Organic Photovoltaics: The Search For More Money

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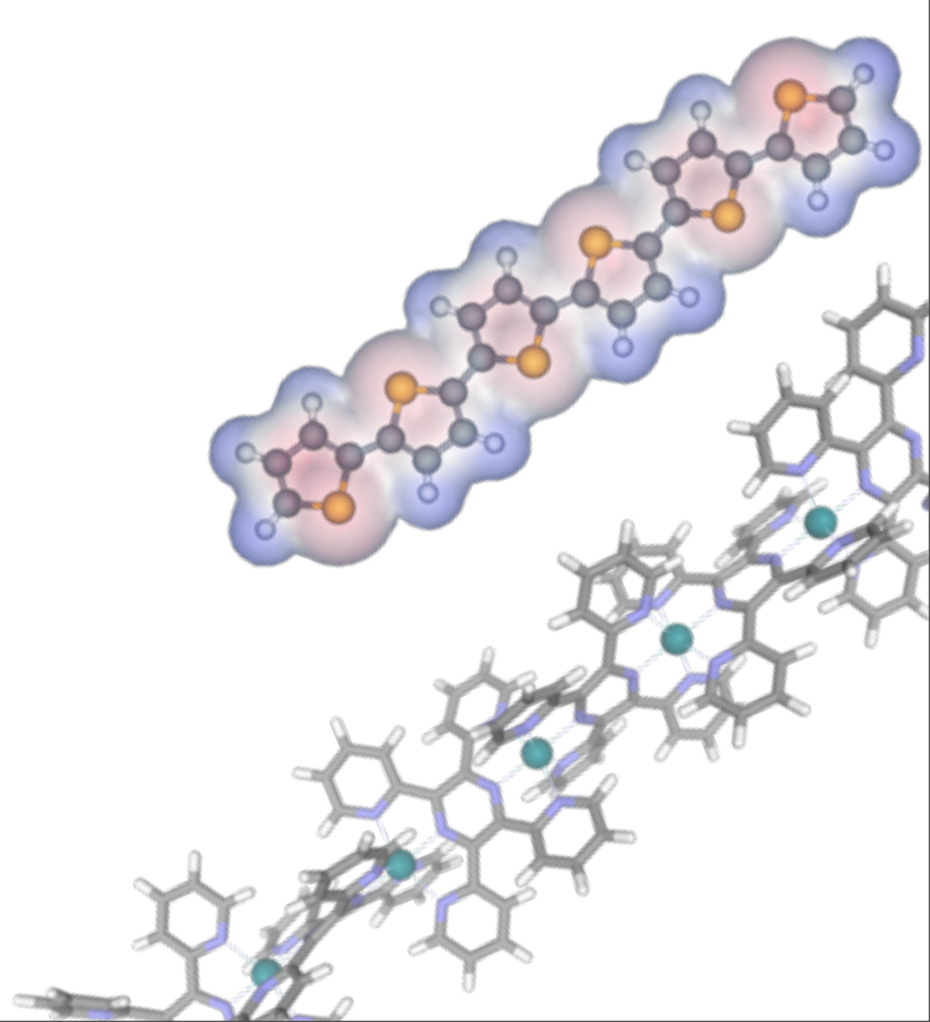
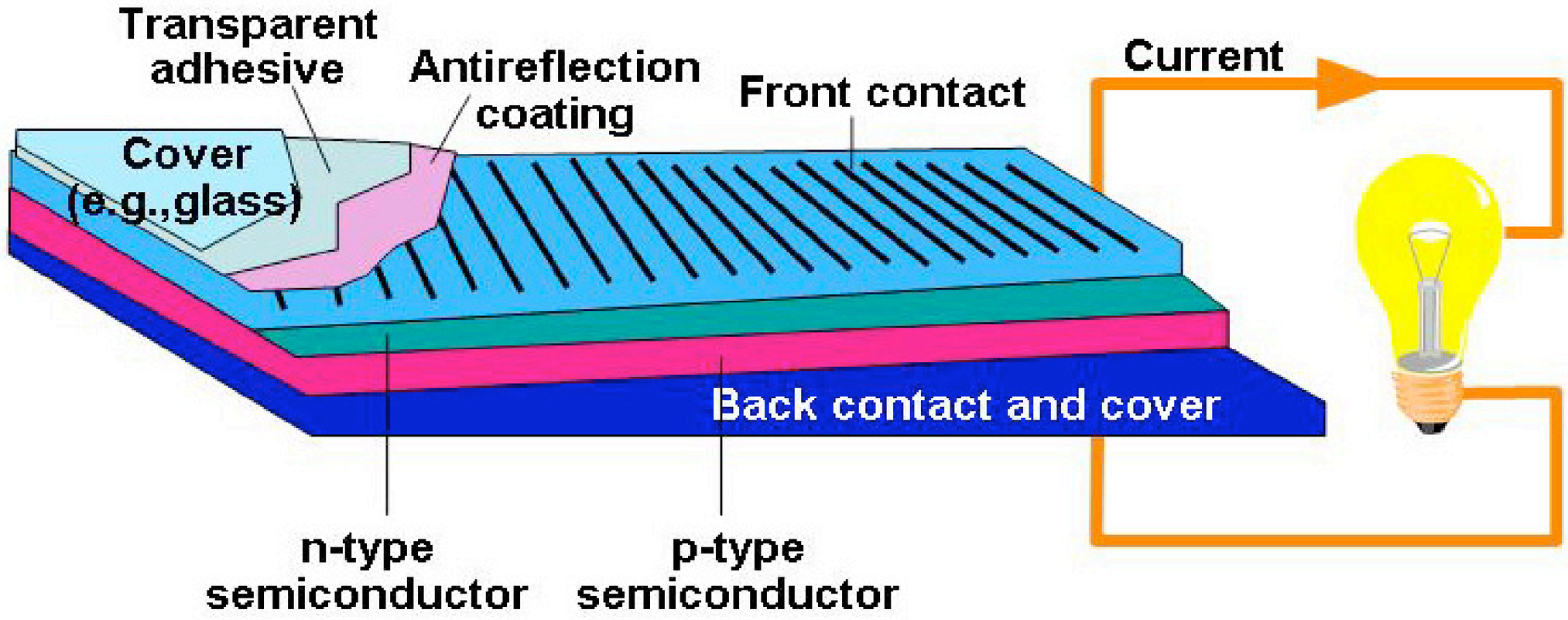


