Electron-Hole Separation with Dual Electron/Hole Acceptors for Organic Photovoltaic Applications

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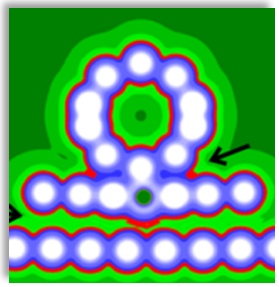


Organic Solar Cells

Cheap and flexible

Boda Boda Operator

Cost

Efficiency

Polymer-fullerene bulk heterojunction solar cells (PSCs) approaching 10%

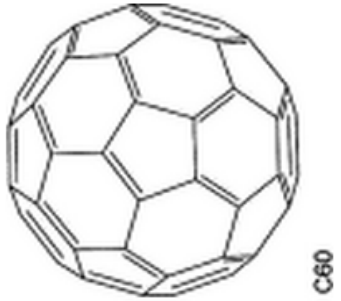
Hoppe, H.; Sariciftci, N. S. *J. Mater. Res.* **2004**, *19*, 1924–1945.

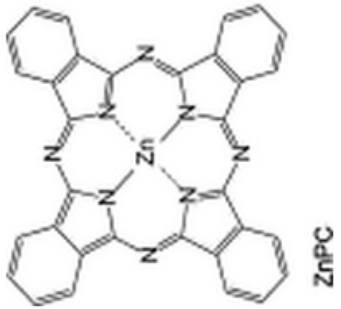
He, Z.; Zhong, C.; Su, S.; Xu, M.; Wu, H.; Cao, Y. *Nat. Photonics* **2012**, *6*, 591–595.

