Electron transport in Organic Materials

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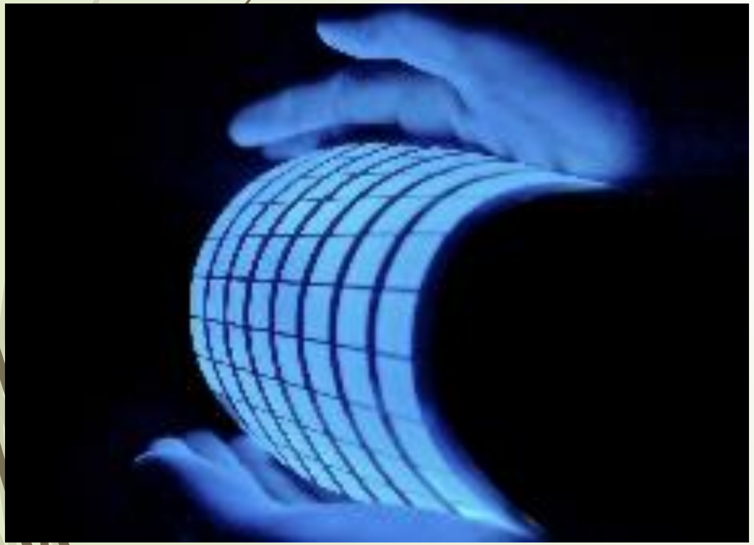
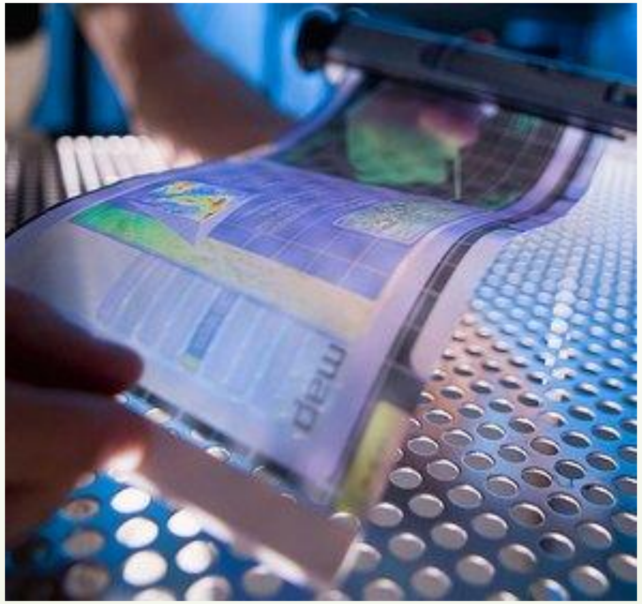
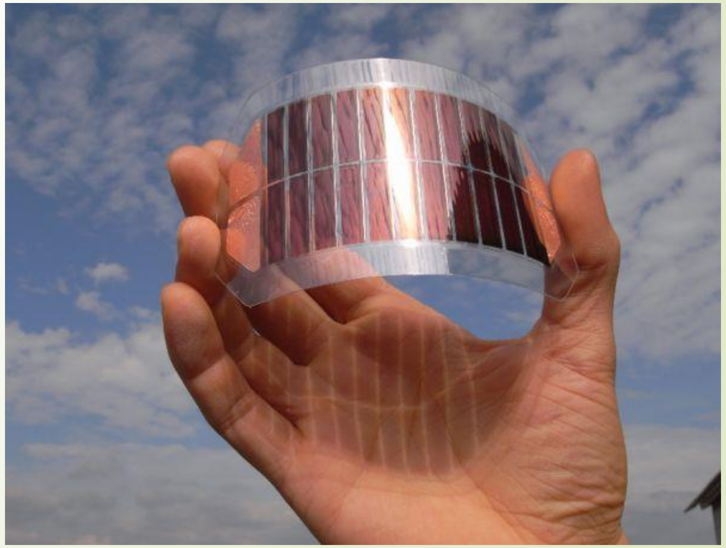
April 25, 2016

Motivation

- Organic materials are abundant
- Organic electronics: more cost effective, easier to process, and can be deposited on flexible substrates.







