Imperial College London

SEPOMO

NETWORK SCHOOL

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Device scale simulation of organic photovoltaic devices

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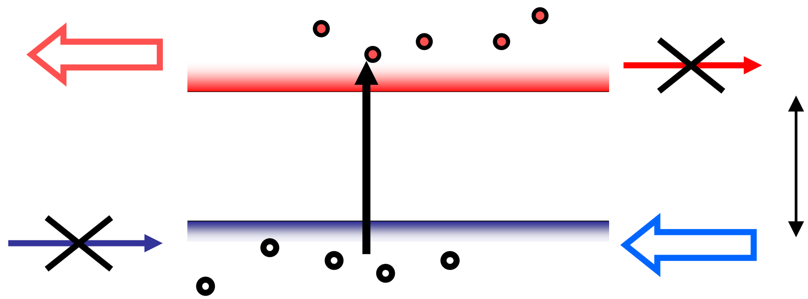
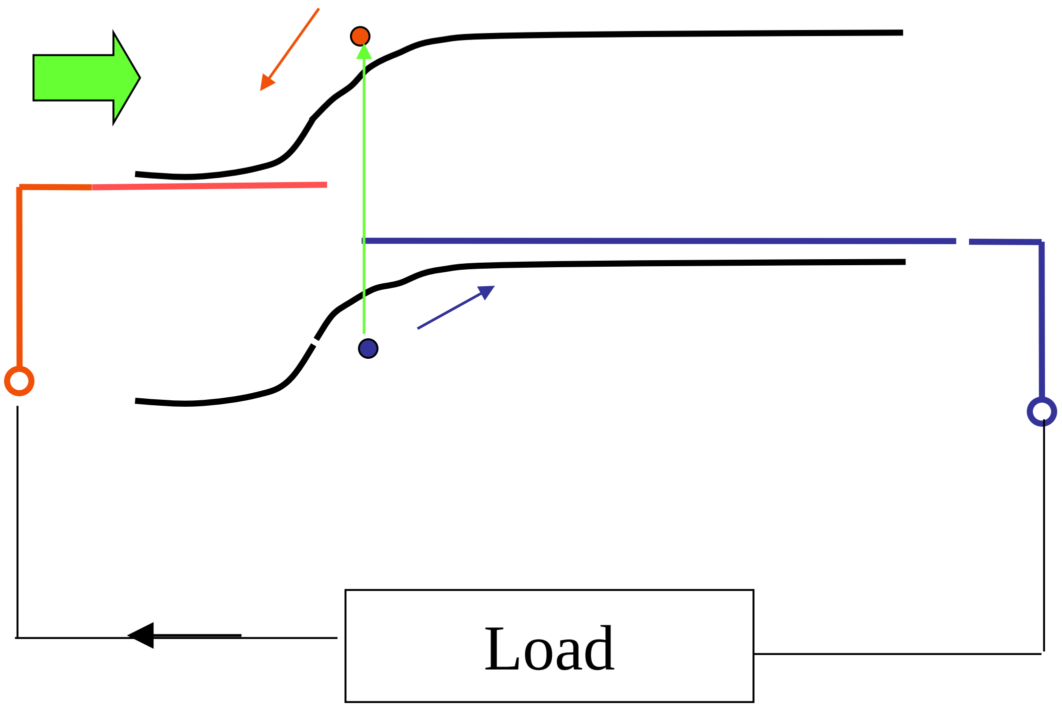
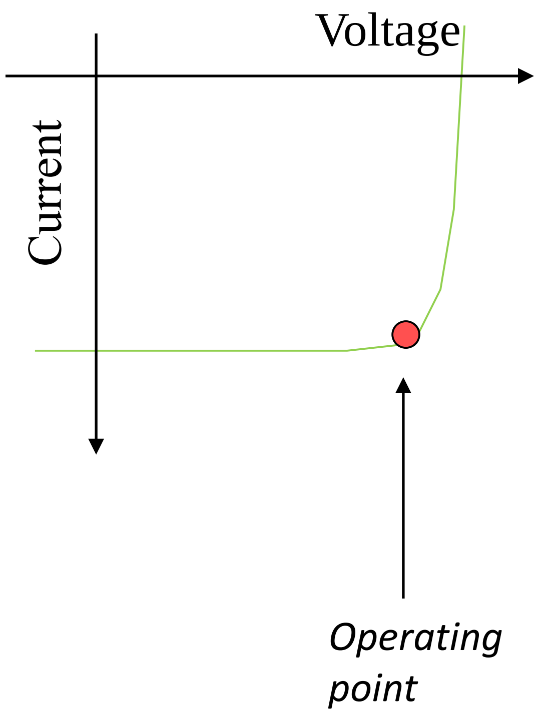


- PV generation requires:
  - photon absorption across an energy gap
  - separation of photogenerated charges
  - asymmetric contacts to an external circuit



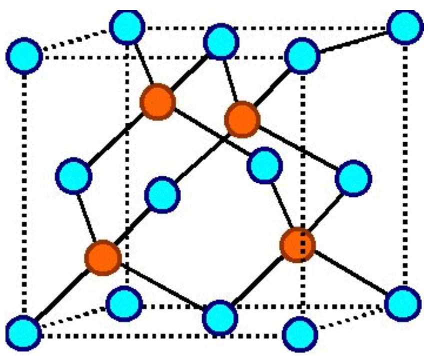


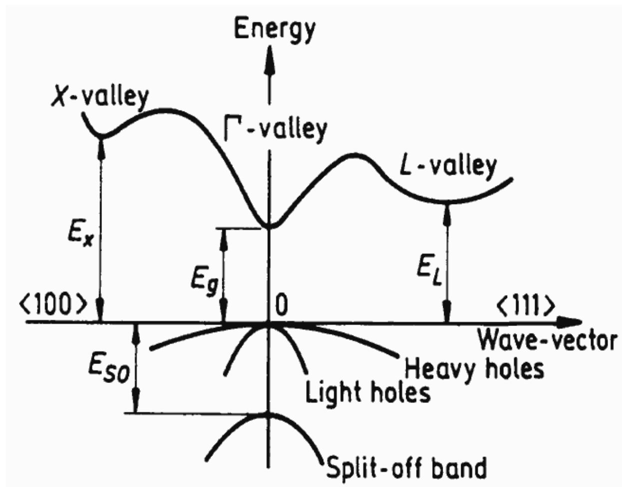
Operating: photovoltage x photocurrent = electric power

