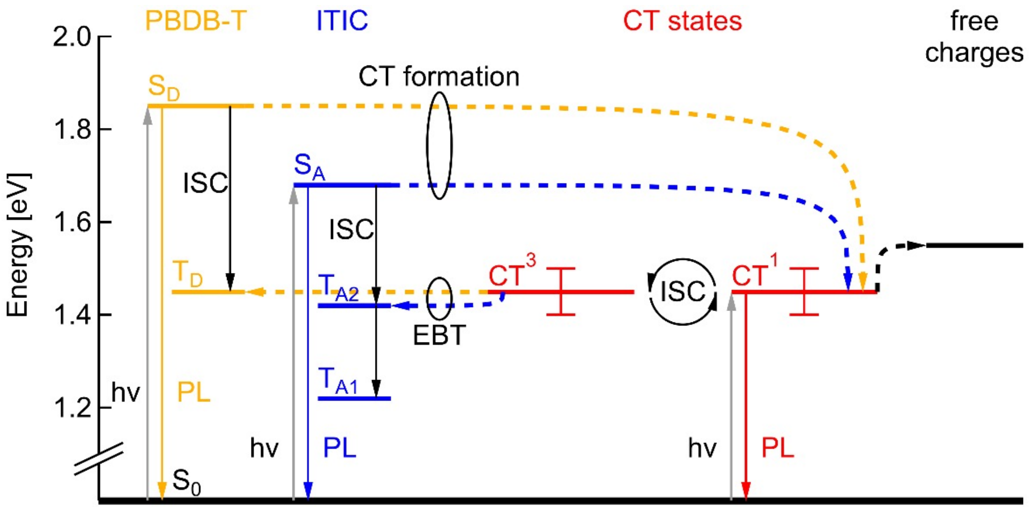
	V_{OC}, mV	J_{SC}, mA/cm^2	FF, %	PCE, %
PBDB-T:$PC_{71}BM$	729	12.4	62	6.1
PBDB-T:ITIC	870	14.2	62	7.7
PM6:Y6	808	18.7	67	10

CT energy

1) $E_{CT}=V_{OC}+0.6$ eV; $E_{CT}= 1.5$ eV
2) V_{OC} (0 K)= 1.40±0.05 eV
3) Fitted reduced EL and the EQE spectra