Difficulty with charge transport

- Large variety
- Variety of molecular interaction
- Tightly bound electrons

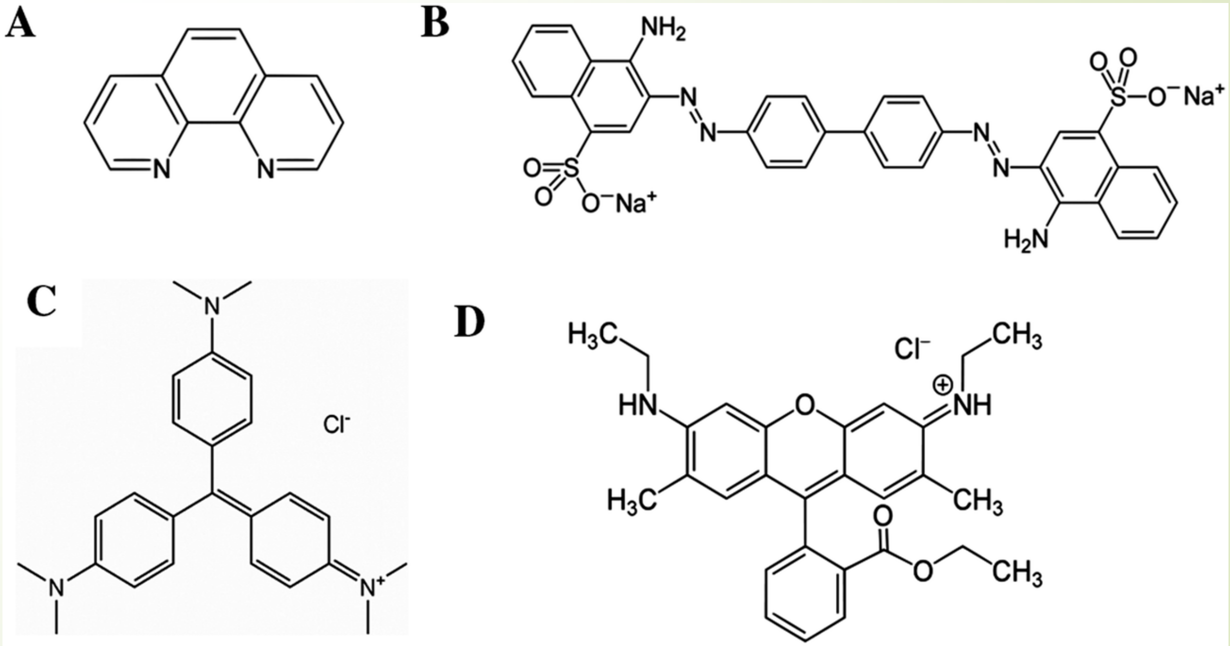
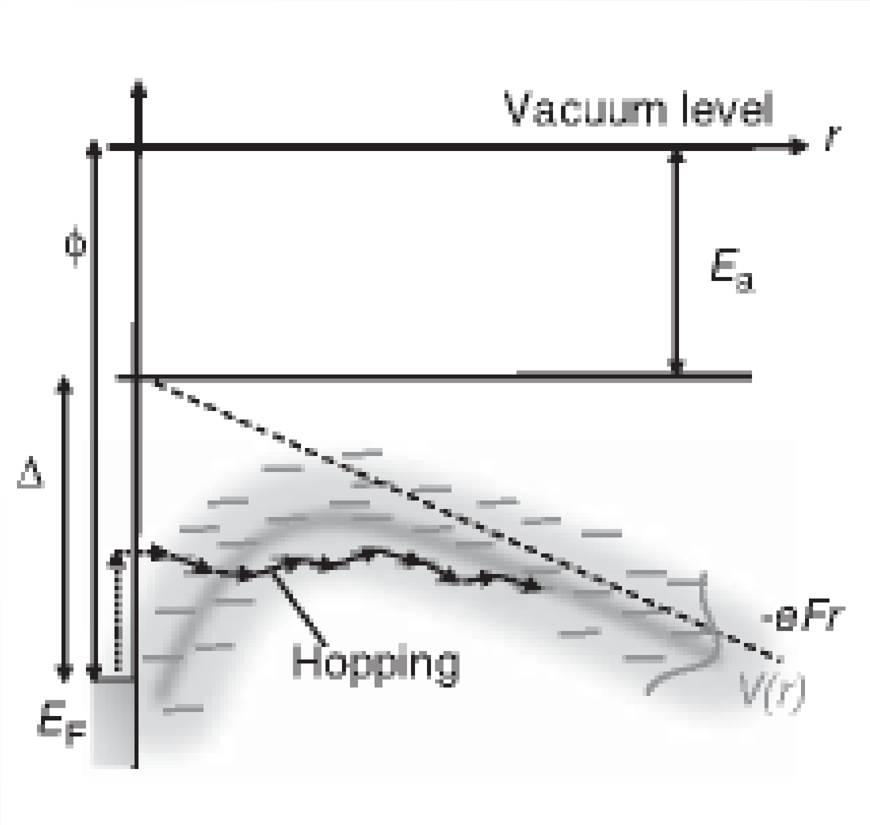


