Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


Supporting Information

# Integrating Theory, Synthesis, Spectroscopy and Device Efficiency to Design and Characterize Donor Materials for Organic Photovoltaics: a Case Study Including 12 Donors.

S.D. Oosterhout,[a] N. Kopidakis,[a] Z.R. Owczarczyk,[a] W.A. Braunecker,[a] R.E. Larsen,[a] E.L. Ratcliff,[b] D.C. Olson[a]

## Additional spectra.

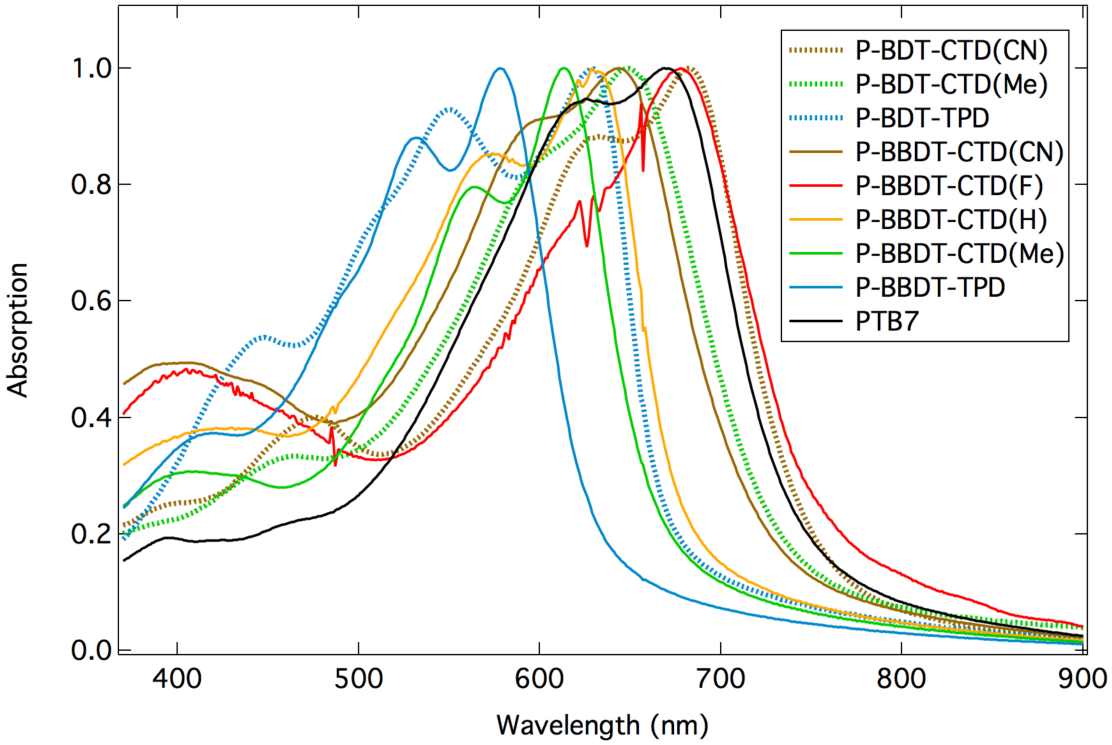



Figure 1. Absorption of various polymers in a thin film, normalized.