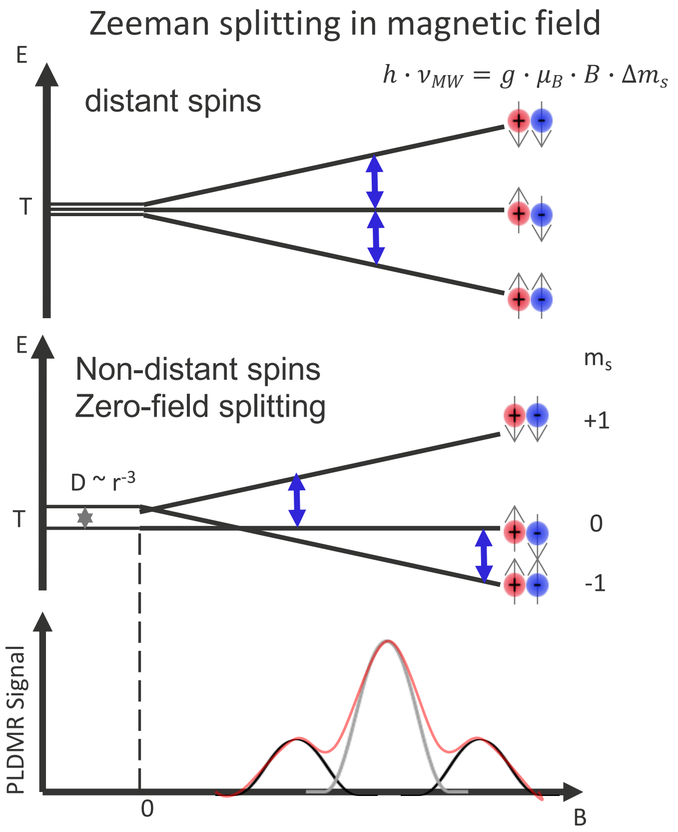
PBDB-T:ITIC Jablonski diagram

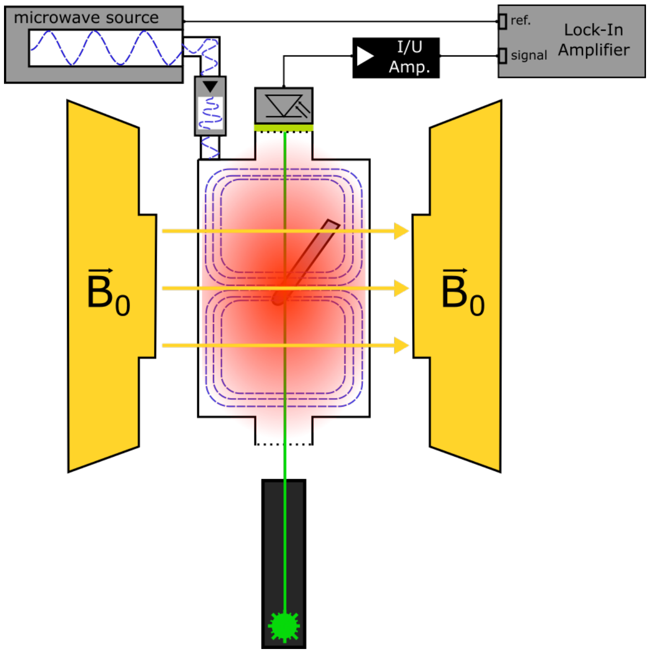


S_D higher than S_A
CT lower than S_A and S_D
Two acceptor triplet states T_{A1}, T_{A2}
EBT energetically possible to T_A and T_D
T population through ISC and EBT

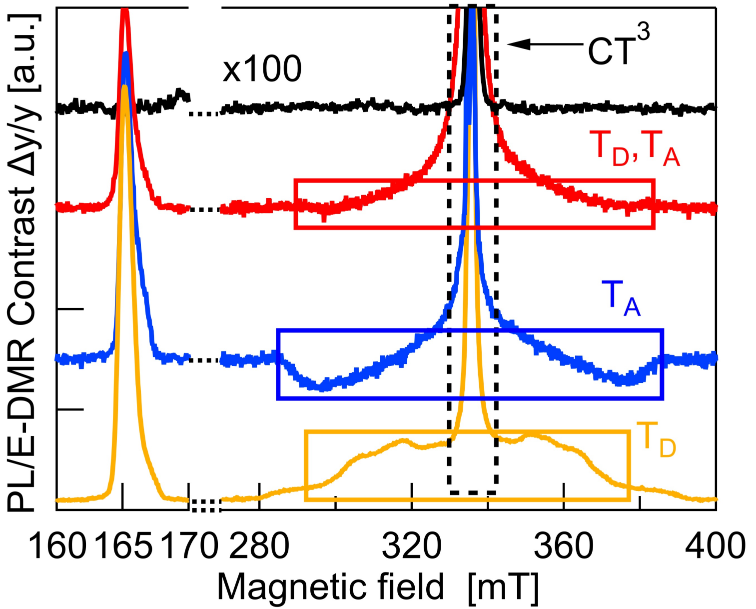
Maria S. Kotova, Giacomo Londi, Johannes Junker, Stefanie Dietz, Alberto Privitera, Kristofer Tvingstedt, David Beljonne, Andreas Sperlich and Vladimir Dyakonov, *Materials Horizons*, 2020, **7**, 1641-1649
doi:10.1039/D0MH00286K

Photo Luminescence Detected Magnetic Resonance (PLDMR)





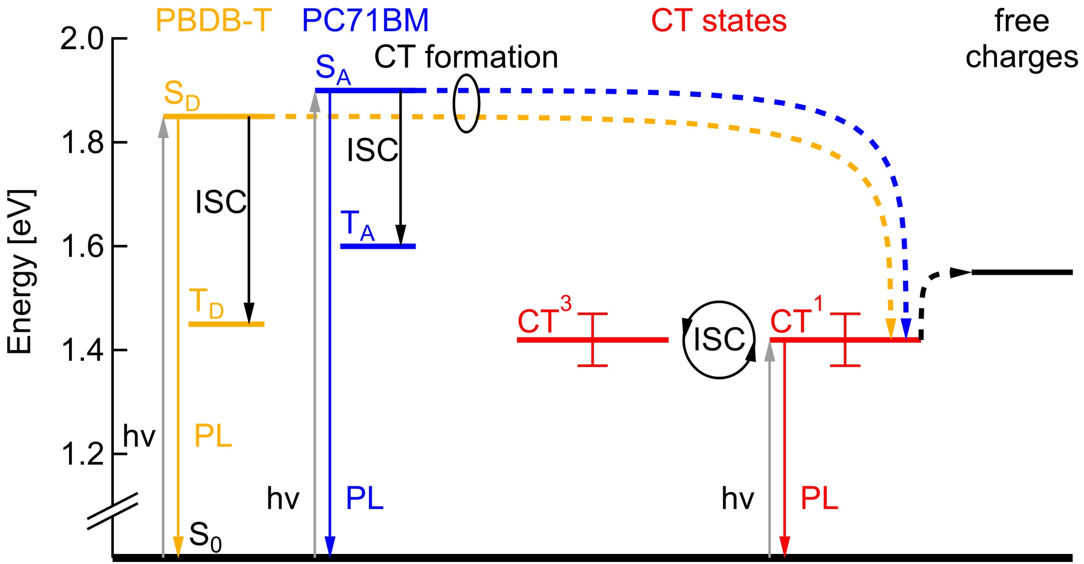
PLDMR on PBDB-T:ITIC



- PLDMR: Drop-cast films at 5 K, Illumination with 532nm
- EDMR: OSC at 250 K under 1 sun illumination