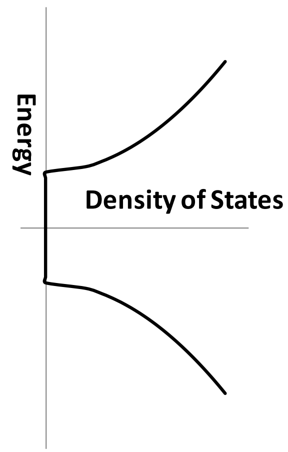
Outline

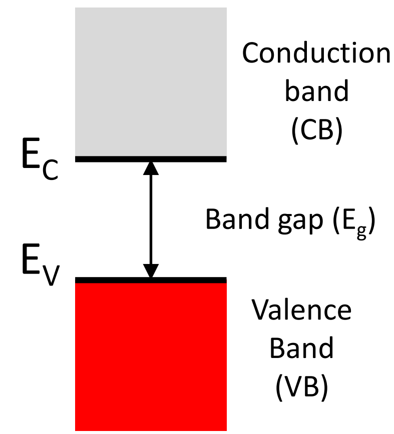
- **Basics of solar cell device modelling**
- What is different about organic solar cells
- Device modelling approaches to OPV
- Case studies: steady state models
- Transient modelling

Semiconductors







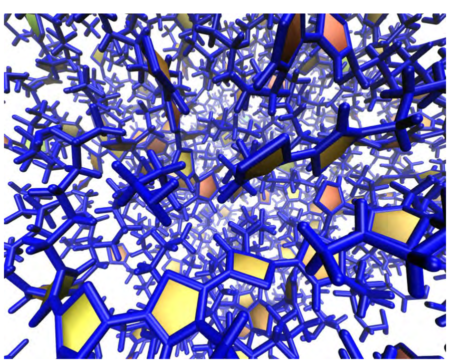


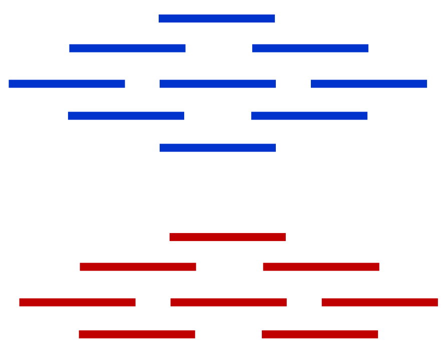
Crystal structure

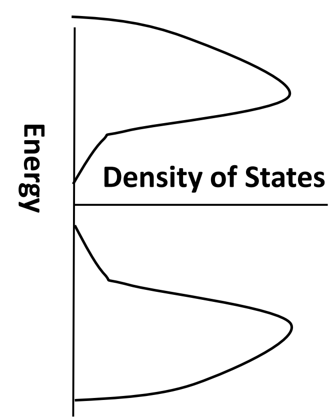
Band structure

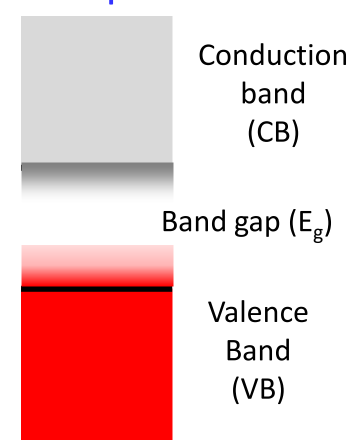
Density of States

Band picture

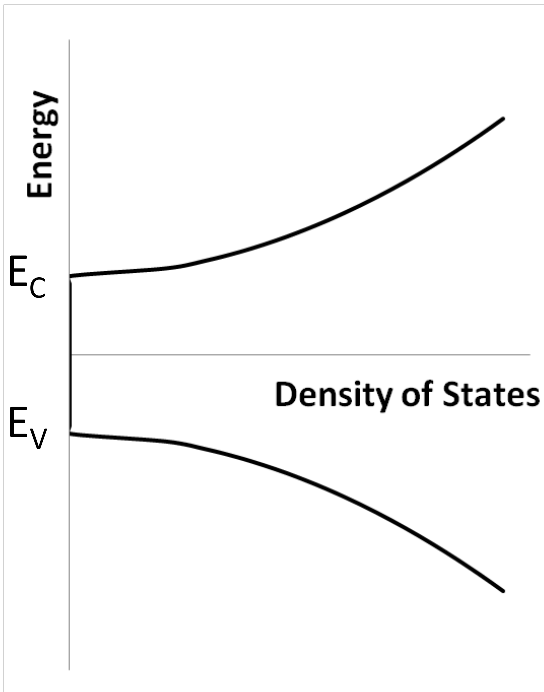


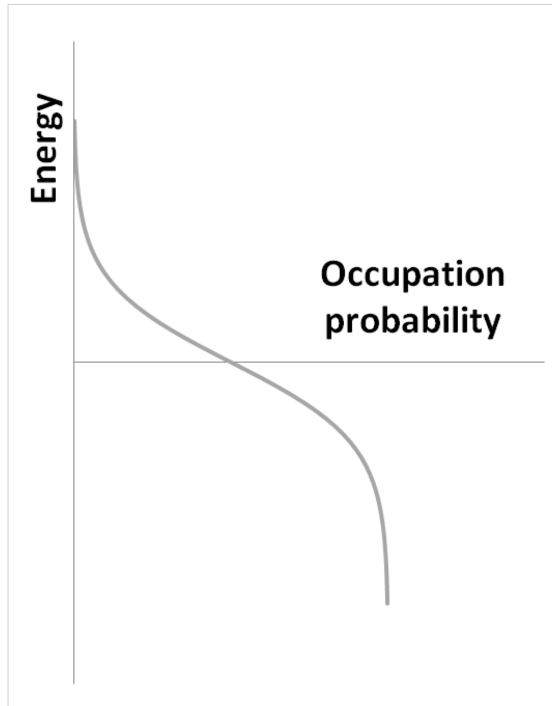


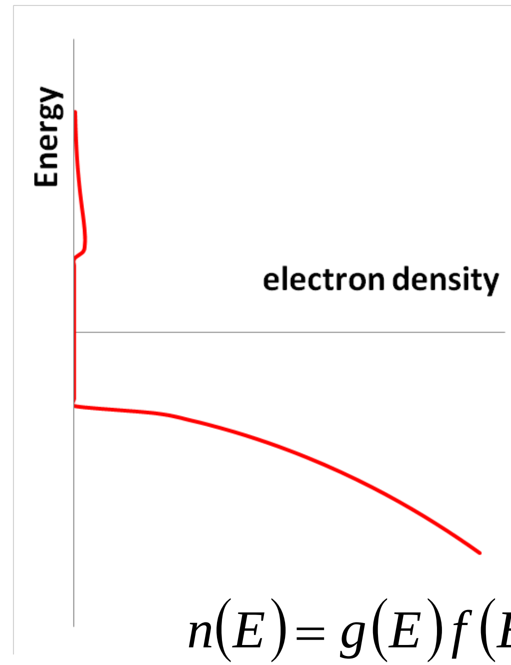




Charge carrier statistics







$$n(E) = g(E)f(E)$$

$$g(E)$$

$$f(E) = \frac{1}{\exp\left(-\frac{E-E_F}{kT}\right)+1}$$

$$n = \int_{E_C}^{\infty} g(E)f(E)dE$$

$$n = \exp\left(-\frac{E_C-E_F}{kT}\right)N_C$$

$$p = \int_{-\infty}^{E_V} g(E)(1-f(E))dE$$

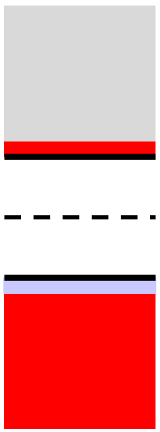
$$p = \exp\left(-\frac{E_F-E_V}{kT}\right)N_V$$

Density of states for electrons and holes