http://www.afrigadget.com/2009/09/05/a-wearable-flexible-solar-panel-idea/

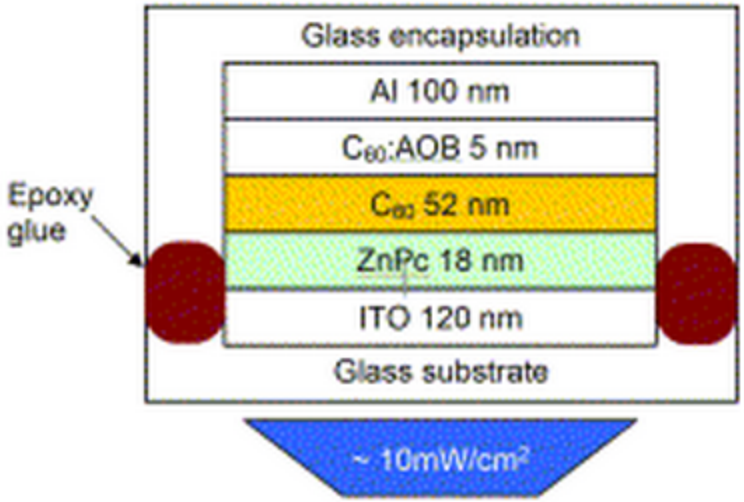
Heterojunctions with Donor-Acceptor

Electron acceptor
High electron affinity



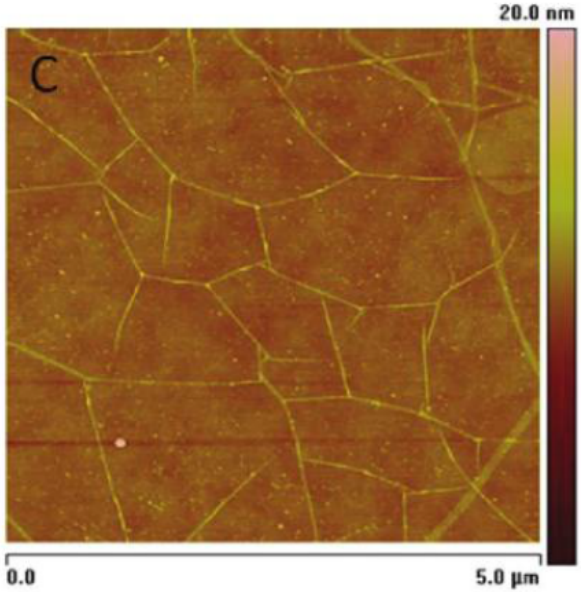


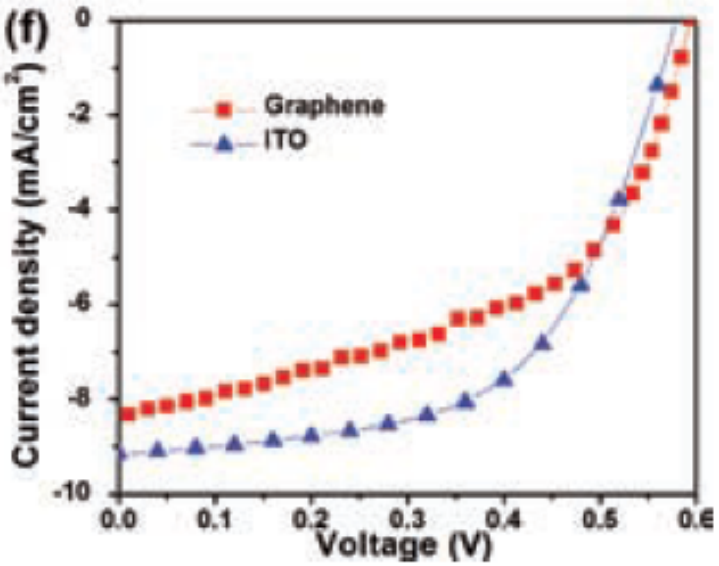
Electron-donor



Kažukauskas et al., Optical Materials 2010, 32 1676.

Graphene as Anode Material





- Low cost, transparency, high electrical conductivity, chemical robustness, Flexibility.
- Impact on hole dynamics.

Park, H.; Brown, P. R.; Bulović, V.; Kong, J. *Nano Lett.* **2012**, *12*, 133–140.
Wang, Y.; Tong, S. W.; Xu, X. F.; Özyilmaz, B.; Loh, K. P. *Adv. Mater.* **2011**, *23*, 1514–1518

Calculation Methods

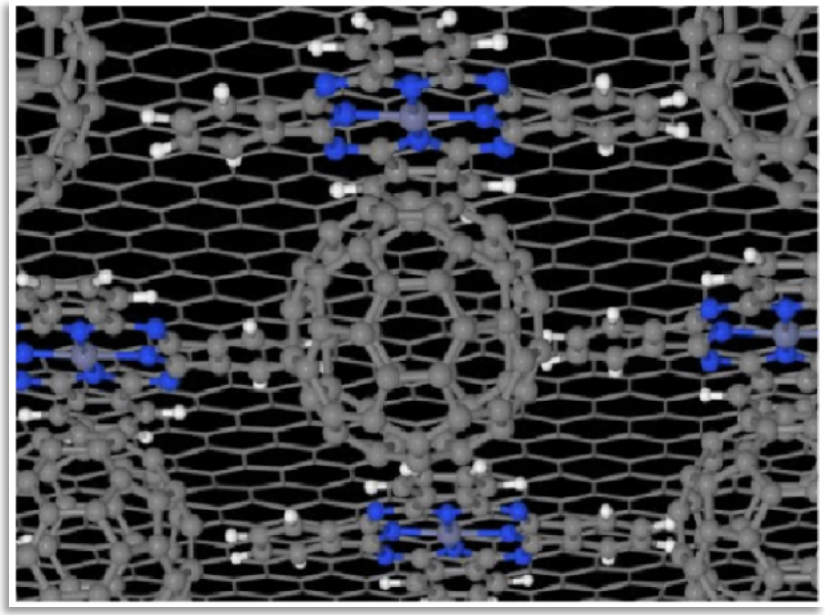
DFT (Siesta):

- Double-ζ plus polarization basis set
- 0.04 eV/Å maximum force convergence criterion
- Mesh cutoff of 200 Ry
- VDW (DRSLL) Van der Waals exchange-correlation density functional