Image from Kumar, V. B., Koltypin, Y., Gedanken, A., & Porat, Z. (2014). Ultrasonic cavitation of molten gallium in water: Entrapment of organic molecules in gallium microspheres. *J. Mater. Chem. A*, 2(5), 1309-1317. doi:10.1039/c3ta13573j

Charge Generation

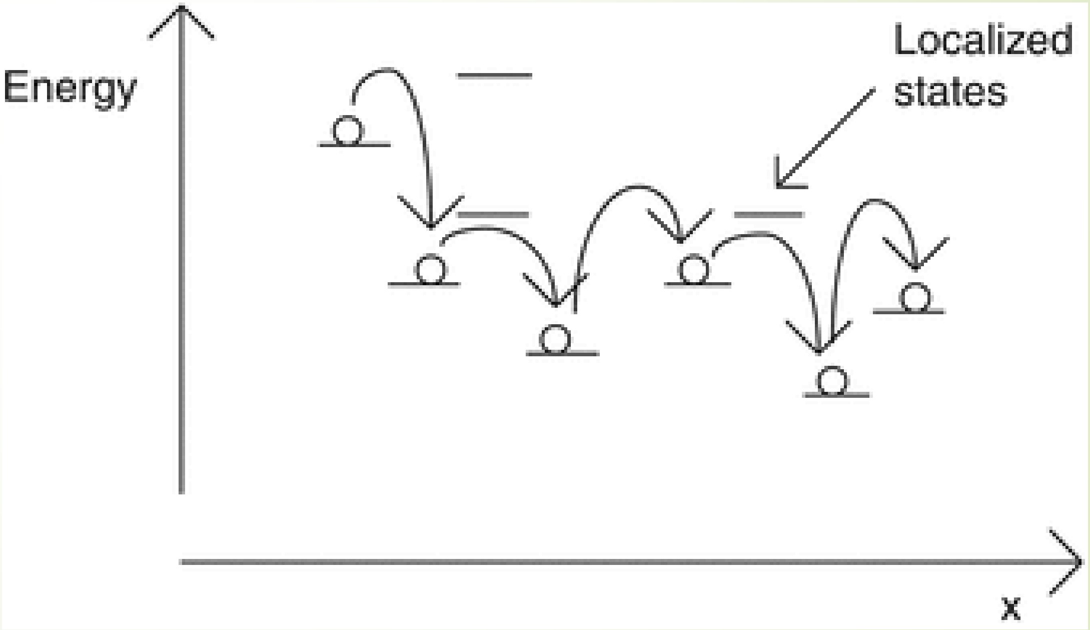
- Charge injection
  - Thermally activated injection
- Optical excitation