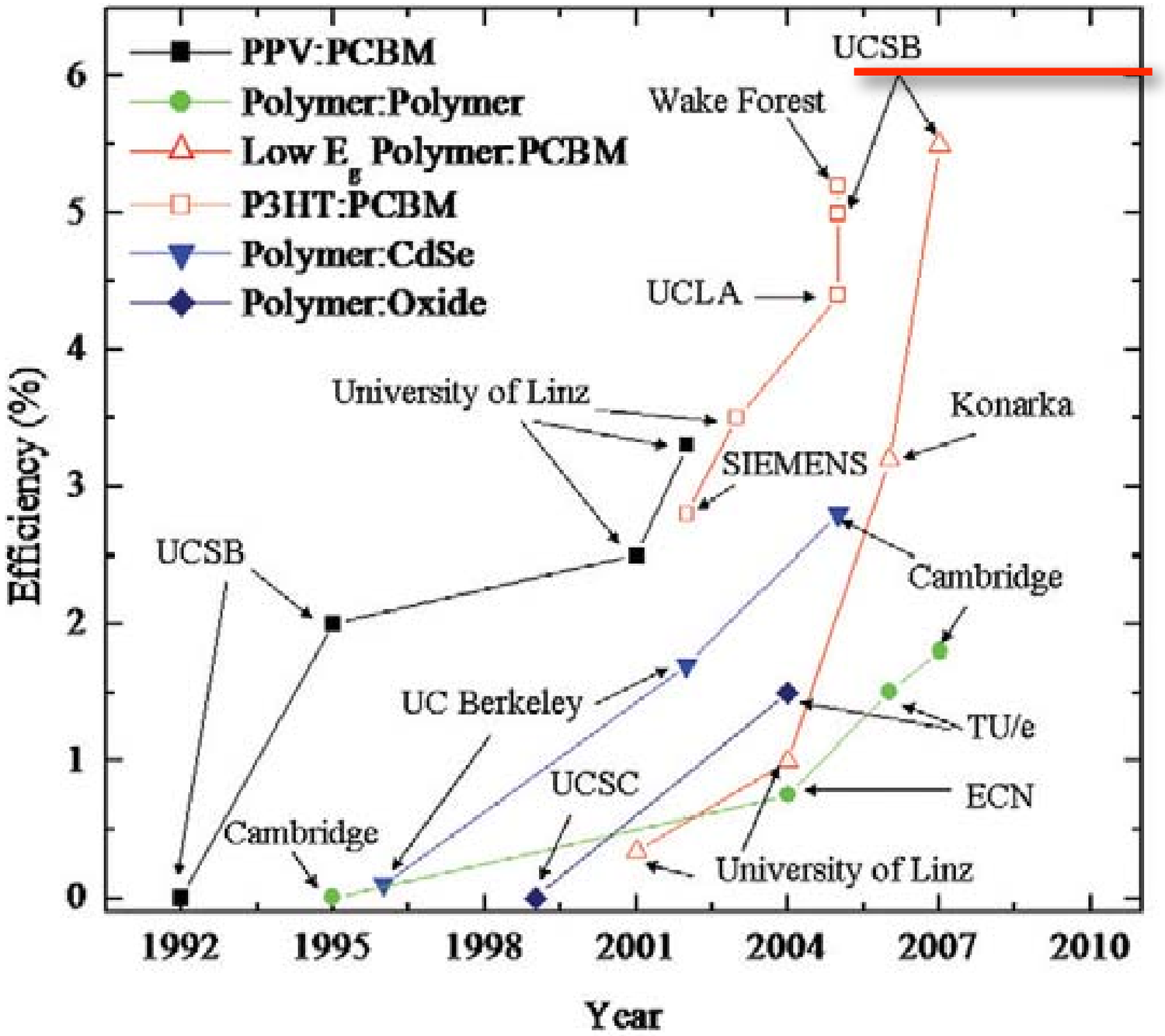
Solar Cell Structure

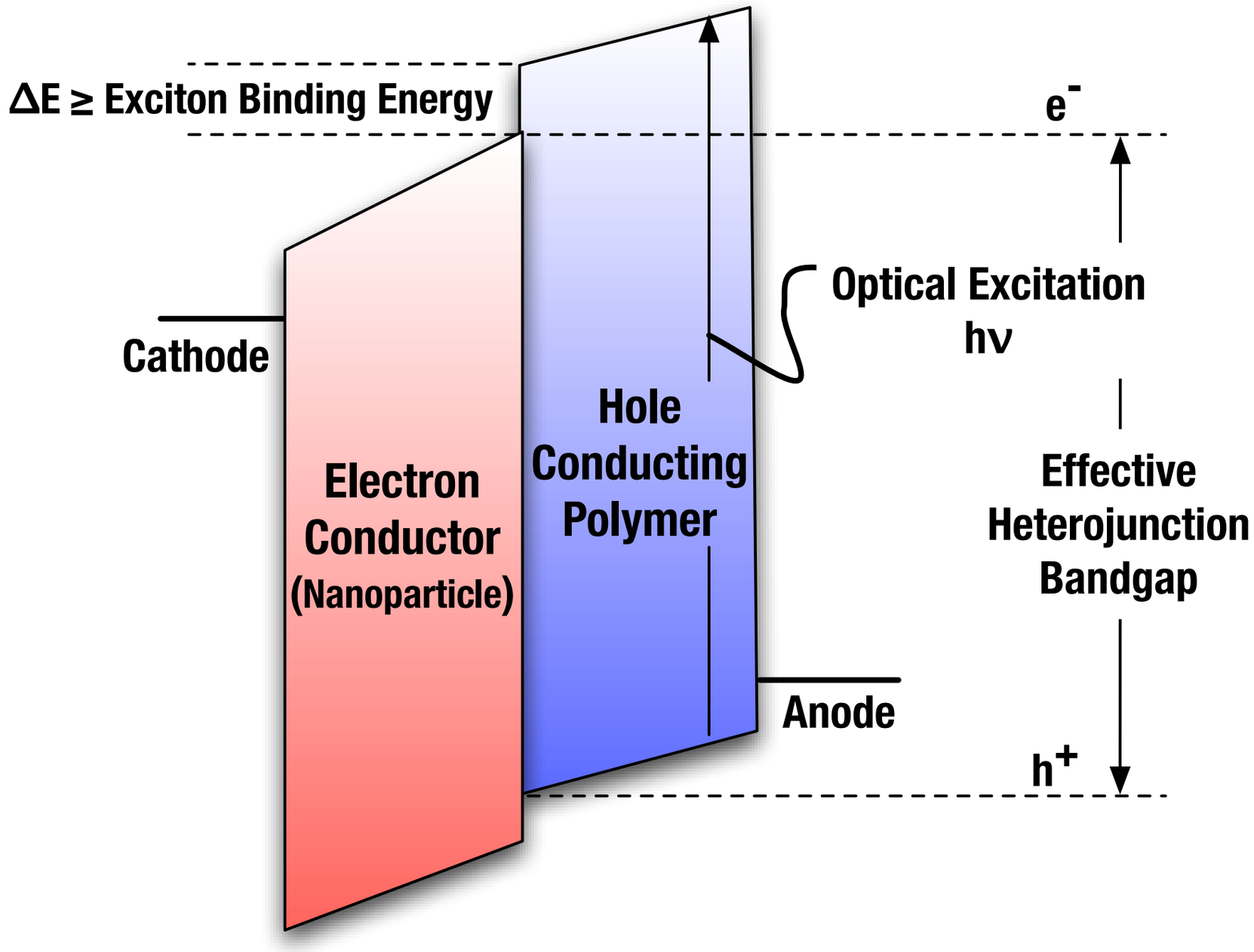


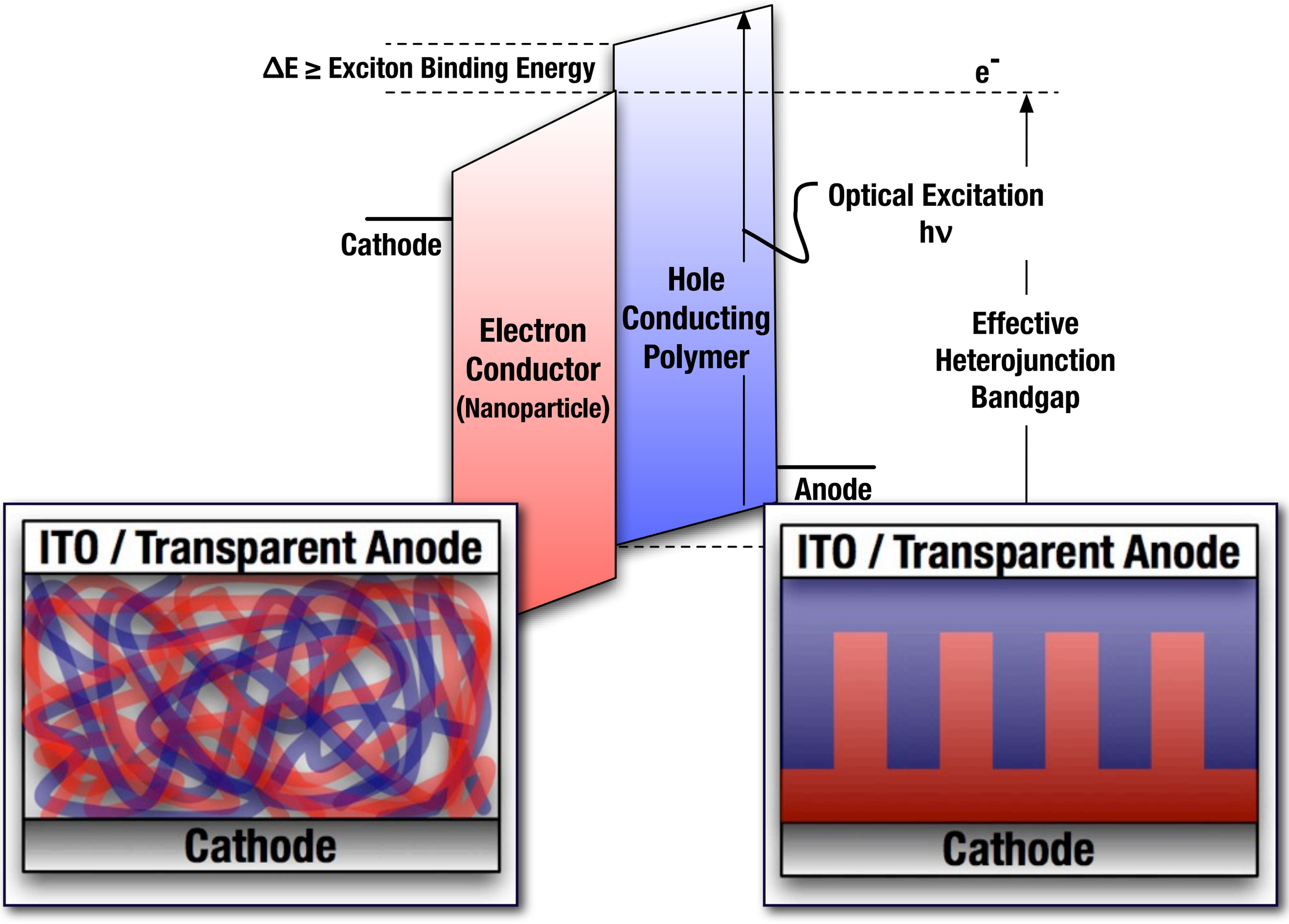
$$\text{Solar cell efficiency (\%)} = \frac{\text{Power out (W)} \times 100\%}{\text{Area (m}^2\text{)} \times 1000\ \text{W/m}^2}$$