Charge carrier populations follow **Fermi Dirac statistics**

Total concentrations of free electrons and holes

Fermi levels and Doping: at equilibrium

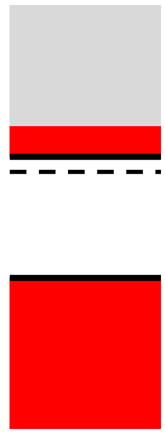


$$n = N_C e^{-(E_C - E_F)/kT}$$

$$p = N_V e^{-(E_F - E_V)/kT}$$

$$np = n_i^{\,2} = N_C N_V e^{-E_g/kT}$$

Intrinsic semiconductor: equal concentrations of free electrons and holes

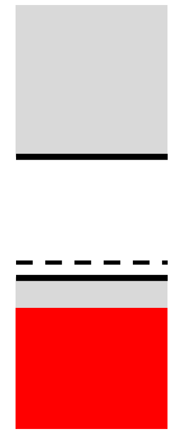


$$n \approx N_D$$

$$p \approx n_i^{\,2} / N_D$$

$$E_F = E_C - kT \ln N_C + kT \ln N_D$$

n doped semiconductor: High density of free electrons introduced by impurity atoms that have one too many valence electrons



$$n \approx n_i^{\,2} / N_A$$

$$p \approx N_A$$

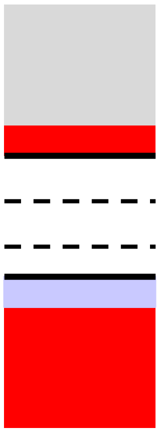
$$E_F = E_V + kT \ln N_V - kT \ln N_A$$

p doped semiconductor: High density of free holes introduced by impurity atoms that have one too few valence electrons

Fermi levels are ***pinned***

Fermi levels and Doping: under bias

Optical or electrical bias increases the concentrations of free electrons and / or holes