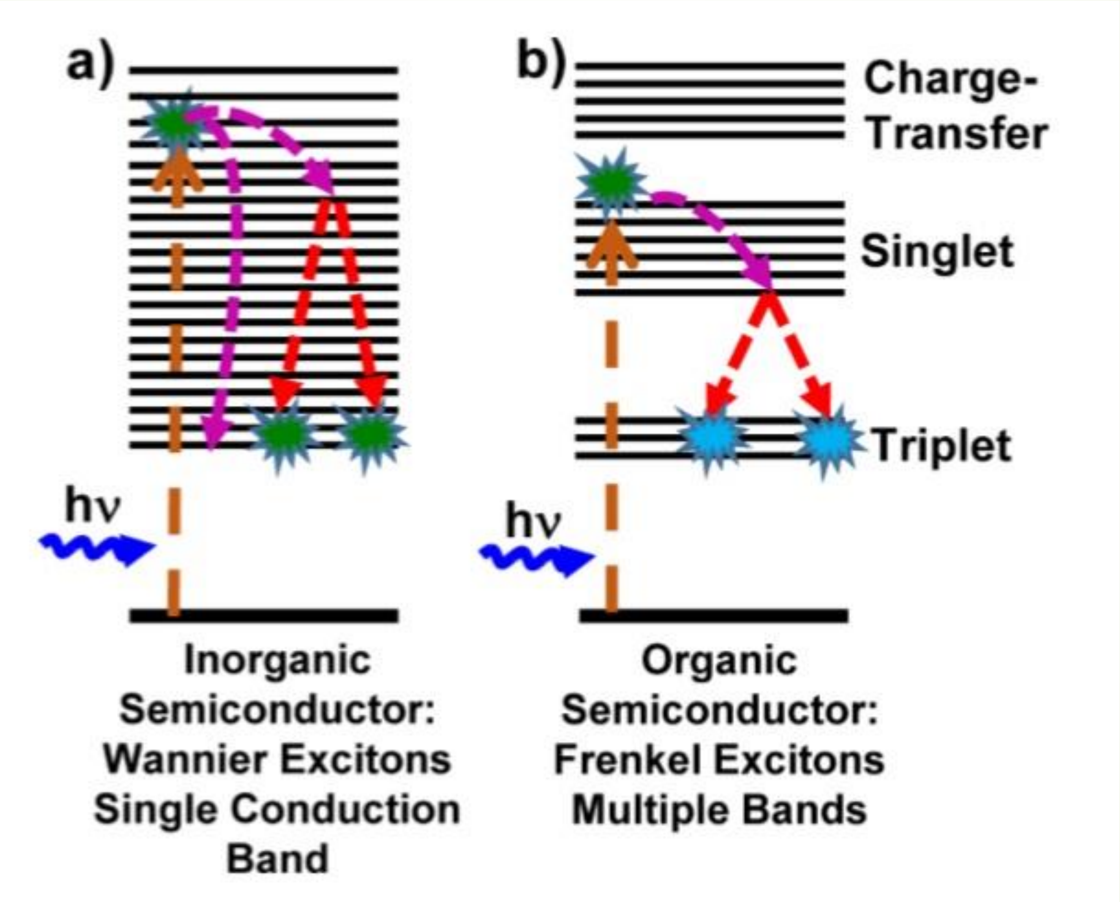
Köhler, A., & Bässler, H. (2015). *Electronic processes in organic semiconductors: An introduction*. Weinheim: Wiley-VCH Verlag GmbH & KGaA.