- Molecular triplet signal both in pure materials and in the blend
- Individual triplet signatures not distinguishable in the blend
- Halffield signal visible, but unclear on which material
- → Molecular triplets in the blend, not distinguishable where
- No molecular triplet signal in EDMR

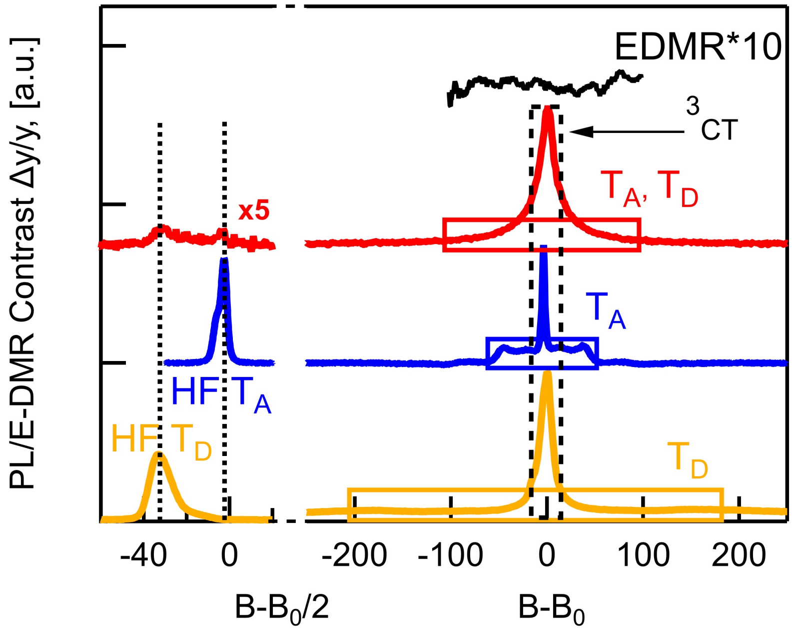
PBDB-T:$PC_{71}BM$ Jablonski diagram



S_D lower than S_A
CT lower than S_A and S_D
One acceptor triplet state T_A
EBT energetically NOT possible to T_A and T_D
T population through ISC

1. H. Kraus, M. C. Heiber, S. Väth, J. Kern, C. Deibel, A. Sperlich, V. Dyakonov, *Scientific Reports*, 2016, **6,** 29158
2. S. Xie, Y. Xia, Z. Zheng, X. Zhang, J. Yuan, H. Zhou, Y. Zhang, *Adv. Funct. Mater.* 2018, **28**, 1705659

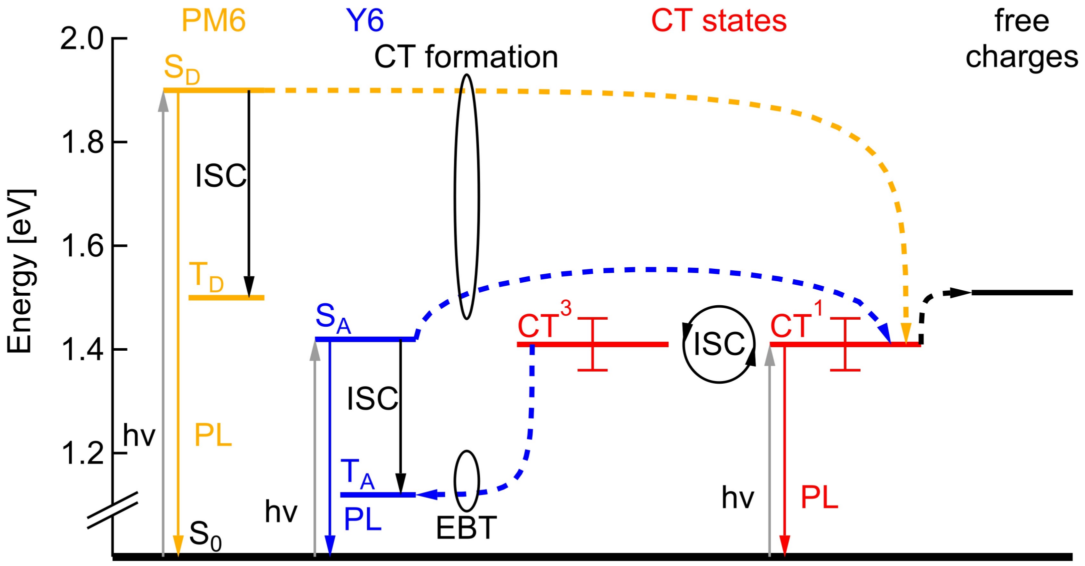
PLDMR on PBDB-T:$PC_{71}BM$



- Molecular triplets both in pure materials and in the blend
- Distinguishable half-field signals for D and A
- In the blend molecular triplets at D and A (HF)
- → Molecular triplets on both materials in the blend
- No molecular EDMR signal