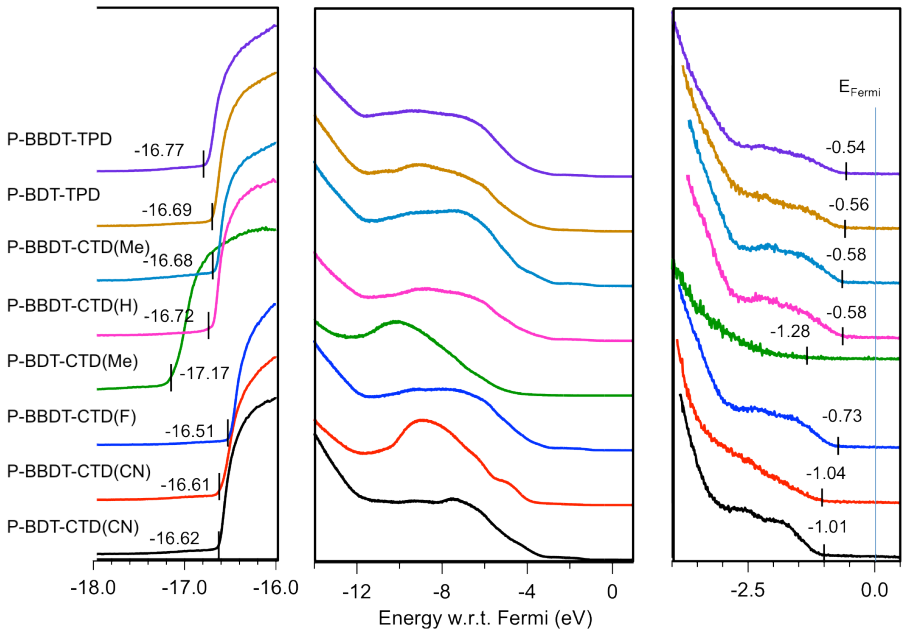
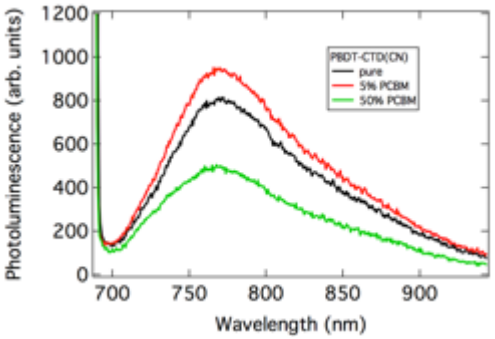
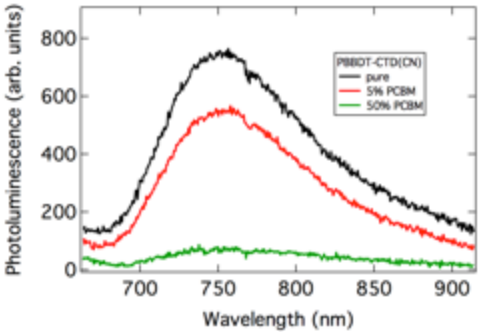
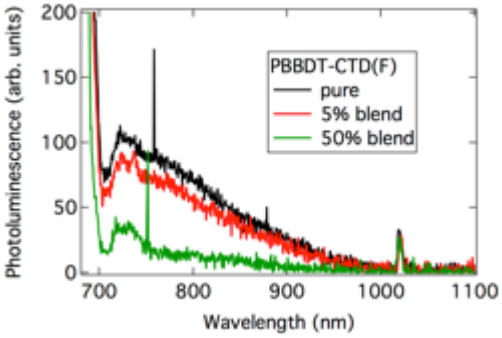
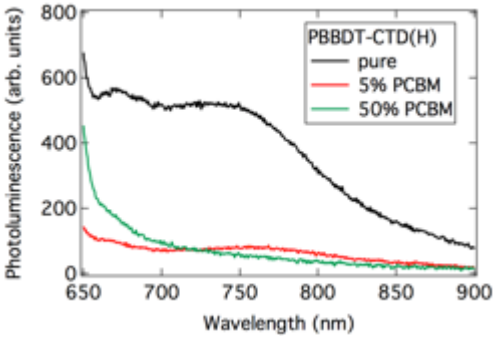