Transport

- Band transport
- Hopping
  - Trapping
  - Singlet fission

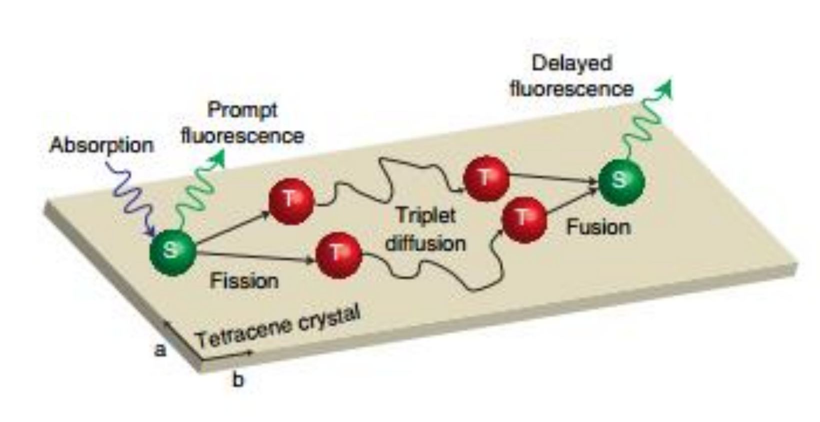


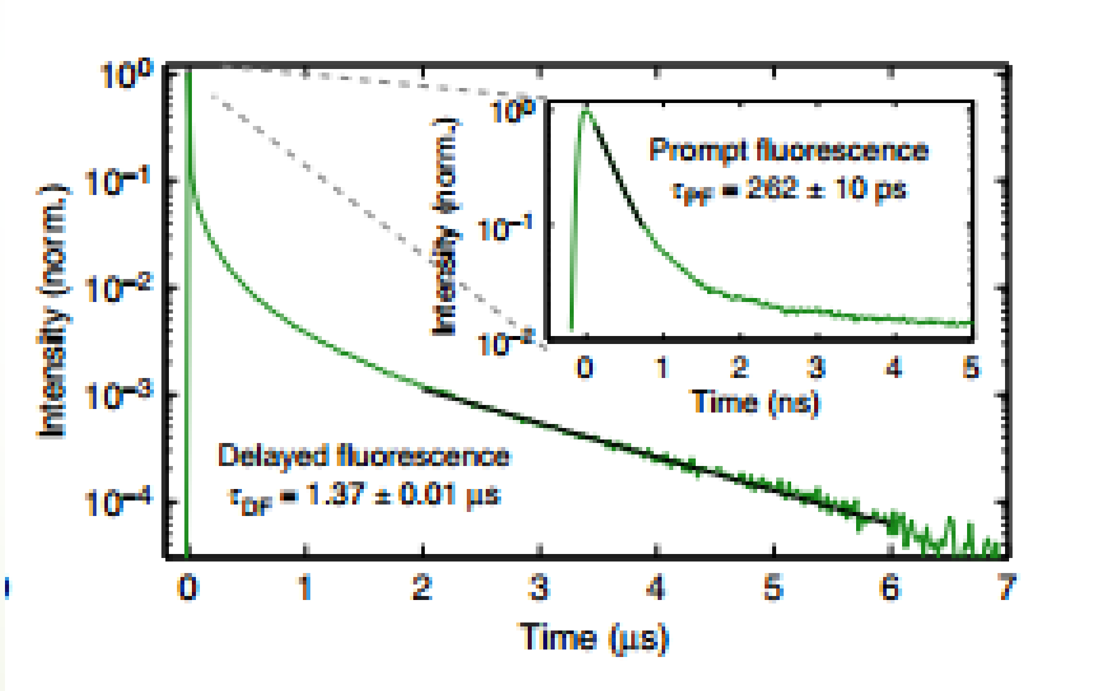
Singlet Fission



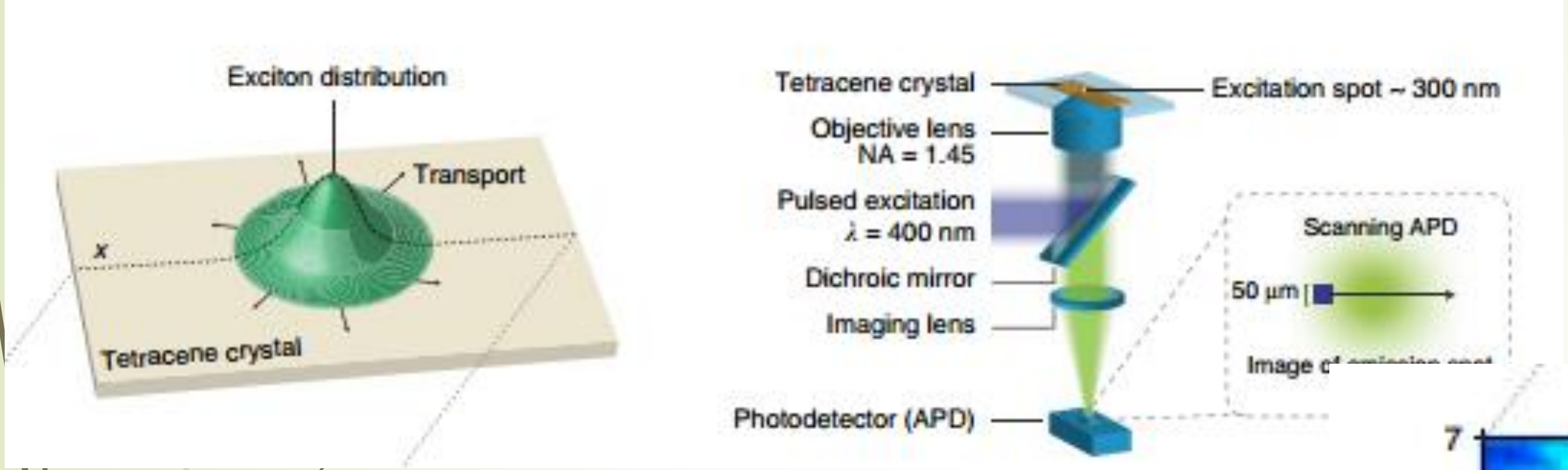
Singlet Fission