10% efficiency = 100 W/m^2 or 10 W/ft^2

Experimental Progress




ΔE ≥ Exciton Binding Energy
e-
Optical Excitation
hν
Cathode
Electron
Conductor
(Nanoparticle)
Hole
Conducting
Polymer
Effective
Heterojunction
Bandgap
Anode
h+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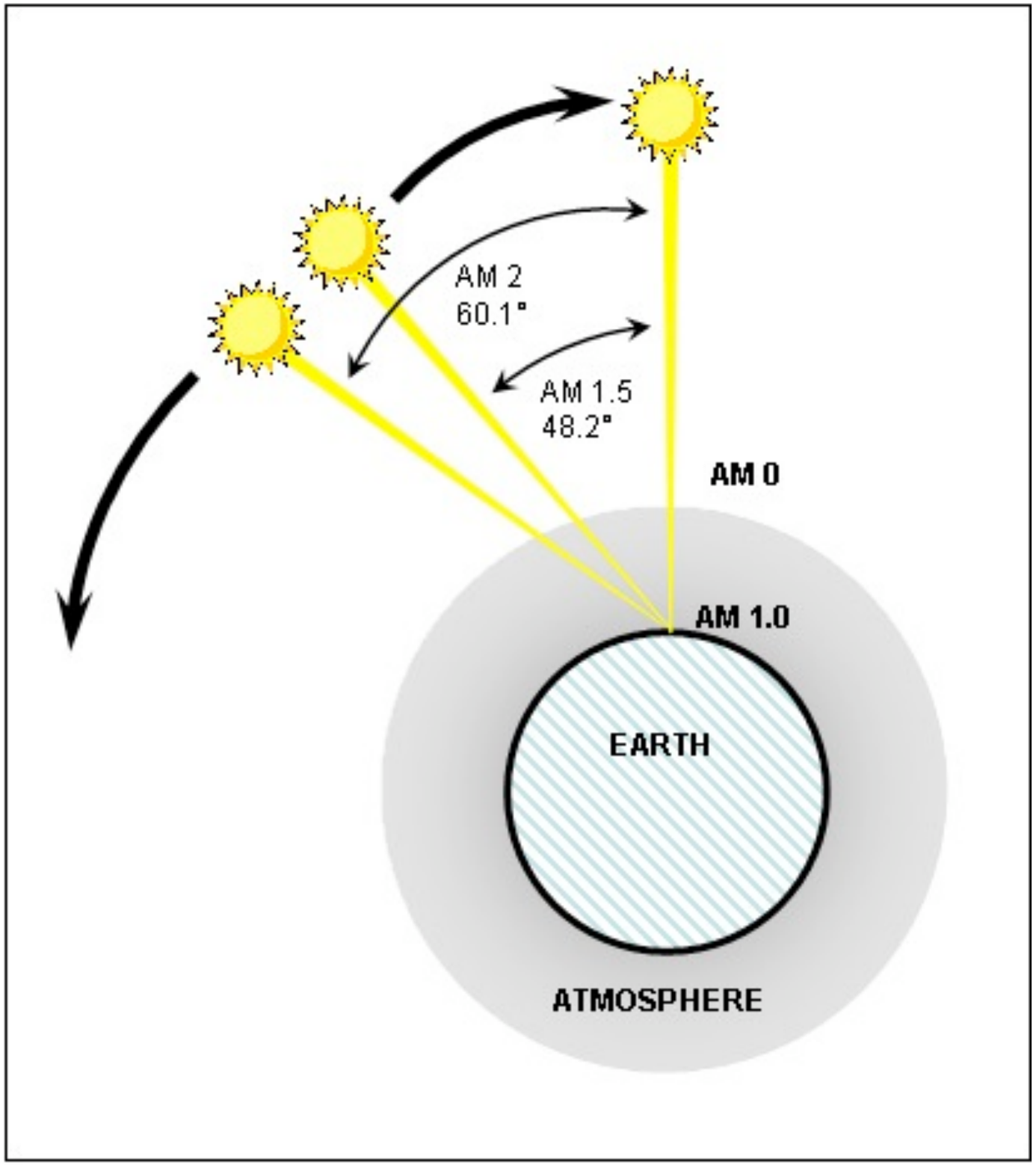
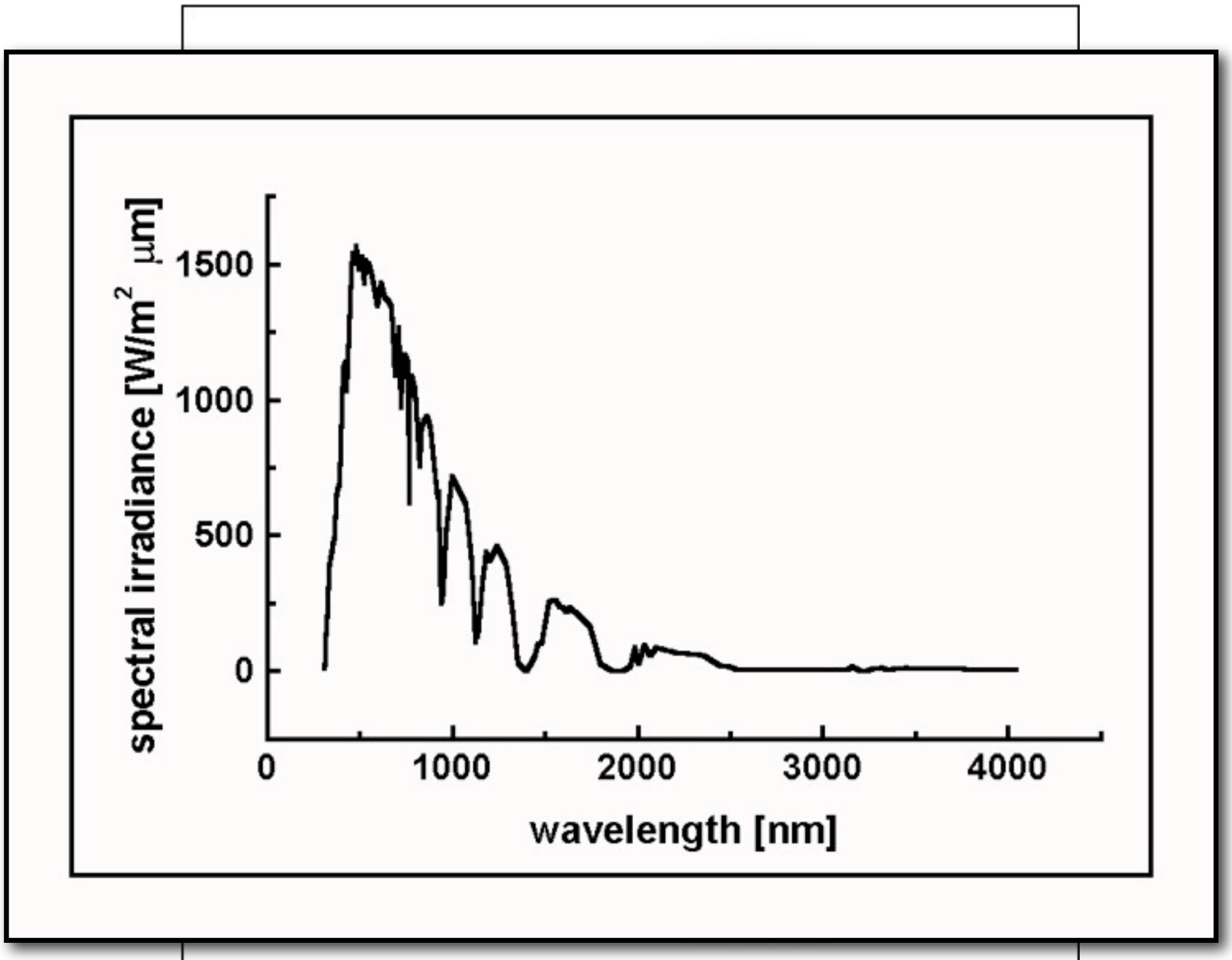
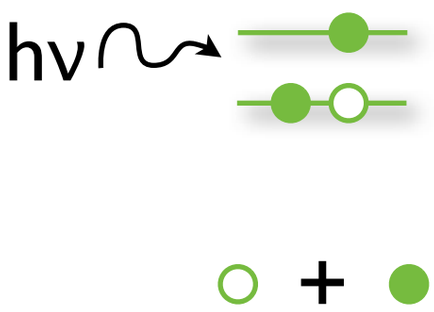
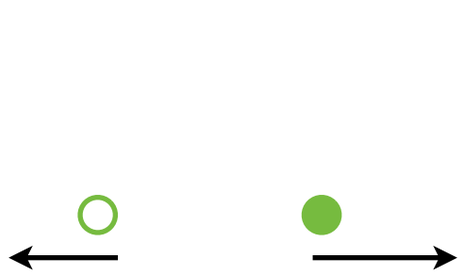
Solar Spectrum



