Paper Introduction

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Triplet Exciton Dissociation in Singlet Exciton Fission Photovoltaics

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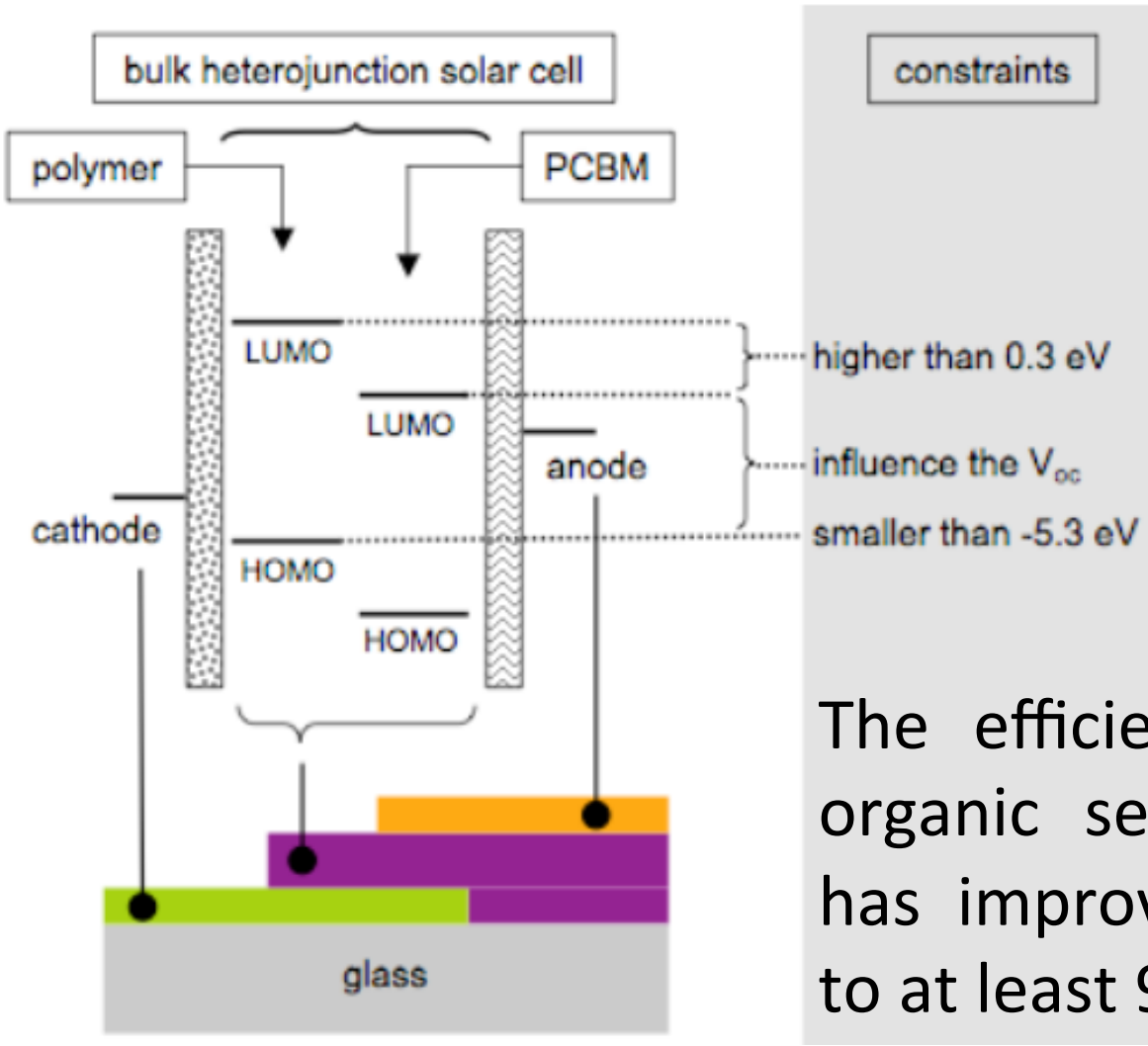
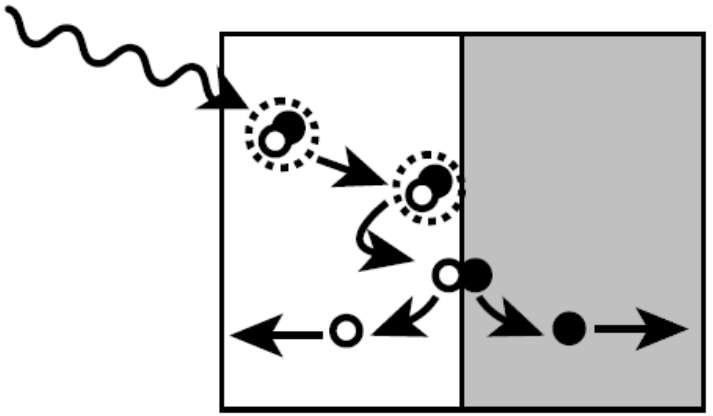
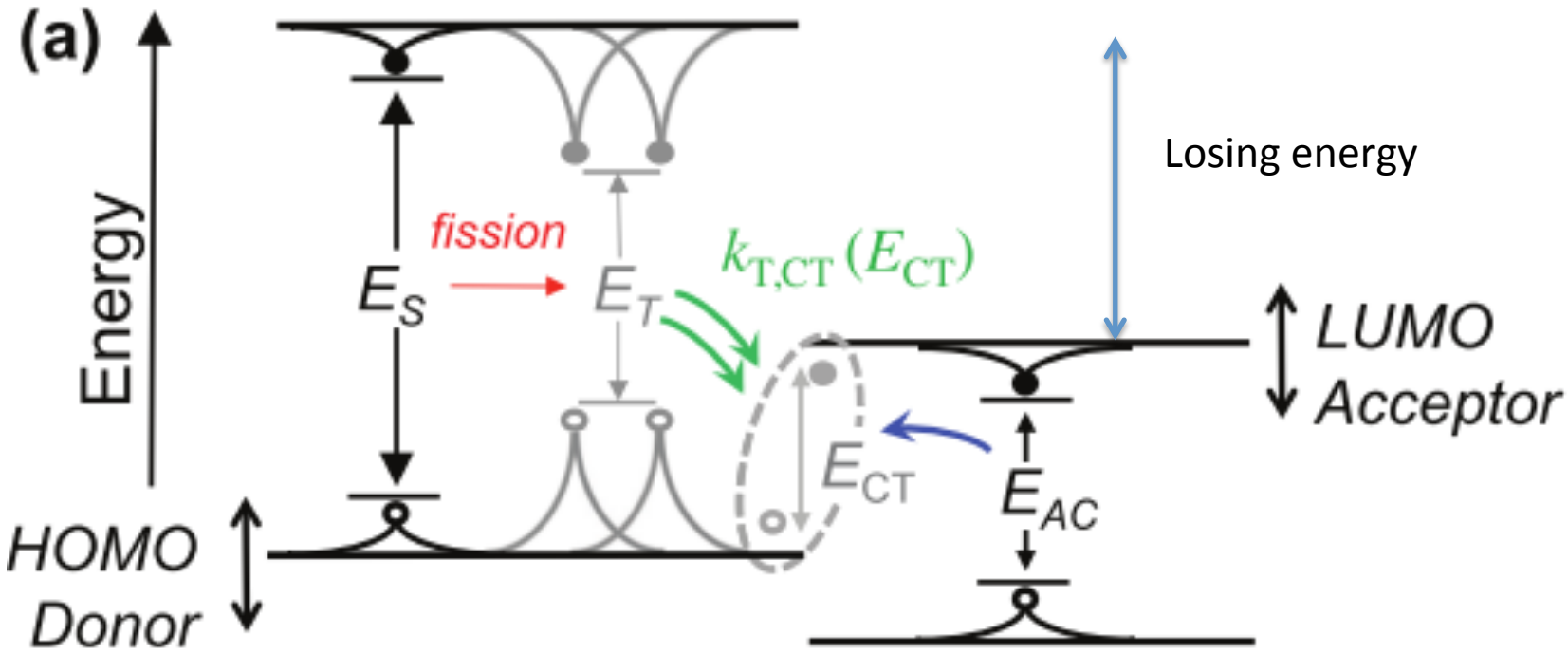
Organic Solar Cell