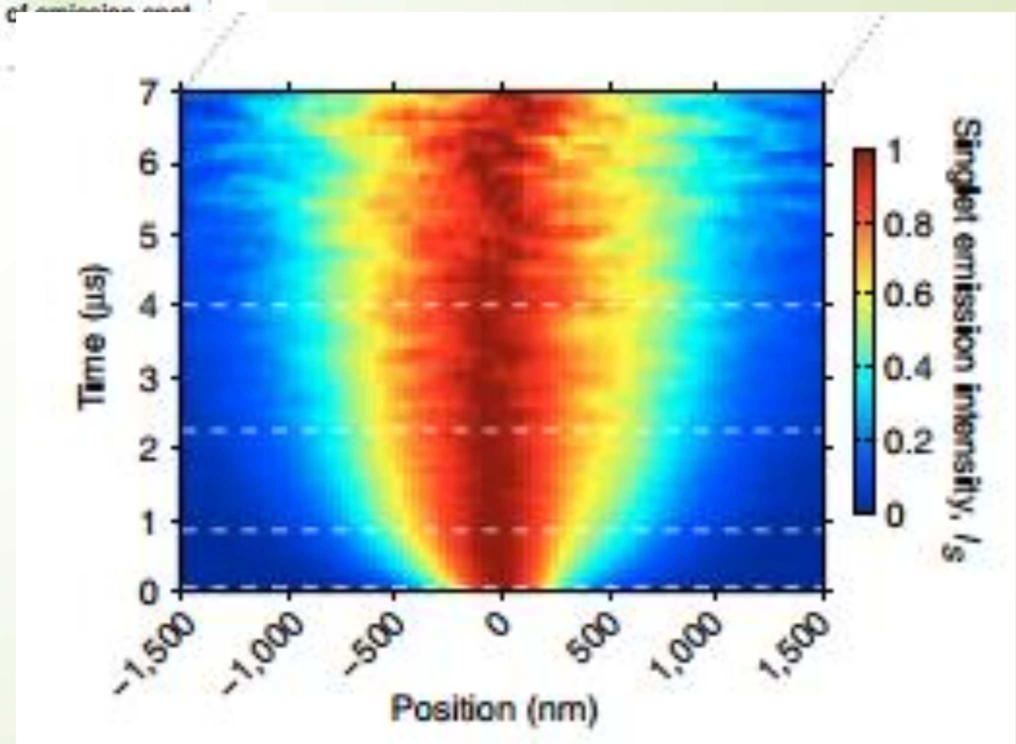
Visualization of exciton transport in ordered and disordered molecular solids.
G. M. Akselrod, P. B. Deotare, N. J. Thompson, J. Lee, W. A. Tisdale, M. A. Baldo, V. M. Menon, & V. Bulovic