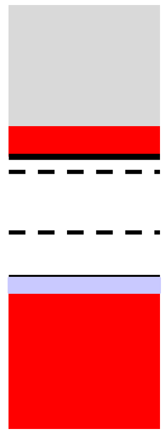


$$n = N_c \exp\left(-\frac{E_c - E_{Fn}}{kT}\right)$$

$$p = N_v \exp\left(\frac{E_v - E_{Fp}}{kT}\right)$$

$$E_{F_n} > E_{F_p}$$

$$np = n_i^{\ 2} e^{\left(E_{F_n} - E_{F_n}\right)/kT}$$

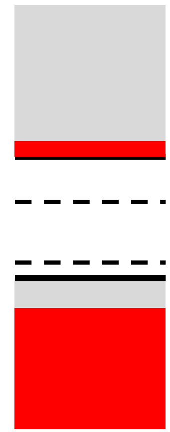


$$n \approx N_D$$

$$p \approx \frac{n_i^2}{N_D} \exp\left(-\frac{E_{Fp} - E_{Fn}}{kT}\right)$$

$$E_{F_n} \approx E_C - kT \ln N_C + kT \ln N_D$$

$$E_{F_p} < E_{F_n}$$



$$n \approx \frac{n_i^2}{N_A} \exp\left(-\frac{E_{Fp} - E_{Fn}}{kT}\right)$$

$$p \approx N_A$$

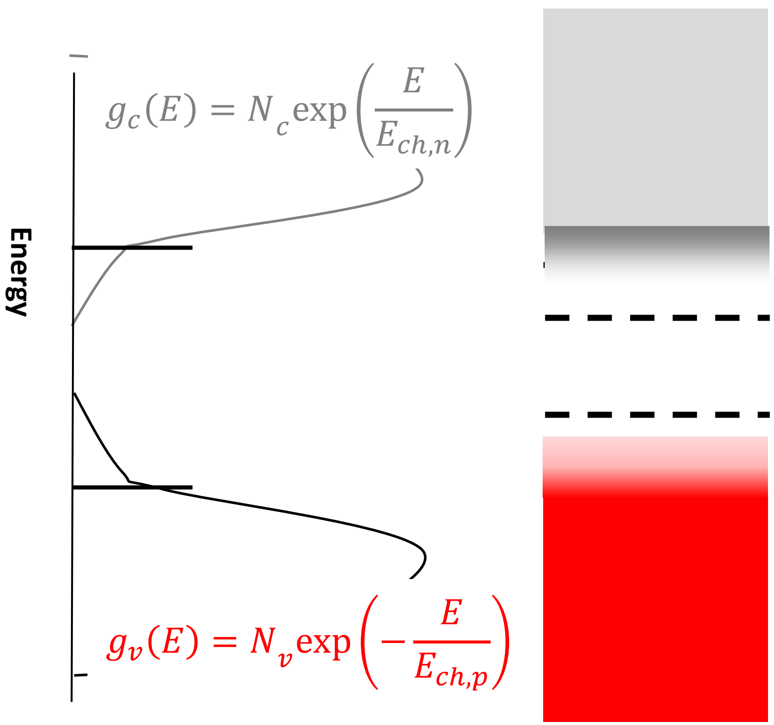
$$E_{F_n} > E_{F_p}$$

$$E_{F_p} = E_V + kT \ln N_V - kT \ln N_A$$

Charge carrier populations are assumed to be in **quasi thermal equilibrium**

This is valid if the rate of scattering within a band is faster than the rate of relaxation between bands (Boltzmann relaxation time approximation)

Fermi levels : with tail states



$$n \approx n_t \propto \exp\left(\frac{E_{Fn}}{E_{ch,n}}\right)$$

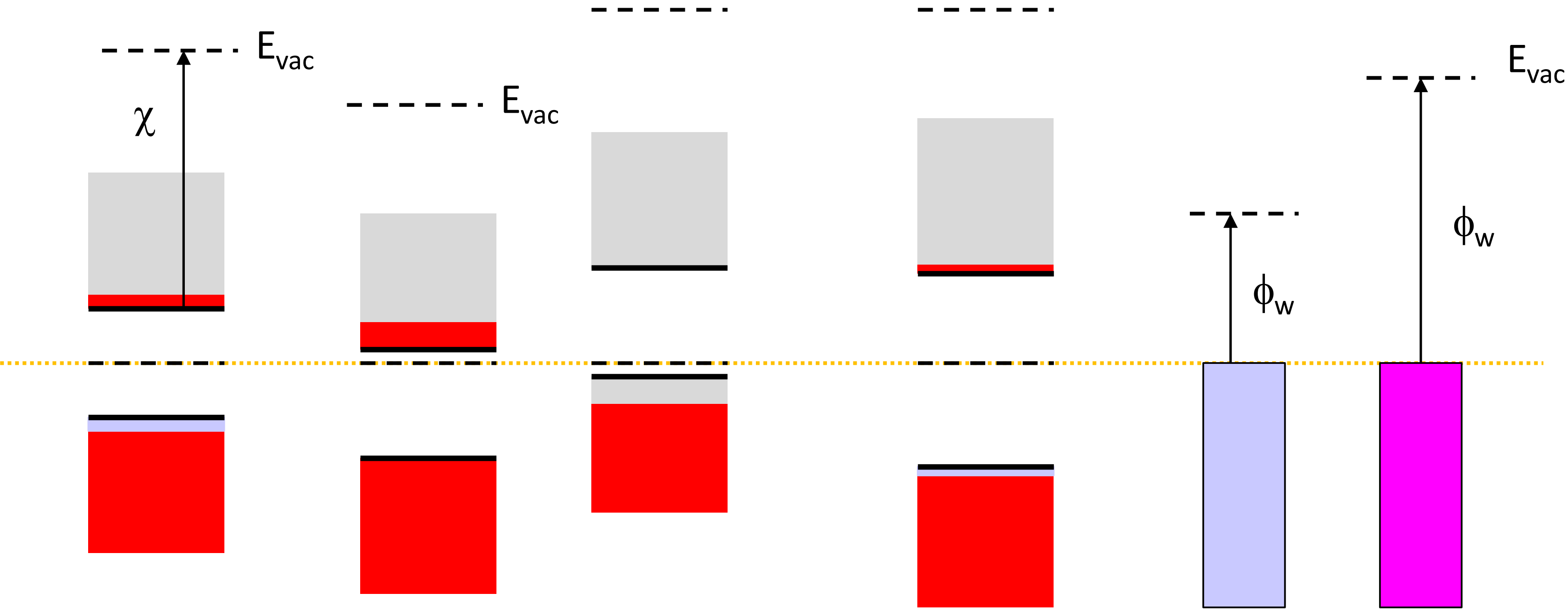
$$p \approx p_t \propto \exp\left(-\frac{E_{Fp}}{E_{ch,p}}\right)$$

Symmetric case:

$$np \propto \exp\left(\frac{E_{Fn} - E_{Fp}}{E_{ch}}\right) \qquad n \propto \exp\left(\frac{qV}{2E_{ch}}\right)$$