- Drop-cast films at 5K, Illumination with 532nm (PBDBT) or 473nm (PC70BM)
- EDMR: OSC at 250 K under 1 sun illumination

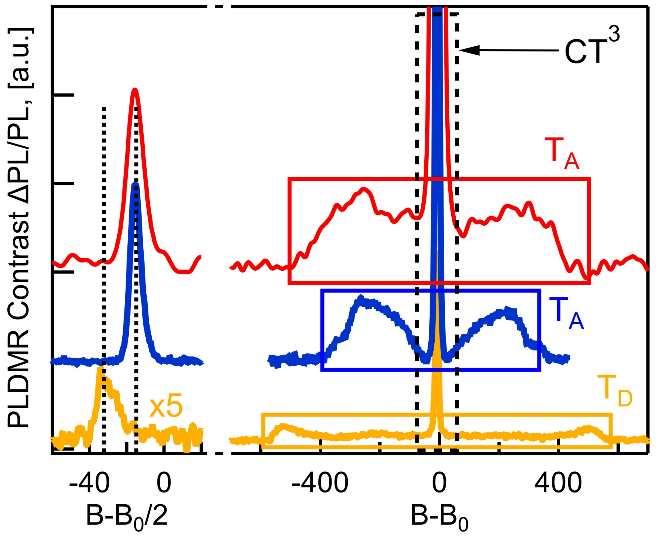
PM6:Y6 Jablonski diagram

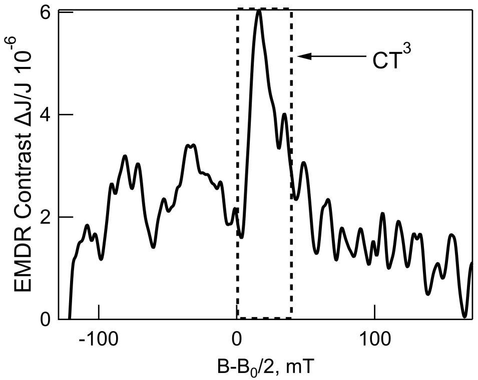


S_D higher than S_A
CT close to S_A
One acceptor triplet state T_A
EBT energetically possible to T_A
T population through ISC and EBT

L. Perdigón-Toro, H. Zhang, A. Markina, J. Yuan, S. M. Hosseini, C. M. Wolff, G. Zuo, M. Stolterfoht, Y. Zou, F. Gao, D. Andrienko, S. Shoaee, D. Neher, *Adv. Mater.,* 2020, 1906763

PLDMR on PM6:Y6





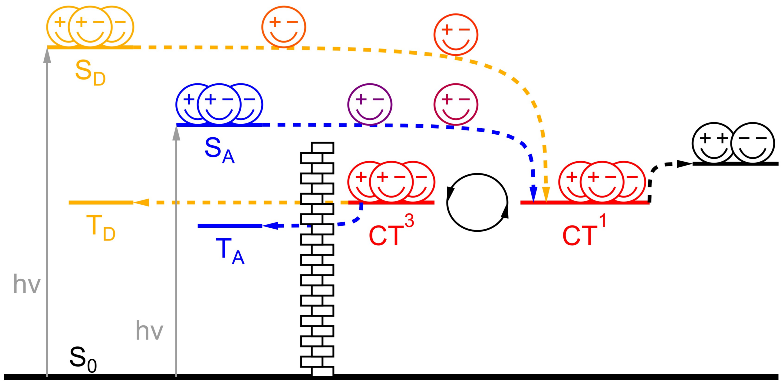
- Molecular triplet signal in both pure materials and in the blend
- Distinguishable half-field signals for D and A
- In the blend molecular triplet only from A
- No molecular triplet signal in EDMR

- PLDMR: Drop-cast films at 5 K, Illumination with 532nm
- EDMR: OSC at 250 K under 1 sun illumination

Conclusions

	T_A at low temperature	T_D at low temperature	T_A in the OSC	T_D in the OSC
PBDB-T:$PC_{71}BM$	✓	✓	✗	✗
PBDB-T:ITIC	✓	✓	✗	✗
PM6:Y6	✓	✗	✗	✗

1. Efficient charge separation can outperform triplet formation
2. Triplet formation has to be checked for every system independently from the Jablonski diagram



Thank you for your attention!

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