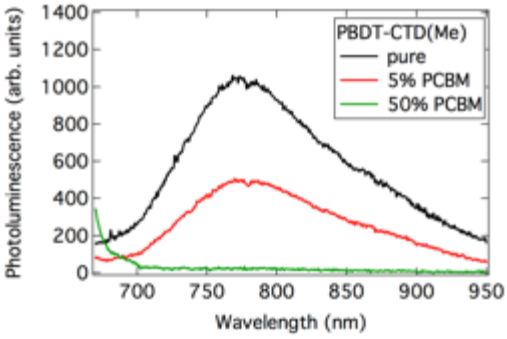

**Figure 2. UPS data on the various polymers studied.**

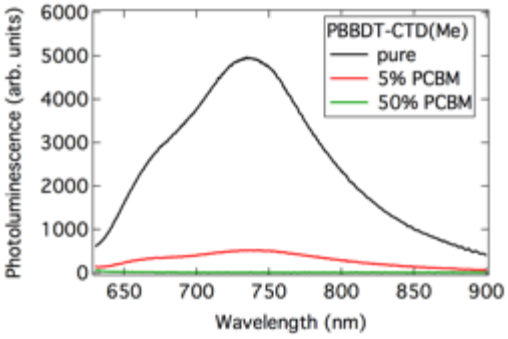

PBDT-CTD(CN)
pure
5% PCBM
50% PCBM
Photoluminescence (arb. units)
Wavelength (nm)


PBBDT-CTD(CN)
pure
5% PCBM
50% PCBM
Photoluminescence (arb. units)
Wavelength (nm)


PBBDT-CTD(F)
pure
5% blend
50% blend
Photoluminescence (arb. units)
Wavelength (nm)


PBBDT-CTD(H)
pure
5% PCBM
50% PCBM
Photoluminescence (arb. units)
Wavelength (nm)


PBDT-CTD(Me)
pure
5% PCBM
50% PCBM
Photoluminescence (arb. units)
Wavelength (nm)


PBBDT-CTD(Me)
pure
5% PCBM
50% PCBM
Photoluminescence (arb. units)
Wavelength (nm)