Solar Spectrum





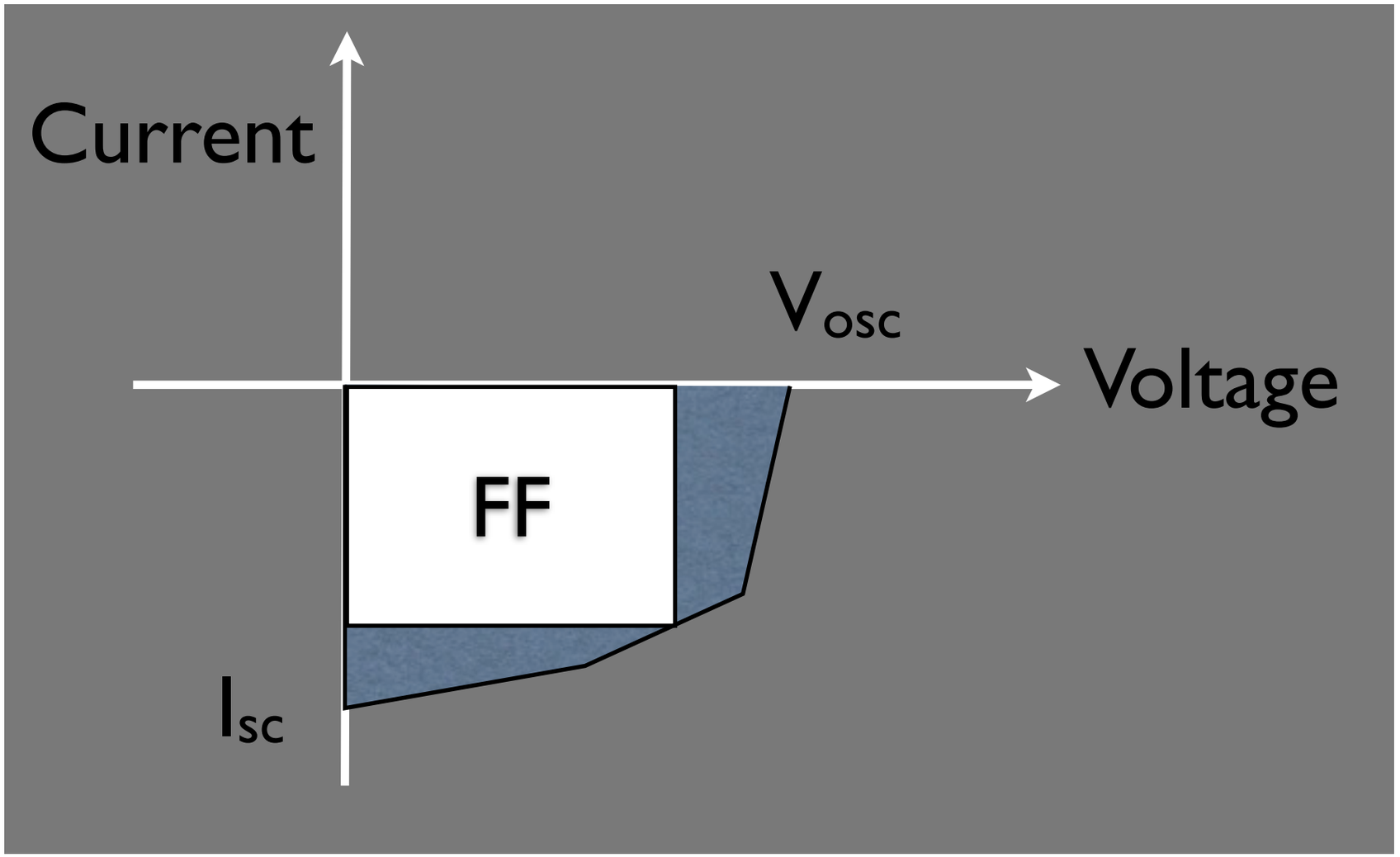


incident photons

Conversion step	Loss mechanism
Light absorption	
exciton creation	Exciton Recombination
exciton diffusion	Charge Recombination
charge separation	
charge transport	
charge collection	