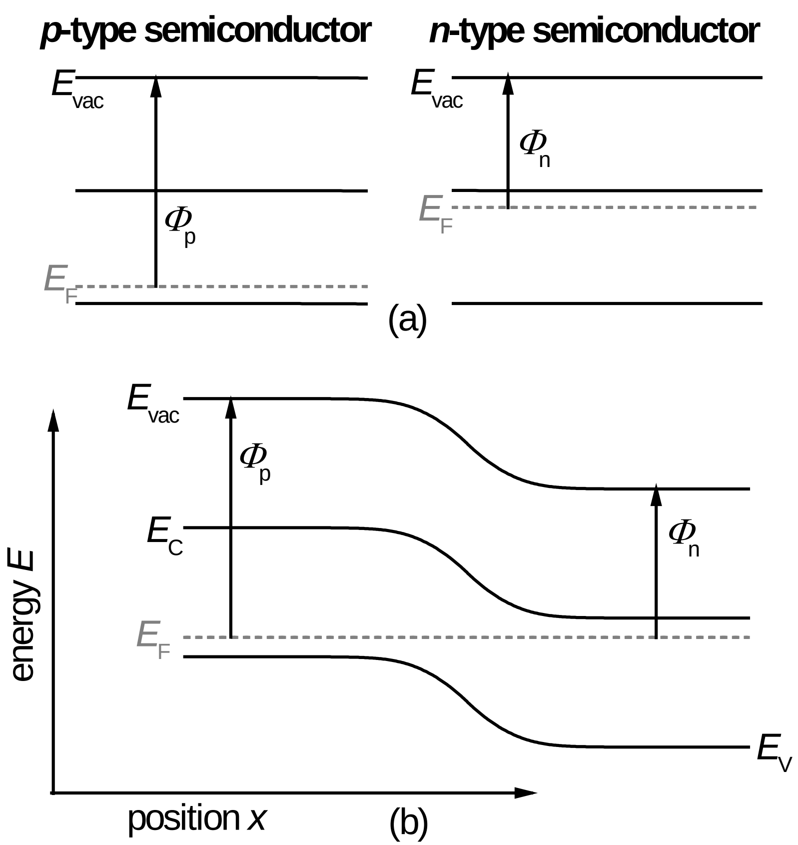
- Typically assume a common quasi Fermi level for all electrons (or holes) in tail states
- May have same or different quasi Fermi level for free charges

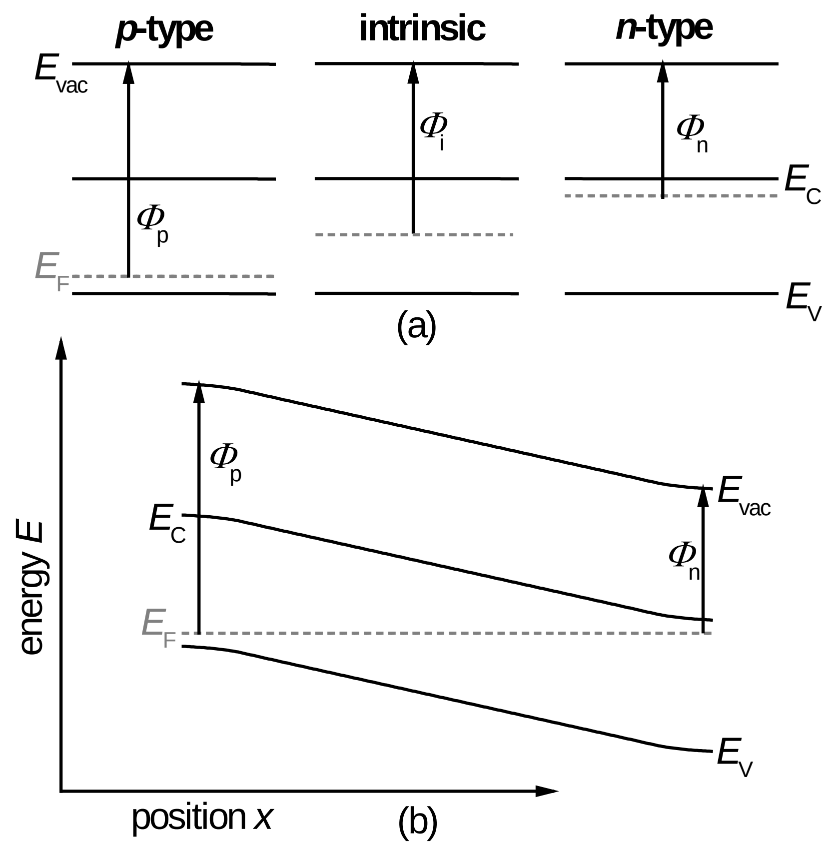
Alignment



- The Fermi level in equilibrium controls band alignment
- Fermi level position is influenced by band gap, doping and electron affinity (or work function)

Band profiles for p-n and p-i-n devices in equilibrium





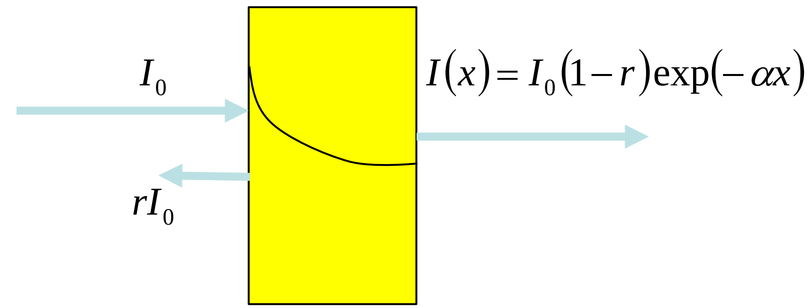
- Band alignment at boundaries controlled by boundary conditions
- Fermi level constant
- Poisson’s equation determines band profile

Photogeneration

Light absorption in the semiconductor increases electron and hole densities above their equilibrium values

Attenuation of light intensity:

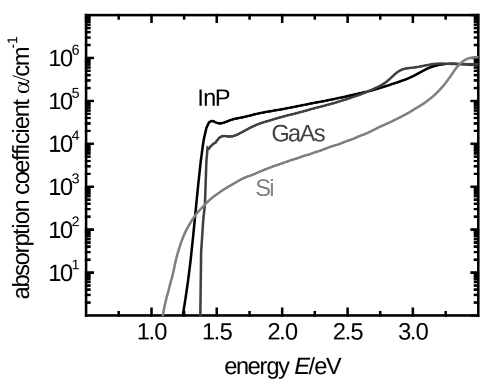
Simple model: Beer Lambert law

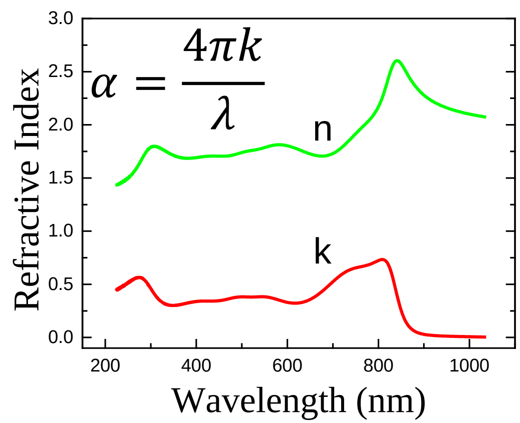


Electron-hole pair *generation rate*

$$G(E,x) = L(E,x) = \alpha(E) b_s(E)\big(1 - r(E)\big)\exp\left(\int_0^x \alpha(E) dx'\right)$$