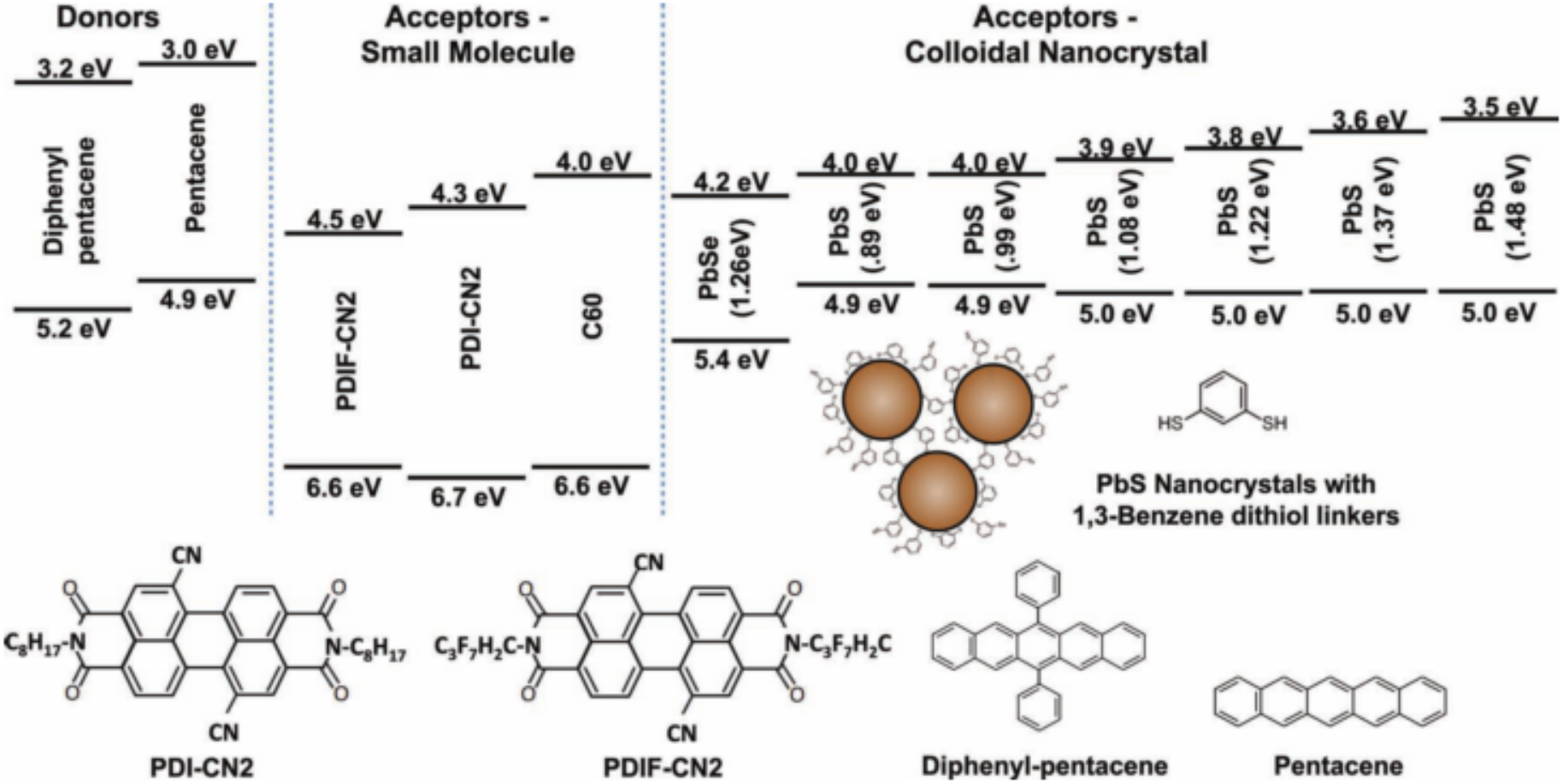
The efficiency of single junction organic semiconductor solar cell has improved rapidly, from 4.4% to at least 9.2% in the last 6 years

Motivation is to improve efficiency of organic Solar cell



Harnessing additional incident photons with wavelengths beyond the absorption energy.

