Dye-attached fullerenes:  
- DPP-C60 (5:6)
- DPP-C60 (6:6)
- TBTDT-C60 (6:6)
- TBTDT-C60 (5:6)*
- PCB-DPP (6:6)
- PCB-TBTDT (6:6)

Pentacene dimers (Htips-Ftips)
DPP-attached to C60 (5:6)

CT energy = 1.42 eV, vEA=2.68 eV
DPP-attached to C60 (6:6)

CT energy = 2.31 eV, vEA = 2.72 eV
TBTDT-6:6 C60

vEA = 2.70 eV

CT energy = 2.35 eV
PCB-TBTDT

CT energy = 2.55 eV, vEA = 2.41 eV
CT energy = 2.74 eV, vEA=2.79 eV
CT energy $= 1.09 \text{ eV} \rightarrow \Delta \text{SCF PBE (No exact exchange, results similar to TDDFT B3LYP)}$

Non-zero, small transition dipole matrix element between H and L.

$v_{\text{IP}} = 5.90 \text{ eV}$ (htip monomer $v_{\text{IP}}=5.96 \text{ eV}$)

$v_{\text{EA}} = 2.55 \text{ eV}$ (ftip monomer $v_{\text{EA}}=2.51 \text{ eV}$)

Trimers are being optimized.
Hetero TIPS Dimer

HOMO - LUMO = 1.524 eV

0.065 eV

TDDFT Excited States:
1: 1.138 eV (1089 nm) (HOMO->LUMO transition)
2: 1.615 eV (768 nm)
3: 1.7272 (717 nm)

vs.
1: 1.8787 eV (HOMO->LUMO + HOMO->LUMO+1)
2: 1.9771 eV

B3LYP predicts low CT state; CAM-B3LYP does not.
dye-adducts LUMO energies are similar to PCBM

electronically, the dye acts independently of the fullerene