Absorption spectrum $\alpha(E)$





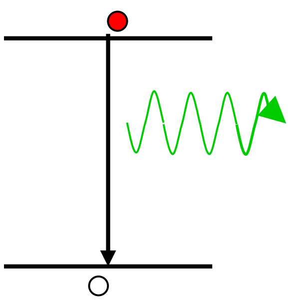
Advanced model: Solve transfer matrix equation using (n,k) data for layers

- In inorganic semiconductors assume generation rate is equal to photon absorption rate $G(E,x) = L(E,x)$. In general, $G = P_{cs}L$

Recombination

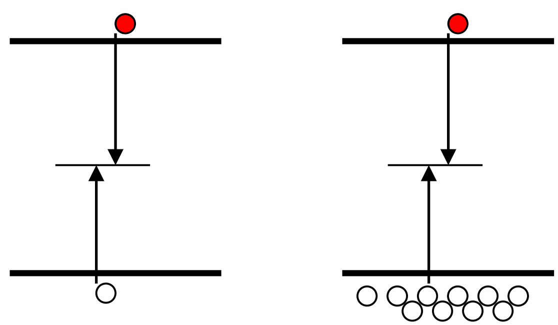
Excess electrons and holes recombine

Radiative



$$R_{rad} = B_{rad}\left(np - n_i^{\ 2}\right)$$
$$\propto \left(e^{eV/kT} - 1\right)$$

Non-radiative (Shockley-Read Hall)

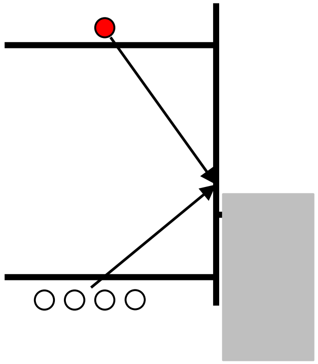


$$R_{SRH} = \frac{np - n_i^2}{(n + n_t)\tau_p + (p + p_t)\tau_n}$$

$$R_{SRH} = \frac{n - n_0}{\tau_n}$$

$$R \propto \left(e^{eV/2kT} - 1\right) \qquad R \propto \left(e^{eV/kT} - 1\right)$$

Surface



$$J_n(x_{surf}) = eS_n(n - n_0)$$

$$R \propto \left(e^{eV/kT} - 1\right)$$

- When tail states or traps are present, distinguish recombination between free or trapped electrons or holes; trapped charge likely to dominate
- $R_{SRH} = R_{SRH}\left(n_{free}, p_{trapped}\right) + R_{SRH}\left(n_{trapped}, p_{free}\right) + R_{SRH}\left(n_{free}, p_{free}\right)$

Current generation

Excess electrons and holes can drive a current

- Electron and hole current densities are defined from the quasi Fermi level gradient

$$J_n(\mathbf{r}) = \mu_n n \nabla_{\mathbf{r}} E_{F_n}$$

$$J_p(\mathbf{r}) = \mu_p p \nabla_{\mathbf{r}} E_{F_p}$$

$$J(\mathbf{r}) = J_n(\mathbf{r}) + J_p(\mathbf{r})$$

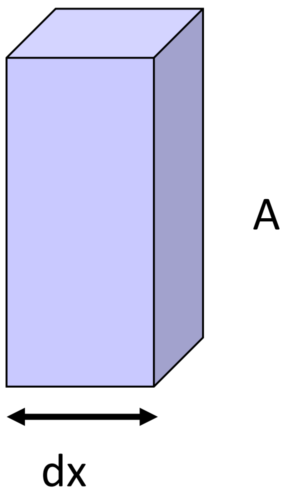
- Fermi level gradient due to gradient in carrier density, electrostatic potential, band edge energy and density of states (We assume no gradient in Temperature .)

$$J_n(\mathbf{r}) = eD_n \nabla n + q\mu_n n\left(F - \nabla\chi - kT\nabla \ln N_c\right) \qquad J_p(\mathbf{r}) = -eD_p \nabla p + q\mu_p p\left(F - \nabla\chi - \nabla E_g + kT\nabla \ln N_v\right)$$

- For a uniform material, current densities J are more commonly written as the sum of drift and diffusion terms

$$J_n(\mathbf{r}) = eD_n \nabla n + e\mu_n F n \qquad J_p(\mathbf{r}) = -eD_n \nabla p + e\mu_p F p$$

Book keeping



In volume A. dx in unit time,

No electrons being generated – no. electrons recombining = no electrons leaving – no electrons entering

$G.Adx$ $\quad R.Adx$ $\quad -\frac{1}{e}J_n(x+dx)A$ $\quad -\frac{1}{e}J_n(x)A$

$$G - R = -\frac{1}{e}\frac{dJ_n}{dx}$$

Semiconductor device equations in steady state

Continuity:

$$-\frac{1}{e}\frac{dJ_n}{dx} = G - R \qquad \frac{1}{e}\frac{dJ_p}{dx} = G - R$$

Any gradient in current density is matched by Generation – Recombination

Current:

electrons: $J_n = eD_n \frac{dn}{dx} + en\mu_n F \quad ⇨ \quad J_n = en\mu_n \frac{dE_{F_n}}{dx}$

holes: $J_p = -eD_p \frac{dp}{dx} + ep\mu_p F \quad ⇨ \quad J_p = ep\mu_p \frac{dE_{F_p}}{dx}$

Poisson's equation:

$$\frac{d^2\phi_i}{dx^2} = \frac{e}{\varepsilon_r \varepsilon_0}\left(N_a - N_d + n - p\right)$$

Charges arrange to minimise electrostatic potential energy

⇨ *set of 3 differential equations, for n, p and* ϕ_i.

Plus: boundary conditions at the electrodes, e.g.