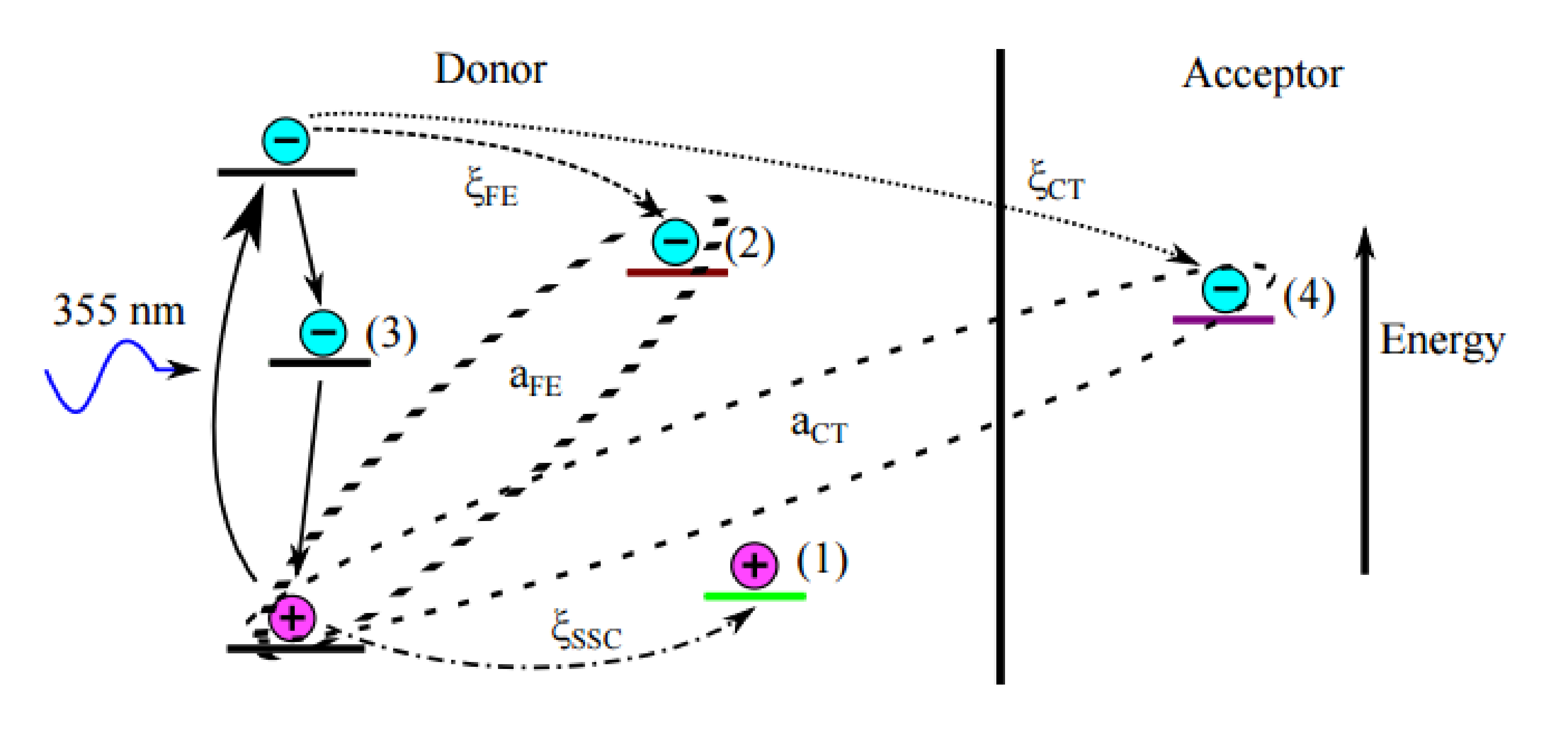




Singlet Fission







Johnson, B. (2015) *Electronic and Optical Properties of Organic Semiconductors: Experiment and Simulation* (PhD Dissertation). Accessed at ScholarsArchive@OSU on April 24, 2016