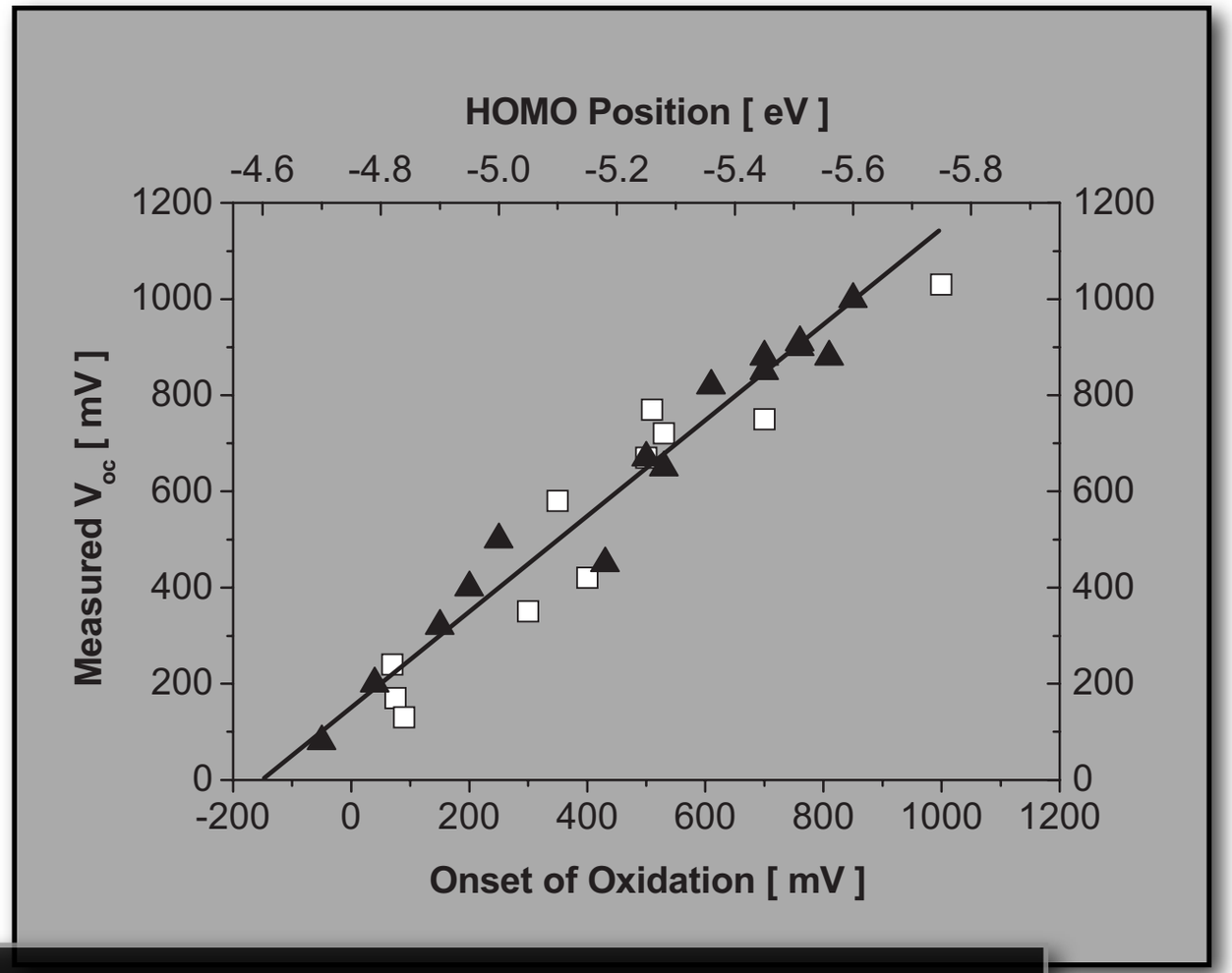
Many steps are important...
We can lose energy at each step