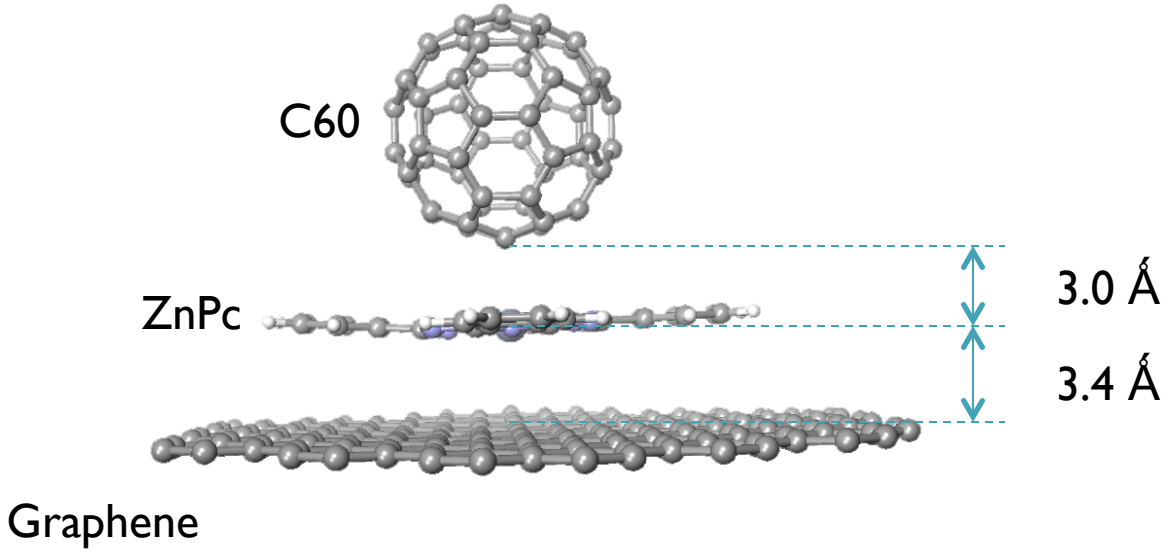
TDDFT (GPAW):

- Absorption spectrum: Casida's formulation of time-dependent DFT (TDDFT) linear response theory
- Evolution of the photo-excited electron-hole pair: non-adiabatic Ehrenfest molecular dynamics
- Periodic boundary conditions used to avoid any spurious finite size effects