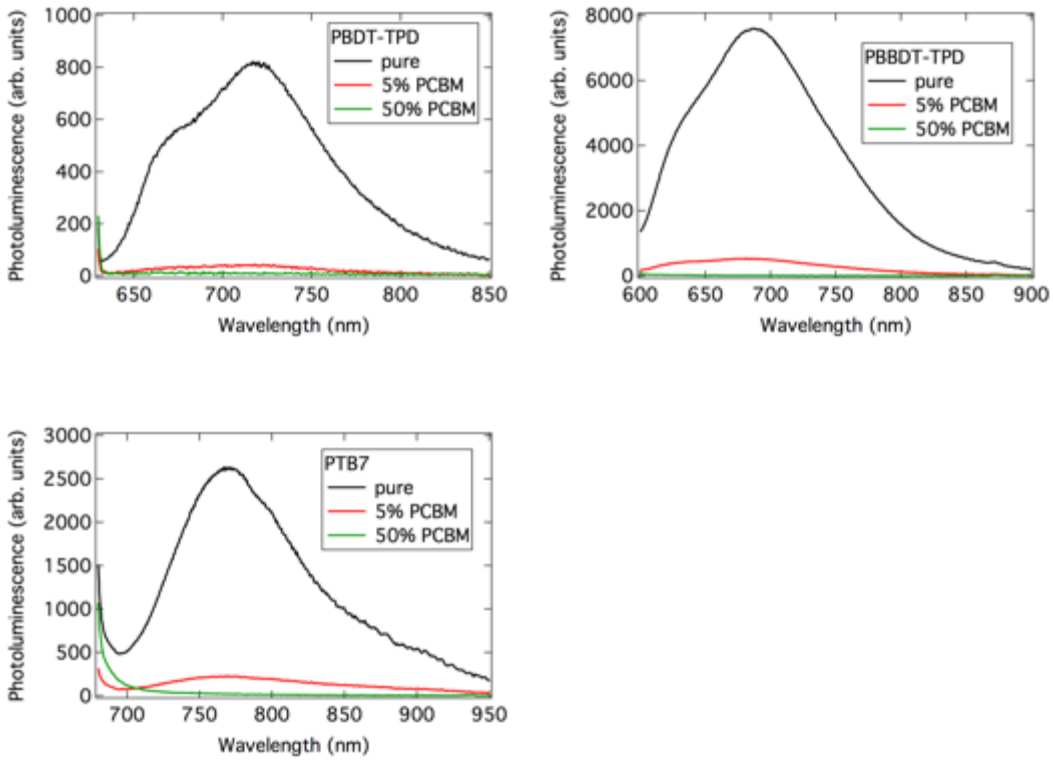
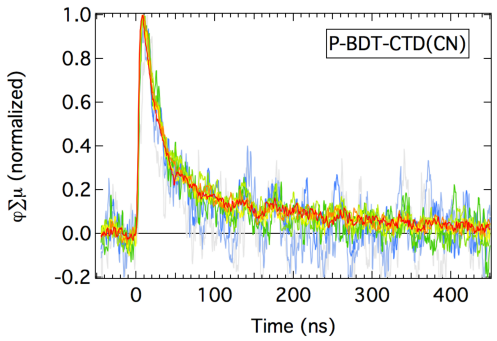
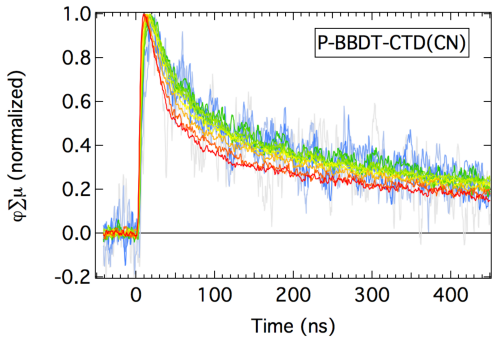
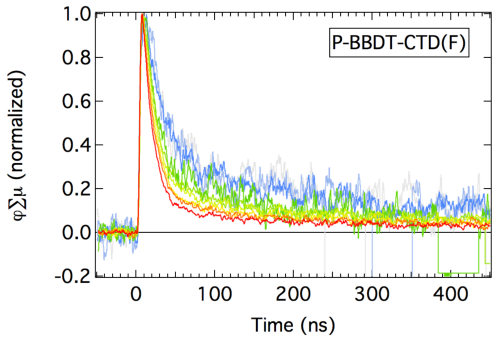
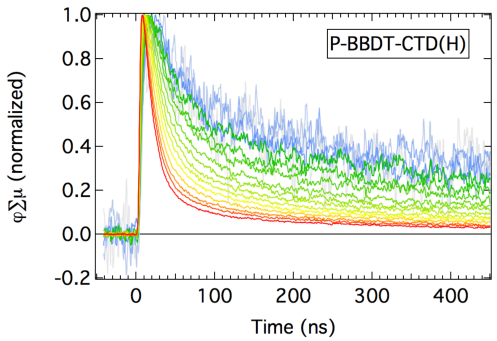


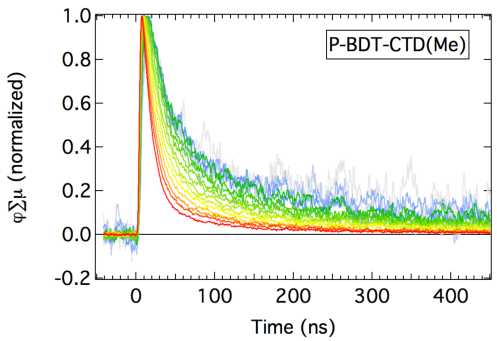

**Figure 3. PL data of the various polymers studied. Percentages indicate weight-% fullerene used in the thin film.**

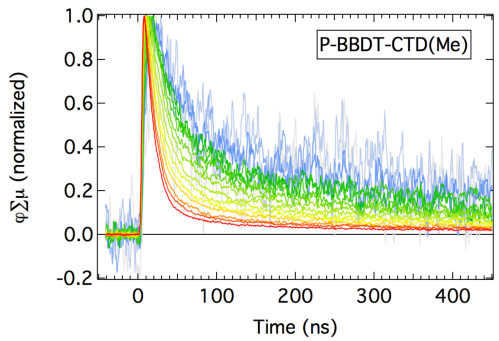

P-BDT-CTD(CN)
φ∑μ (normalized)
Time (ns)