Efficiency



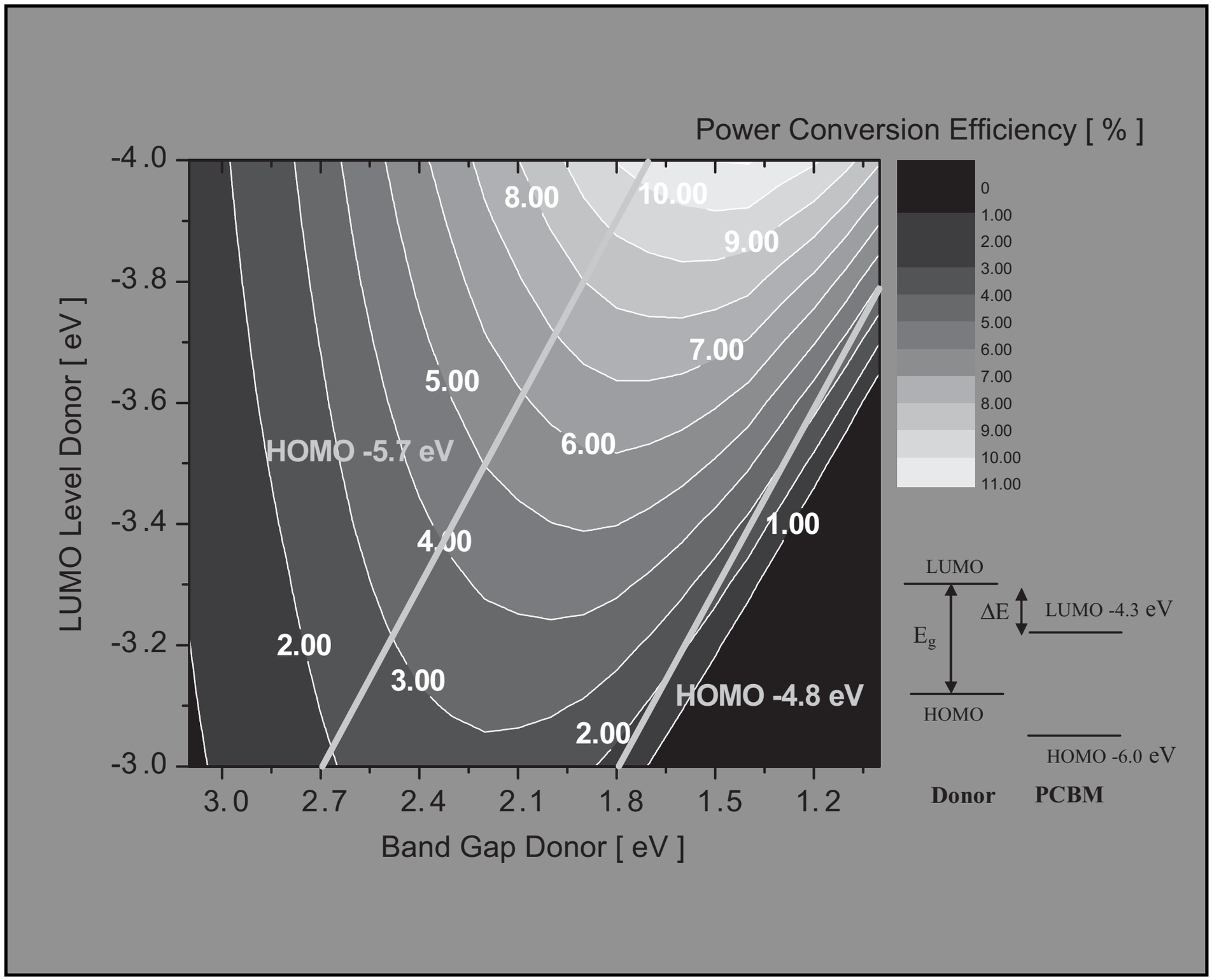
Open Circuit Potential

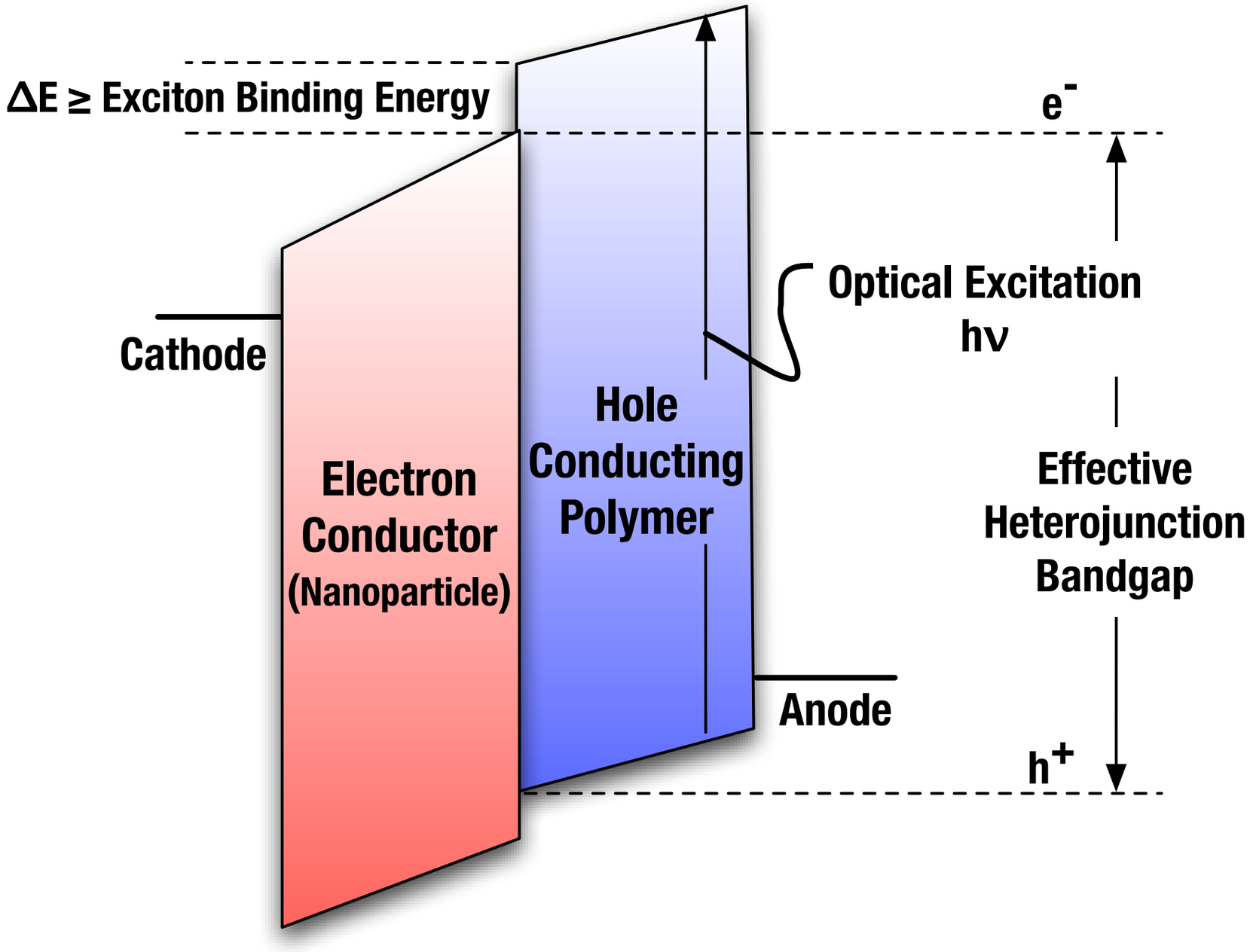
- Fill factor = max power / (V_{oc} x I_{sc})
- Improving open circuit potential is a key goal
- OCP appears to be directly correlated with the HOMO energy



We want something with high ionization potential.

Heeger Efficiency Criterion

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h+

Heeger's Proposed 10% Efficiency Targets

- Suggest that band gap should be
  ≈1.8-1.5 eV
- LUMO energy of donor ≤ 3.9eV
- Balance between optical absorption and voltage
- Decreases energy loss going from donor to acceptor

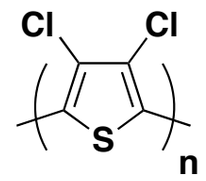
What we don't know...
What molecule fits these criteria?

What Compound?

- Electronic parameters do not tell us what molecule to make…
- “Inverse design” problem
- Parameters to consider:
  - Electron-donating / Electron-withdrawing
  - Greater delocalization / non-aromatic
  - etc...

First Step.... "Diversity Library"

- Primitive level:
  Do we find anything which meets our target?
- Secondary:
  Key "structural features"
- And...
  What do you need to model the full polymer?



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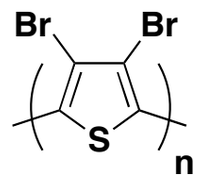

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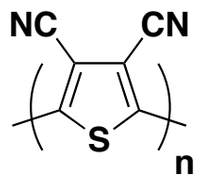

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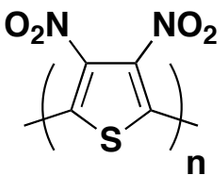

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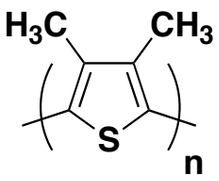

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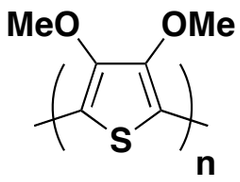

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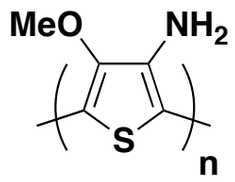

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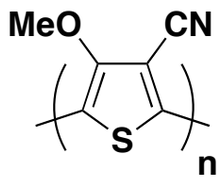