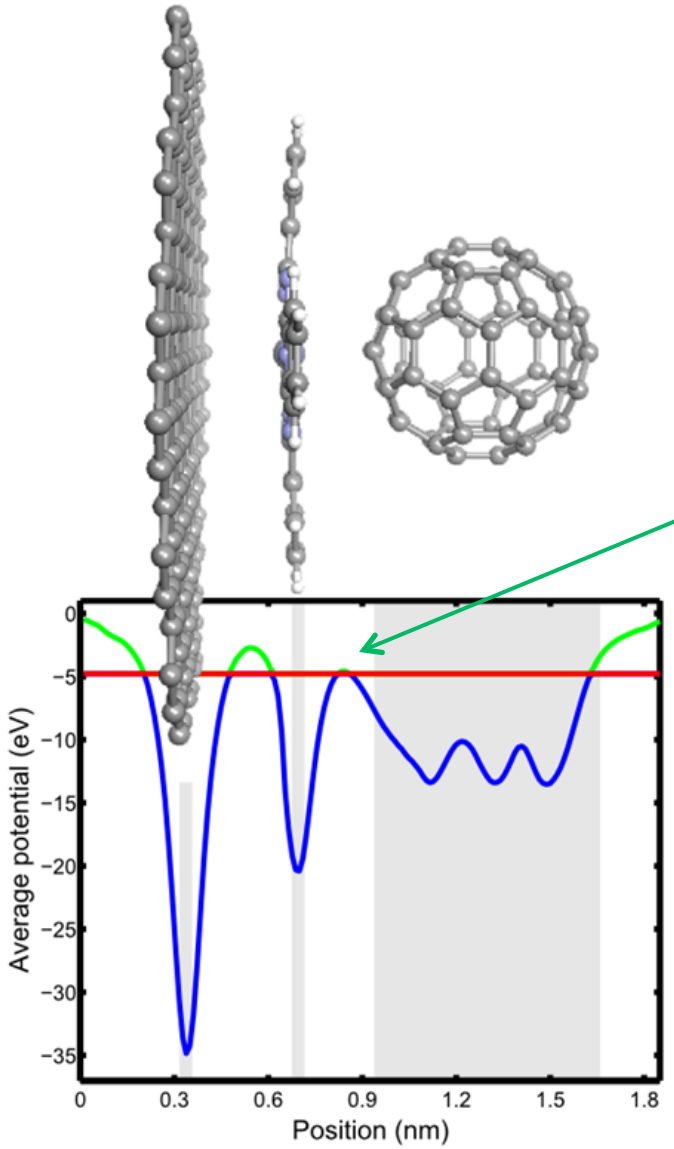
Sandwich Structure



Dia. Variation <1%

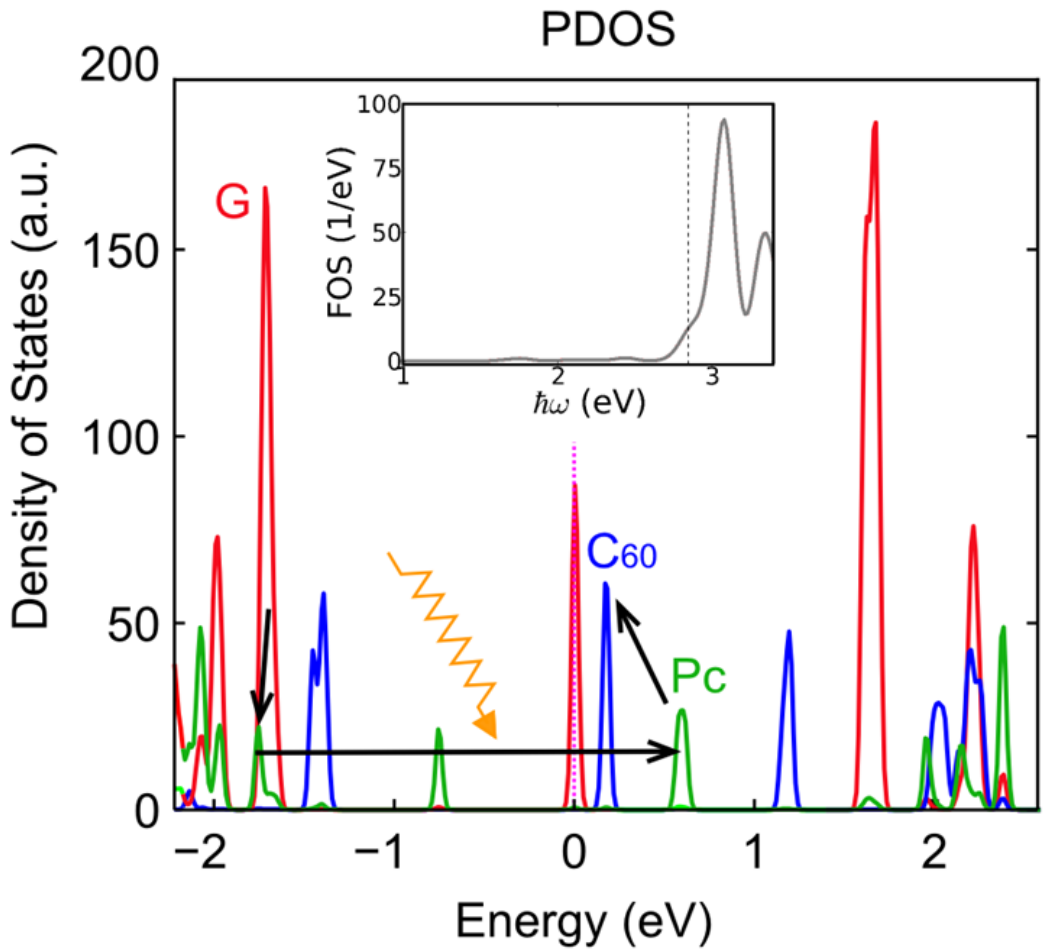