Materials


Donors
3.2 eV
3.0 eV
Diphenyl pentacene
Pentacene
4.9 eV
5.2 eV
Acceptors - Small Molecule
4.5 eV
4.3 eV
4.0 eV
PDIF-CN2
PDI-CN2
C60
6.6 eV
6.7 eV
6.6 eV
Acceptors - Colloidal Nanocrystal
4.2 eV
PbSe (1.26eV)
5.4 eV
4.0 eV
PbS (.89 eV)
4.9 eV
4.0 eV
PbS (.99 eV)
4.9 eV
3.9 eV
PbS (1.08 eV)
5.0 eV
3.8 eV
PbS (1.22 eV)
5.0 eV
3.6 eV
PbS (1.37 eV)
5.0 eV
3.5 eV
PbS (1.48 eV)
5.0 eV
HS
SH
PbS Nanocrystals with 1,3-Benzene dithiol linkers
CN
C8H17-N
N-C8H17
CN
PDI-CN2
CN
C3F7H2C-N
N-C3F7H2C
CN
PDIF-CN2
Diphenyl-pentacene
Pentacene

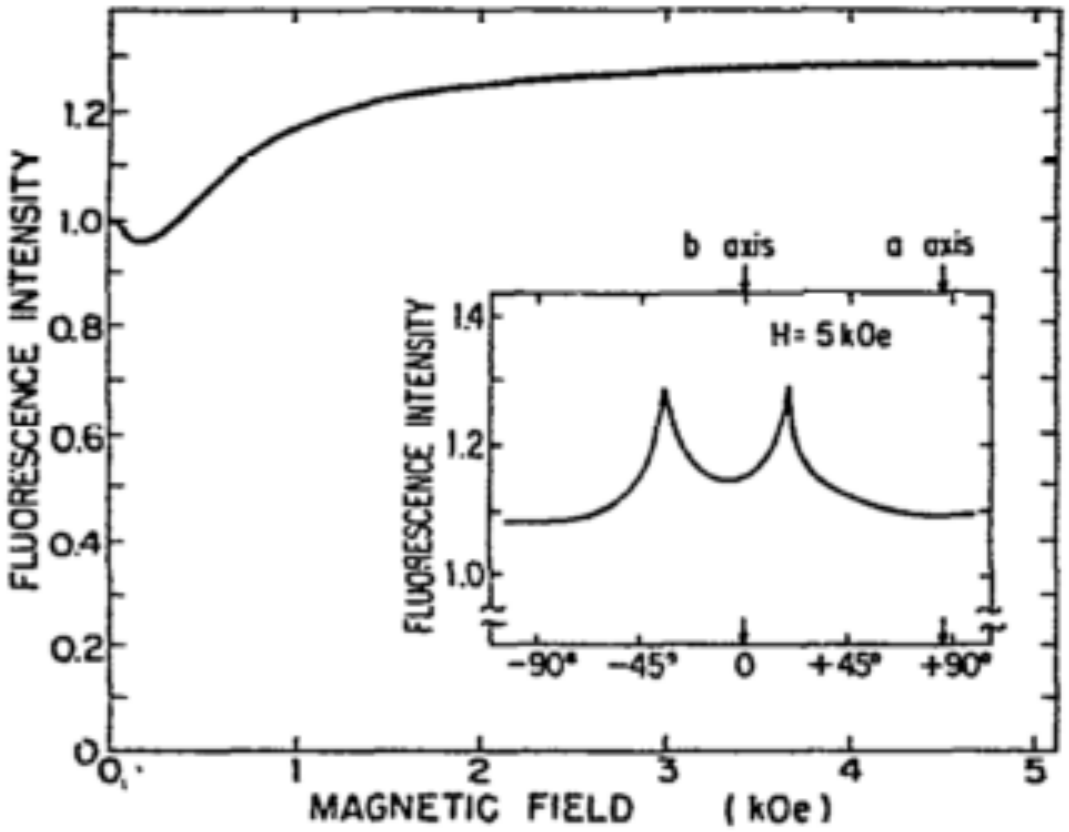