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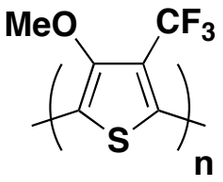

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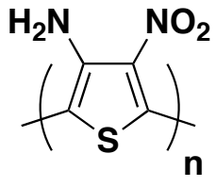

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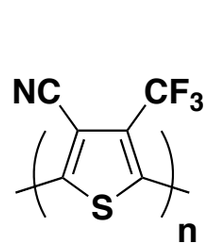

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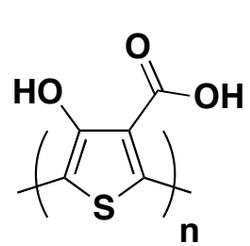

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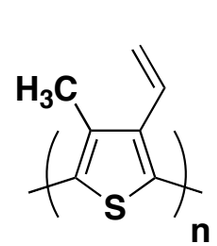

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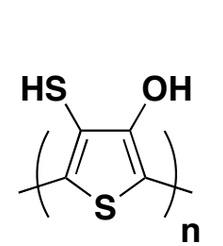

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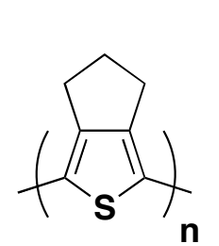

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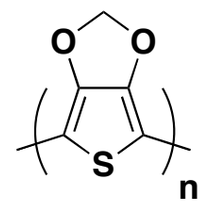

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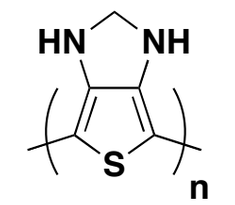

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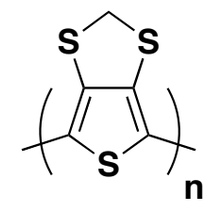

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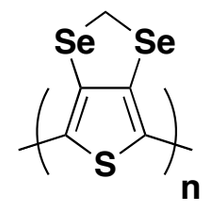

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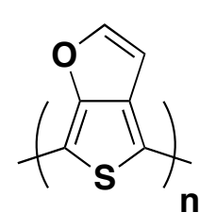

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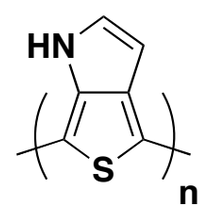

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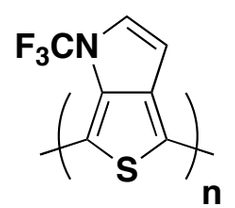

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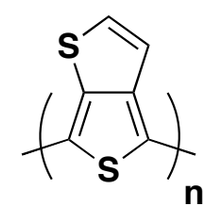

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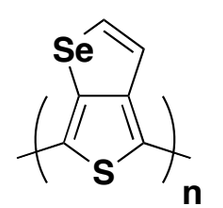

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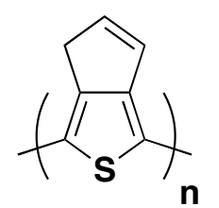

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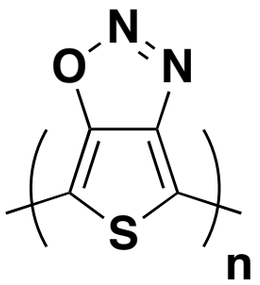
New Targets?



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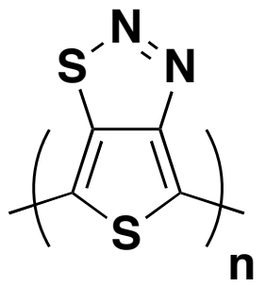

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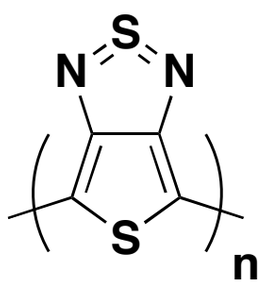

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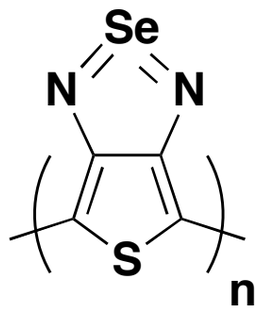

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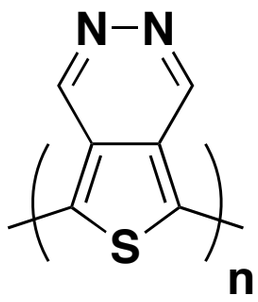

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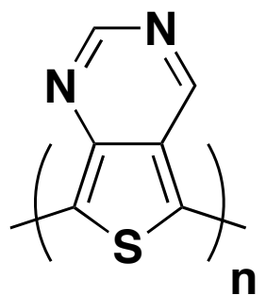

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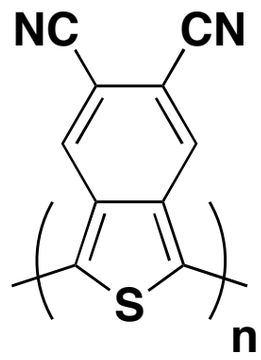

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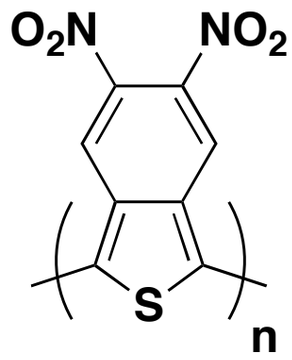

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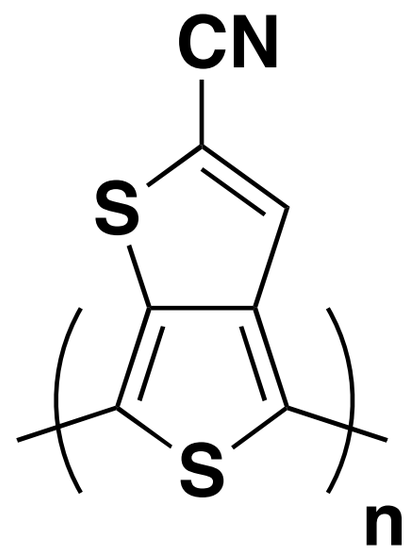

Wait... What About Everything Else?

- Heeger criteria only address first 2 steps
- Still need to understand
  - exciton diffusion
  - charge recombination
  - charge separation
  - charge transport

    ...
- Not to mention:
  - **Disorder**
  - **Defects**
  - **Stability**