P-BBDT-CTD(CN)
φ∑μ (normalized)
Time (ns)


P-BBDT-CTD(F)
φ∑μ (normalized)
Time (ns)


P-BBDT-CTD(H)
φ∑μ (normalized)
Time (ns)


P-BDT-CTD(Me)
φ∑μ (normalized)
Time (ns)


P-BBDT-CTD(Me)
φ∑μ (normalized)
Time (ns)

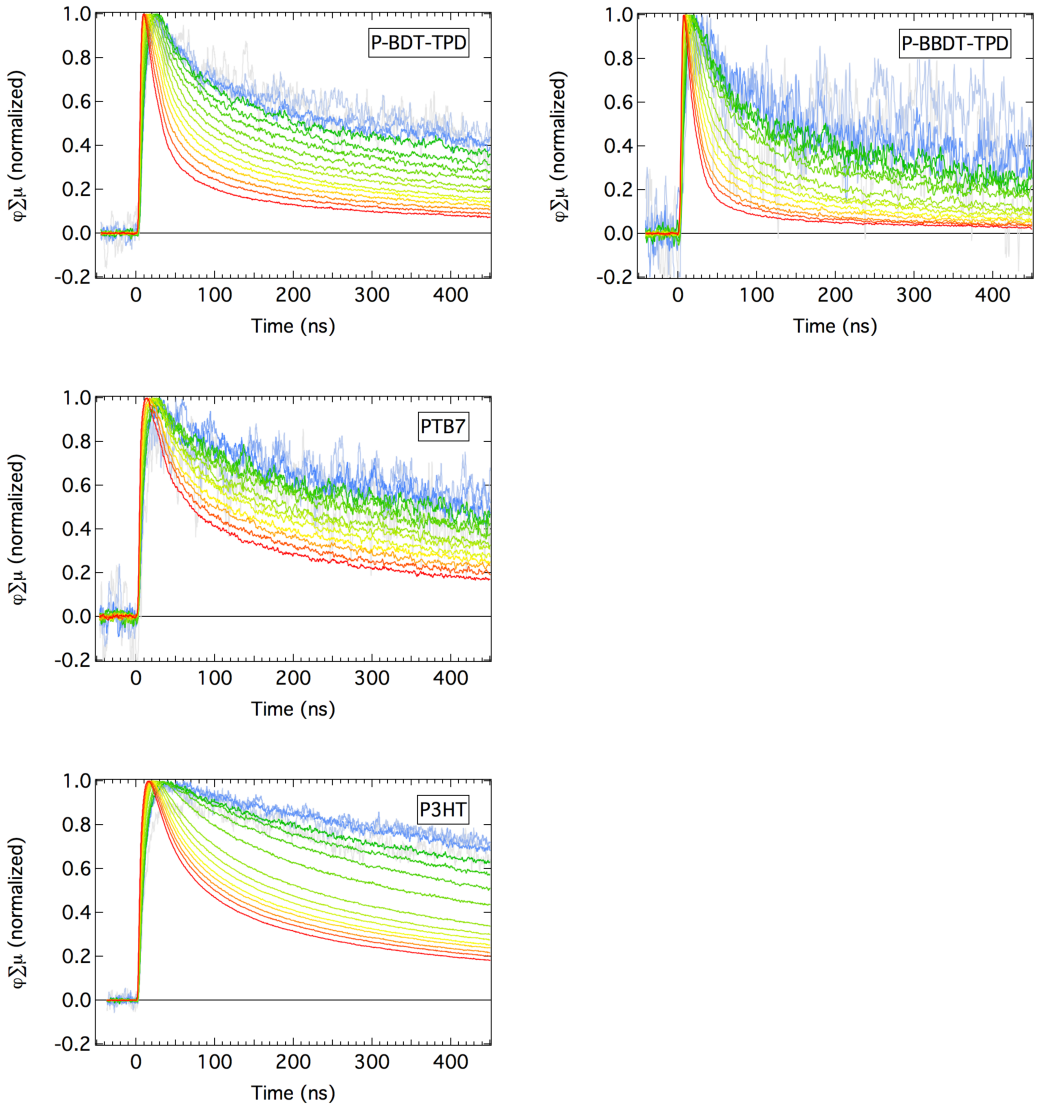



**Figure 4. TRMC transients of 50% blends with PCBM of the polymers studied. The curves in red are at the highest laser intensity, going to lower intensity towards the blue curves. We are currently investigating how these transients can give additional insight into predicting device performance.**

**Table 1. Device fabrication parameters for optimized devices. [a]CB=chlorobenzene, DIO=1,8-diodooctane, CN=chloronaphtalene, additives in vol-%. [b]PEDOT:PSS= poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (35 nm), $MoO_3$=molybdenum oxide (10 nm), [c]layer thickness of polymer:PCBM blend, [d]spun from hot solution (100°C). The top electrode consisted of calcium (20 nm) and aluminum (100 nm) for all devices.**

| Polymer | Polymer: PCBM ratio (w/w) | solvent[a] | Polymer concentration (mg/mL) | Spin rate (rpm) | Hole contact[b] | d (nm)[c] |
|---|---|---|---|---|---|---|
| P-BDT-CTD(CN) | 1:2 | CF | 6 | 1500 | PEDOT:PSS | |
| P-BBDT-CTD(CN) | 1:2 | CB | 8 | 2500 | PEDOT:PSS | 45 |