Differential Equations

$$n_f' = \xi_{SSC}(E)G(t) + k_{diss,FE}X_{FE} - \gamma n_f p_f - B_n(N_n - n_t)n_f - B_{n_f p_t} n_f p_t \; [+k_{diss,CT}X_{CT}]$$

$$n_t' = B_n(N_n - n_t)n_f - B_{n_t p_f} n_t p_f$$

$$p_f' = \xi_{SSC}(E)G(t) + k_{diss,FE}X_{FE} + B_{p_t}p_t - \gamma n_f p_f - B_p(N_p - p_t)p_f$$
$$- B_{n_t p_f} n_t p_f \; [+k_{diss,CT}X_{CT}]$$

$$p_t' = B_p(N_p - p_t)p_f - B_{n_f p_t} n_f p_t - B_{p_t}p_t$$

$$X_{FE(CT)}' = \xi_{FE(CT)}(E)G(t) - k_{diss,FE(CT)}X_{FE(CT)} - k_{r,FE(CT)}X_{FE(CT)}$$

Numerical Values

- In a few published papers the (cited below) they were seeing currents of 1-10 mA/cm^2. In Brian's dissertation, he published results of around 60 mA/m
- Brian's was finding electron mobilities between 0.01-0.1 cm^2/Vs and hole mobilities of 0.3-0.6 cm^2/Vs

Jeong, W., Lee, Y. E., Shim, H., Kim, T., Kim, S., & Kim, J. (2012). Photoconductivity of C60 as an Origin of Bias-Dependent Photocurrent in Organic Photovoltaics. *Adv. Funct. Mater. Advanced Functional Materials, 22*(14), 3089-3094. doi:10.1002/adfm.201200069

Schlenker, C. W., Chen, K., Yip, H., Li, C., Bradshaw, L. R., Ochsenbein, S. T., . . . Ginger, D. S. (2012). Polymer Triplet Energy Levels Need Not Limit Photocurrent Collection in Organic Solar Cells. *J. Am. Chem. Soc. Journal of the American Chemical Society, 134*(48), 19661-19668. doi:10.1021/ja306110b

Thank you!

- Questions?

Sources

- Kumar, V. B., Koltypin, Y., Gedanken, A., & Porat, Z. (2014). Ultrasonic cavitation of molten gallium in water: Entrapment of organic molecules in gallium microspheres. *J. Mater. Chem. A, 2*(5), 1309-1317. doi:10.1039/c3ta13573j
- Köhler, A., & Bässler, H. (2015). *Electronic processes in organic semiconductors: An introduction*. Weinheim: Wiley-VCH Verlag GmbH & KGaA.
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- Jeong, W., Lee, Y. E., Shim, H., Kim, T., Kim, S., & Kim, J. (2012). Photoconductivity of C60 as an Origin of Bias-Dependent Photocurrent in Organic Photovoltaics. *Adv. Funct. Mater. Advanced Functional Materials, 22*(14), 3089-3094. doi:10.1002/adfm.201200069
- Schlenker, C. W., Chen, K., Yip, H., Li, C., Bradshaw, L. R., Ochsenbein, S. T., . . . Ginger, D. S. (2012). Polymer Triplet Energy Levels Need Not Limit Photocurrent Collection in Organic Solar Cells. *J. Am. Chem. Soc. Journal of the American Chemical Society, 134*(48), 19661-19668. doi:10.1021/ja306110b