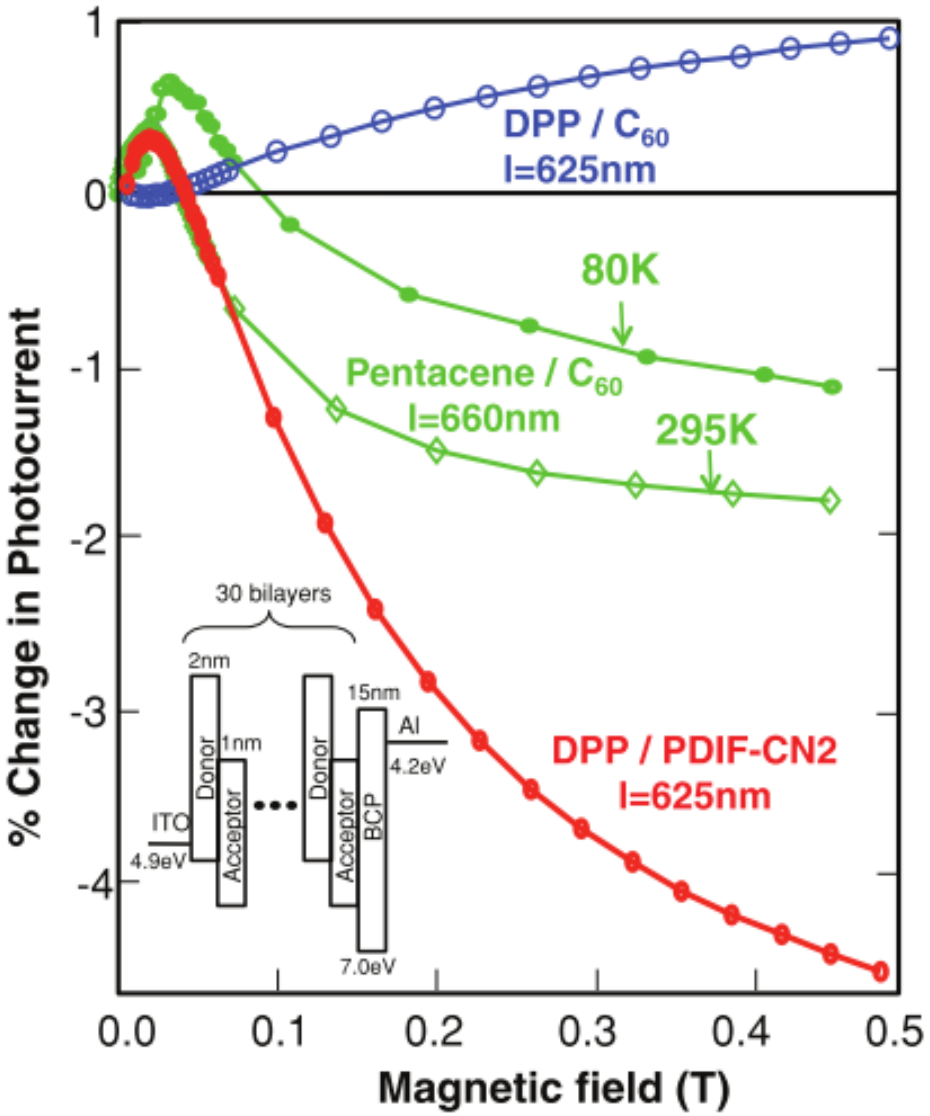


Fig. 1. Magnetic field dependence of fluorescence intensity from a tetracene crystal at room temperature with the magnetic field in the *ab* plane of the crystal at +18° with respect to the *b* axis. The insert shows the dependence of the fluorescence intensity on the orientation of a 5 kOe magnetic field in the *ab* plane of the crystal.

Chemical Physics Letters 3, 155–157 (1969).



Rate of singlet fission(k_f) in pentacene is very fast (1/80 fs) and dependent on the magnetic field, increasing slightly initially and then decreasing at fields higher that 50 mT.