Potential Profiles across the Sandwich Structure



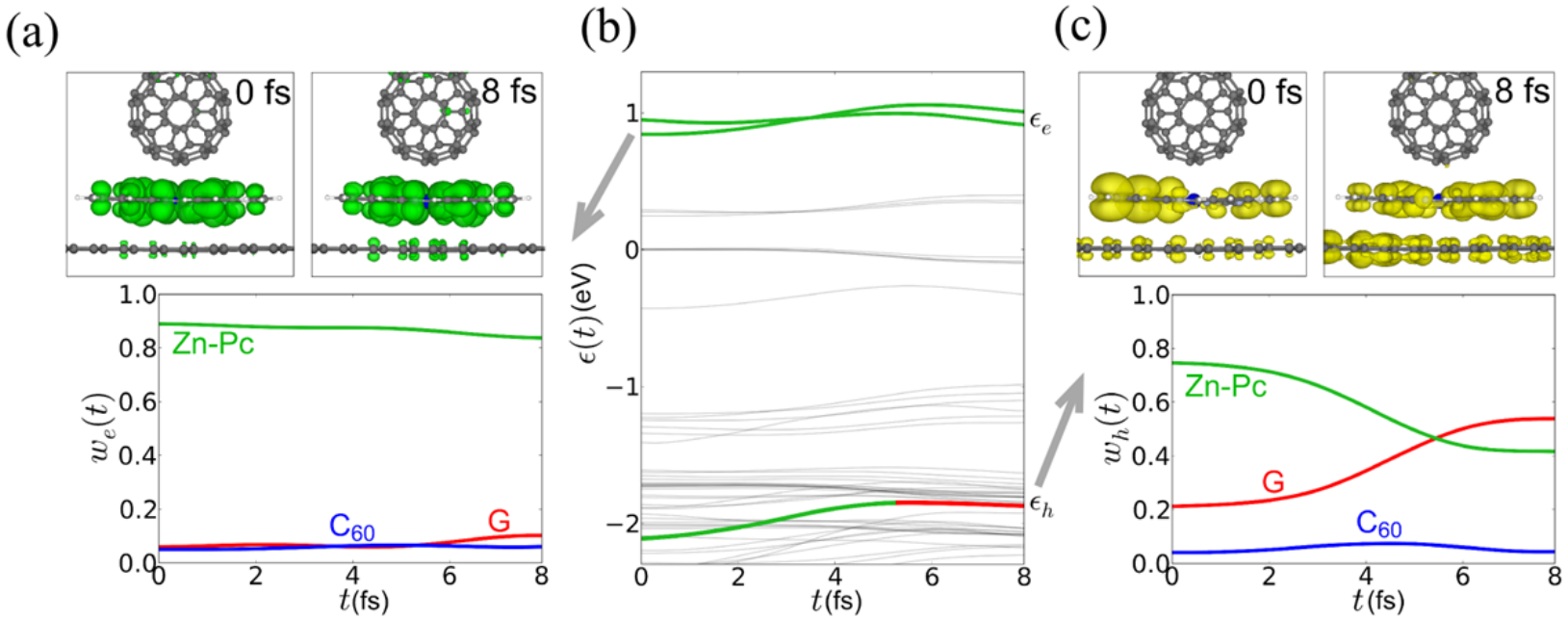
Lower barrier for electron to transport to C60