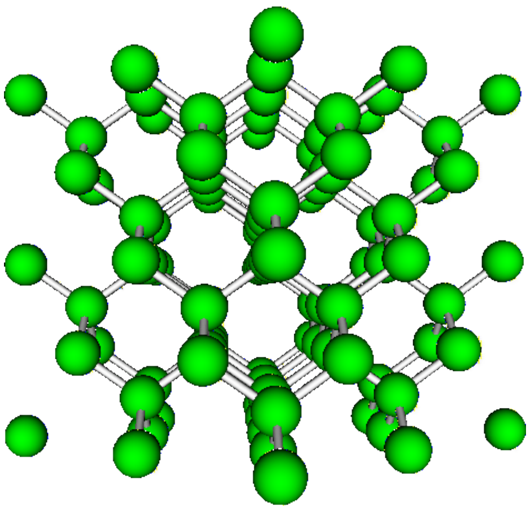
$$J_n(x_{surf}) = eS_n(n - n_0)$$

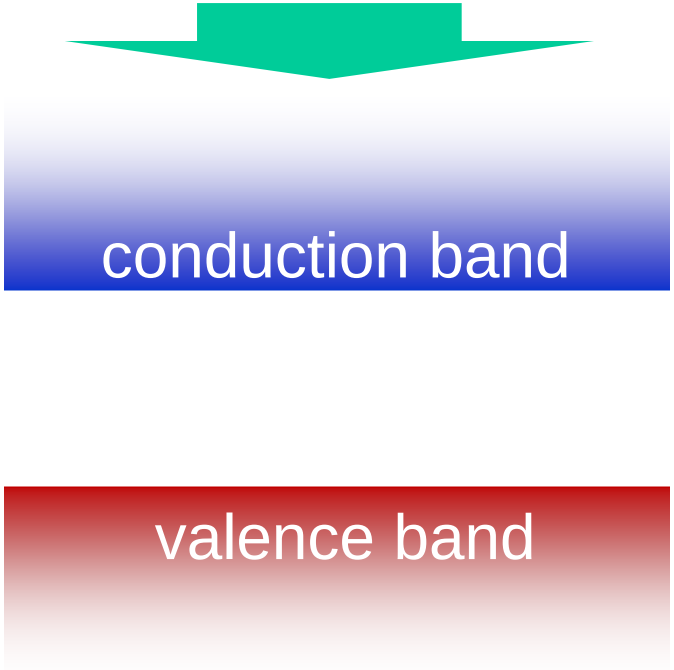
$$\phi(x_{front}) - \phi(x_{rear}) = V$$

Outline

- Basics of solar cell device modelling
- **What is different about organic solar cells**
- Device modelling approaches to OPV
- Case studies: steady state models
- Transient device modelling

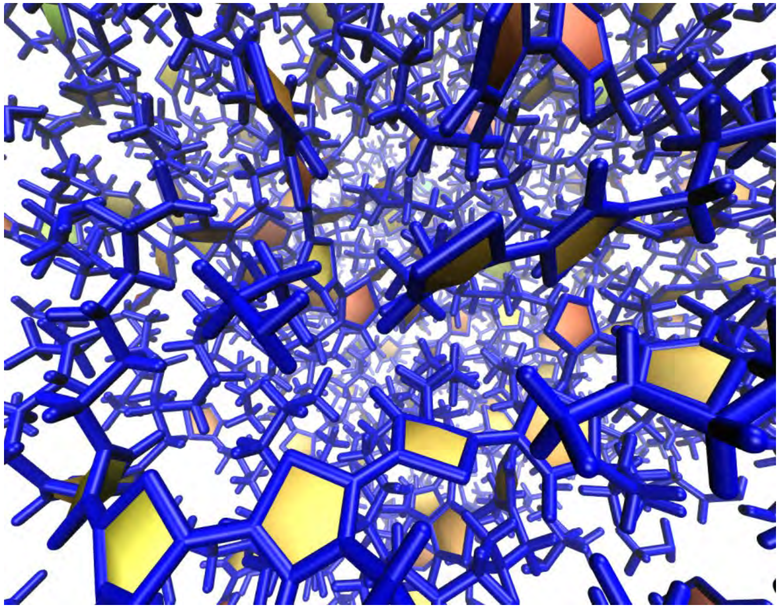
Inorganic vs. organic semiconductor: Density of States