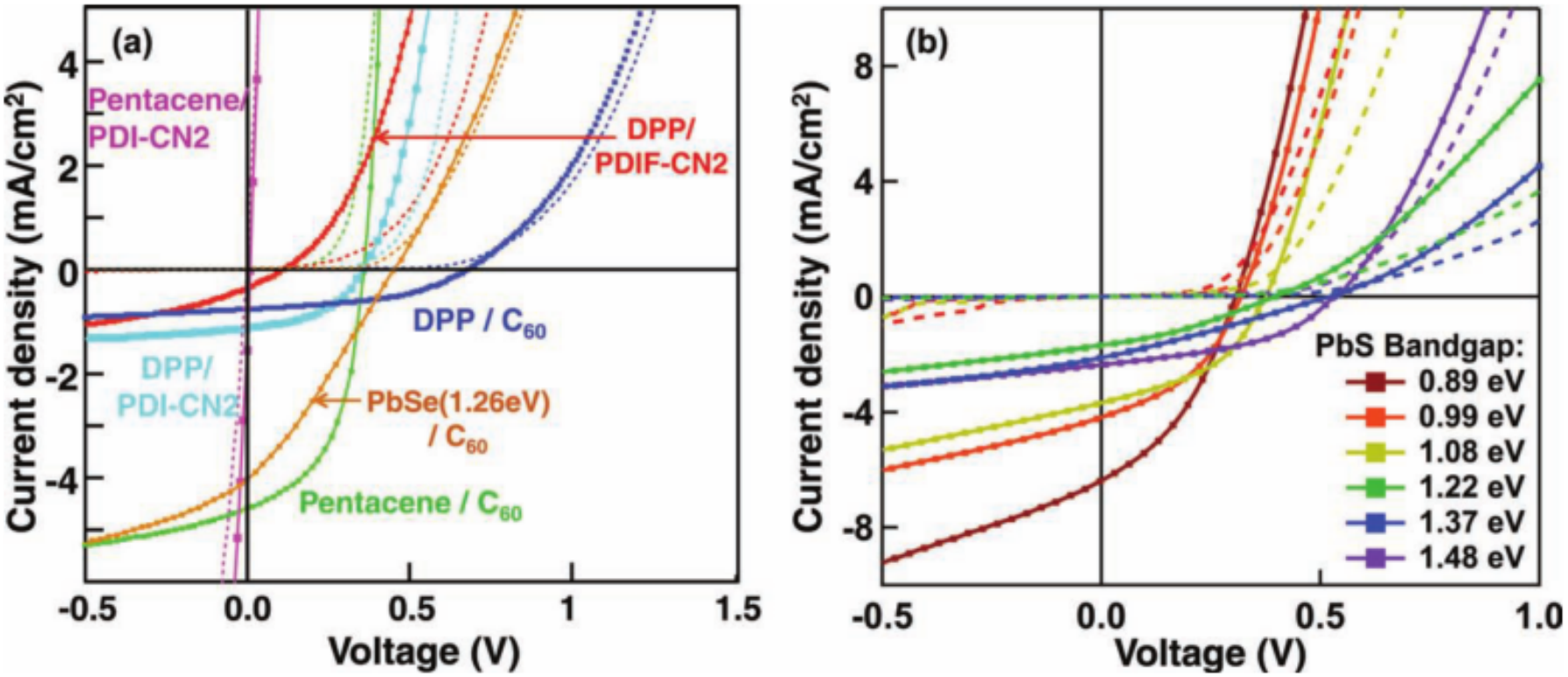
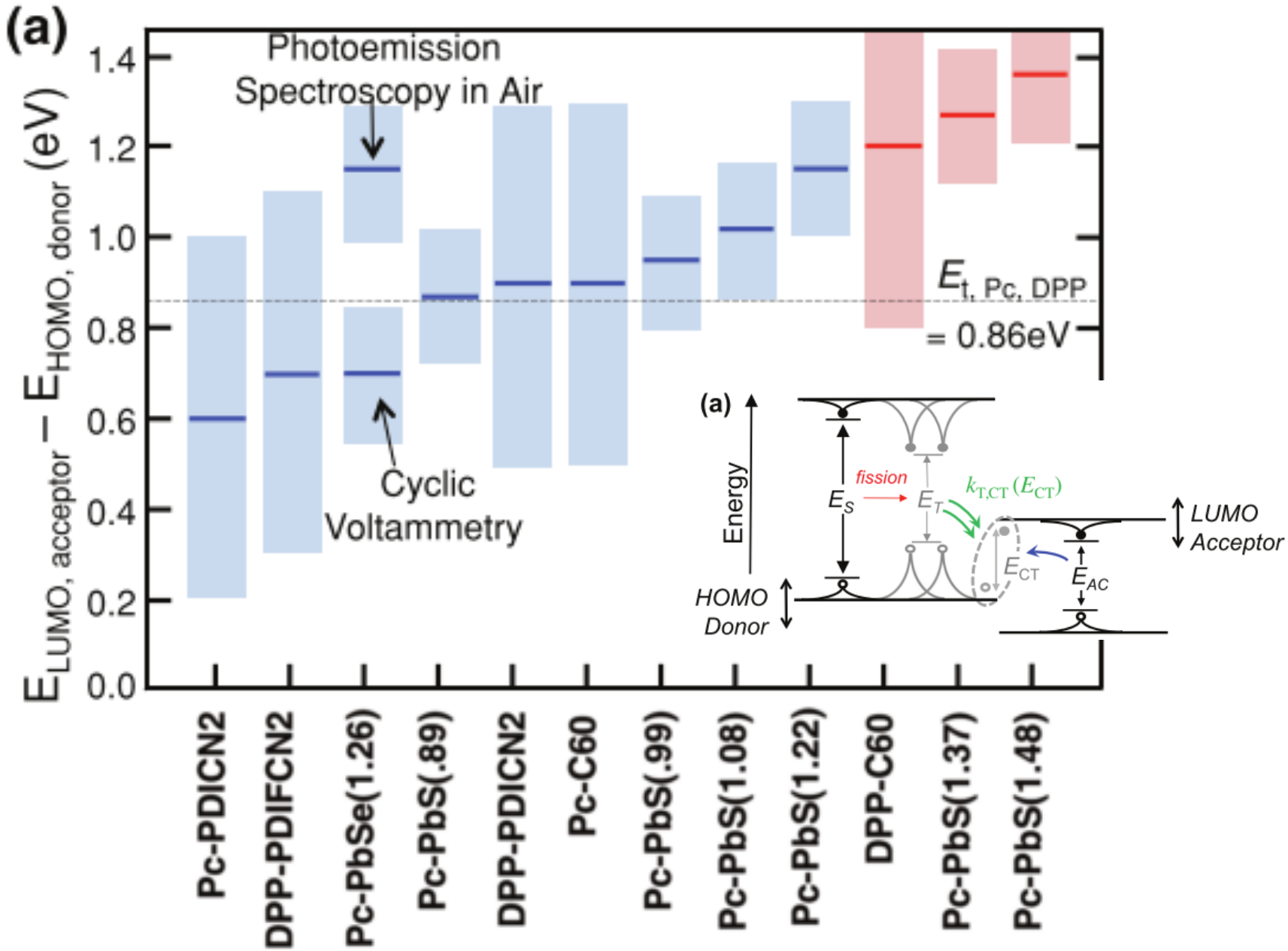