Pumping mechanism with dual electron/ hole acceptors

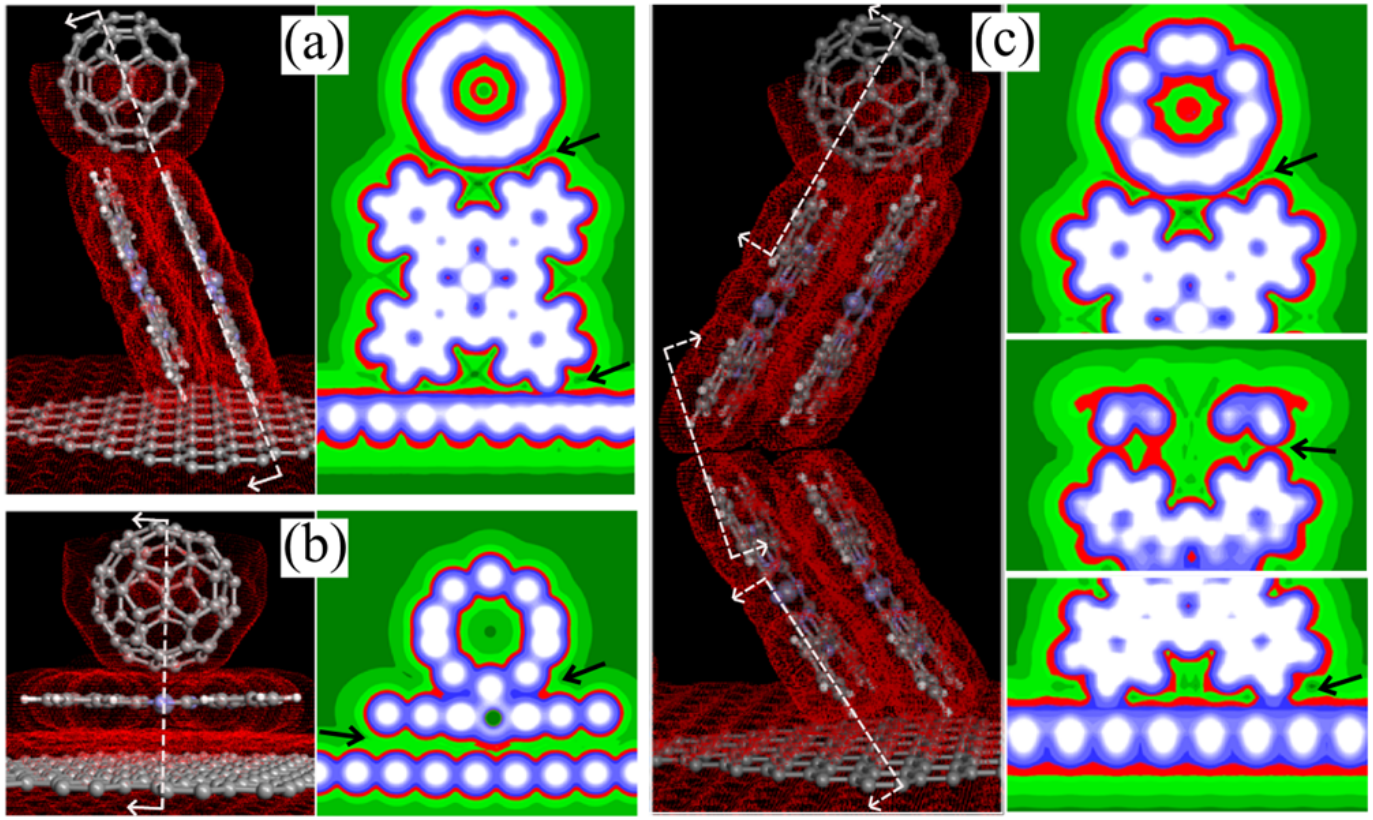


TDDFT: 2.8 eV
DFT: 2.3 eV

Dynamics of Electron and Hole Transfer



Comparison between Various Interface Morphology



The flat configuration (b) is favored due to stronger coupling and asymmetric barriers

Summary

- Dual electron/hole acceptors for high efficiency
- Graphene is a promising hole collecting anode material
- The flat configuration for G/ZnPc/C60 structure is favored

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