| P-BBDT-CTD(F) | 1:2 | CB/3% CN | 6 | 800 | $MoO_3$ | 60 |
| P-BDT-CTD(Me) | 1:2 | CF | 4 | 3000 | $MoO_3$ | 75 |
| P-BBDT-CTD(H) | 1:2 | CF | 4 | 3000 | $MoO_3$ | 75 |
| P-BBDT-CTD(Me) | 1:2 | CB/3% CN | 6 | 1000 | $MoO_3$ | 95 |
| P-BDT-TPD | 1:2 | CB/4% DIO[d] | 8 | 2000 | PEDOT:PSS | 200 |
| P-BBDT-TPD | 1:2 | ODCB | 10 | 2000 | PEDOT:PSS | 130 |
| PTB7 | 1:1.5 | CB 3% DIO | 10 | 1500 | PEDOT:PSS | 215 |

**Table 2. Electronic properties of polymers.**

| **Polymer** | **-ΔH (calc)[a] (eV)** | **-ΔH (measured)[b] (eV)** |
|---|---|---|
| P-BDT-CTD(CN) | -0.20 | 0.01 |
| P-BBDT-CTD(CN) | 0.10 | 0.08 |
| P-**B**BDT -CTD(F) | 0.15 | 0.19 |
| P-BDT -CTD(Me) | 0.36 | 0.38 |
| P-**B**BDT-CTD(H) | 0.47 | 0.68 |
| P-**B**BDT -CTD(Me) | 0.50 | 0.70 |
| P-BDT-TPD | 0.49 | 0.68 |
| P-**B**BDT -TPD | 0.61 | 0.96 |
| PTB7 | 0.66 | 0.51[c] |

*[a]$\Delta H = (IE_{donor} - EA_{fullerene}) - E_{exc}$, using the calculated HOMO as IE and optical band gap as $E_{exc}$, as described in the main article. The EA of PCBM is assumed to be -3.80 eV.*[3] *[b]using the ionization potential from UPS measurements and the band gap measured in a thin film of pure material ($\lambda_{max}$) as $E_{exc}$ [c]Literature value is used for the band gap and IE*[4]