Figure 4. Current-voltage characteristics for (a) organic acceptor devices and the pentacene-PbSe(1.26 eV) device, and (b) pentacene-PbS devices. Solid lines are taken under simulated AM1.5 conditions. Dashed lines are the dark response.

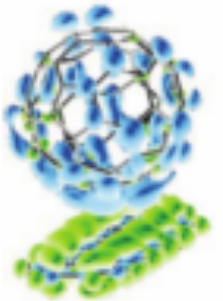


The binding energy of a triplet exciton in pentacene is signified by the horizontal at 0.86 eV

head-to-tail

(b)

0.9 – 1.0 eV



1.1 – 1.3 eV

the face-to-face

The HOMO-LUMO energy of the geometry is 1.0–1.1 eV and the binding energy of the CT state is found to be roughly 0.1 eV

→ CT state energy of 0.9–1.0 eV

→ Low enough to break up the pentacene triplet state.

HOMO-LUMO energy is 1.4–1.6 eV, and the CT binding energy is roughly 0.3 eV

→ CT state energy of 1.1–1.3 eV.

Their conclusion

- C_{60} are sensitive to small changes in the donor and acceptor energy levels

- The most technologically promising acceptor is PbSe(1.26 eV). It efficiently dissociates pentacene triplet excitons and also absorbs long wavelength light.