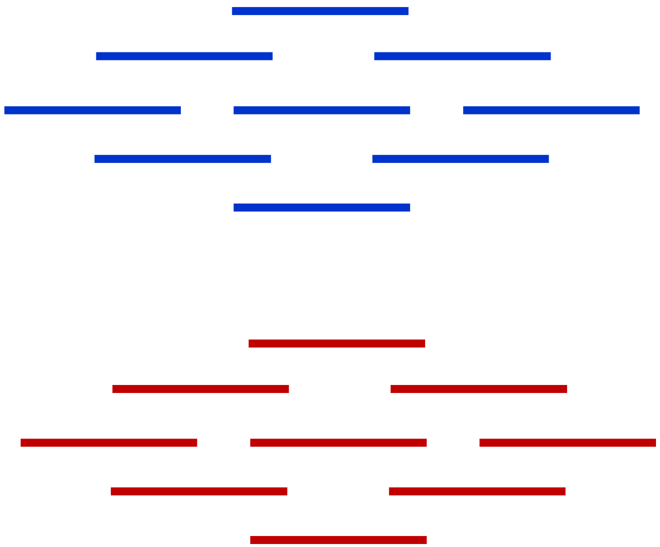




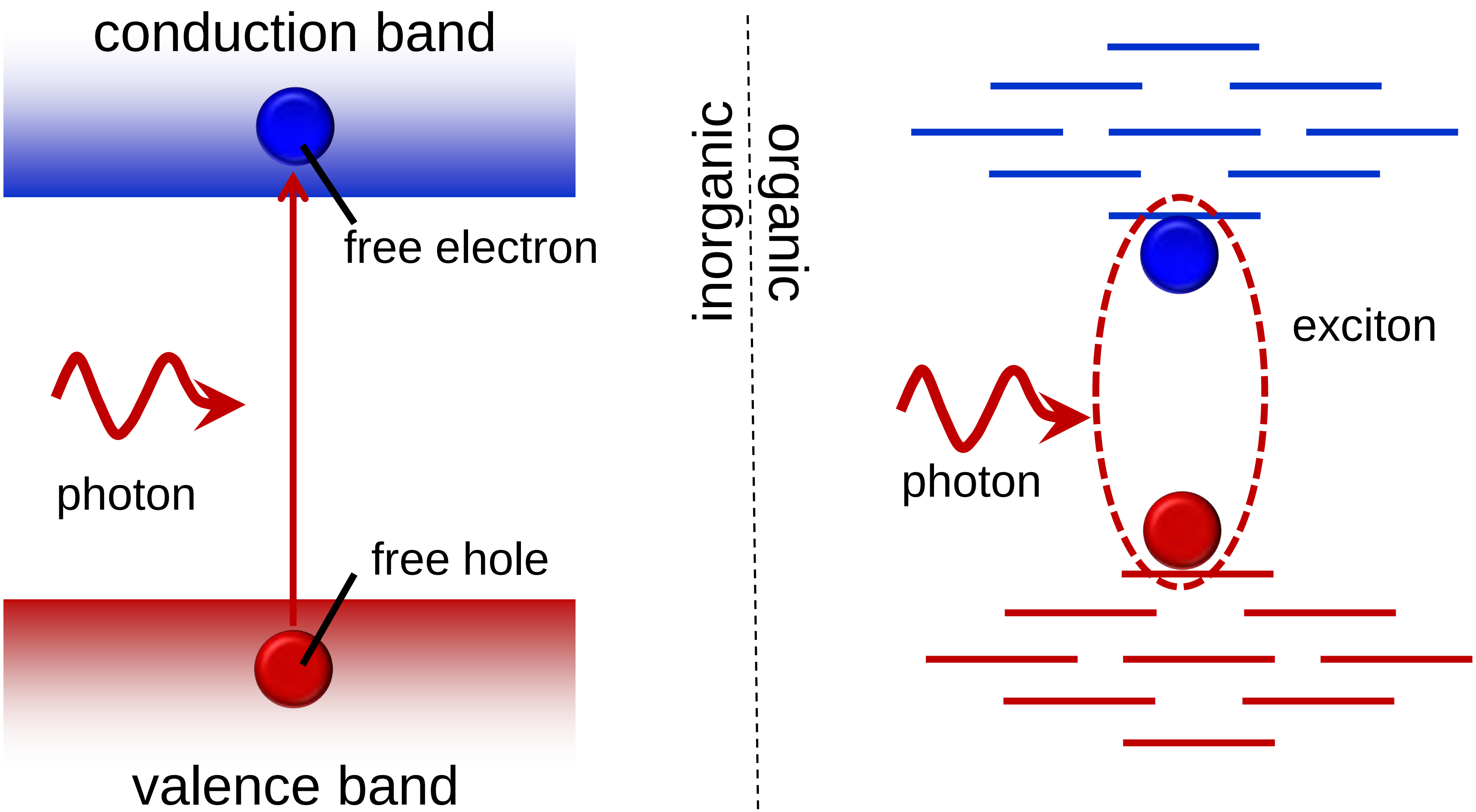
inorganic

organic





Photoexcitation in inorganic vs. organic semiconductors

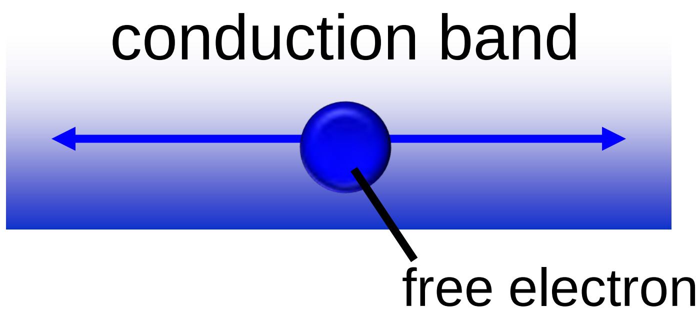


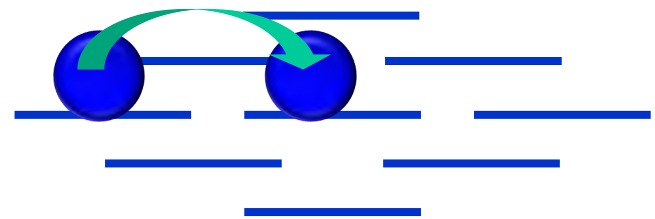
Coulomb binding of exciton

dielectric constant $\varepsilon_r > 10$

dielectric constant $\varepsilon_r \approx 3 - 4$

Transport in inorganic vs. organic semiconductors

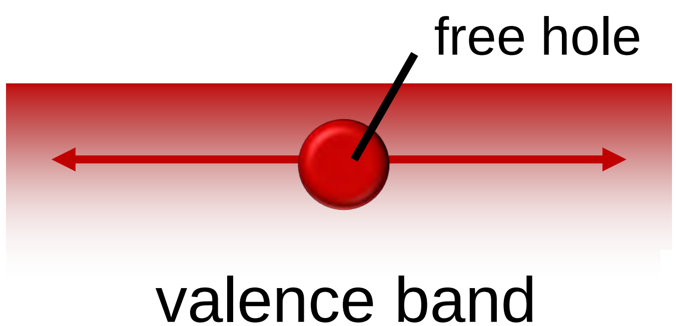


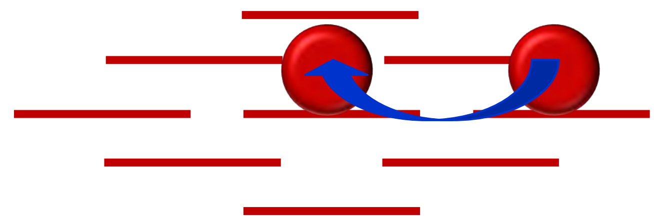


inorganic | organic

mobility:
μ = 1 to 10^4 cm^2/Vs

mobility:
$\mu \approx 10^{-4}$ cm^2/Vs



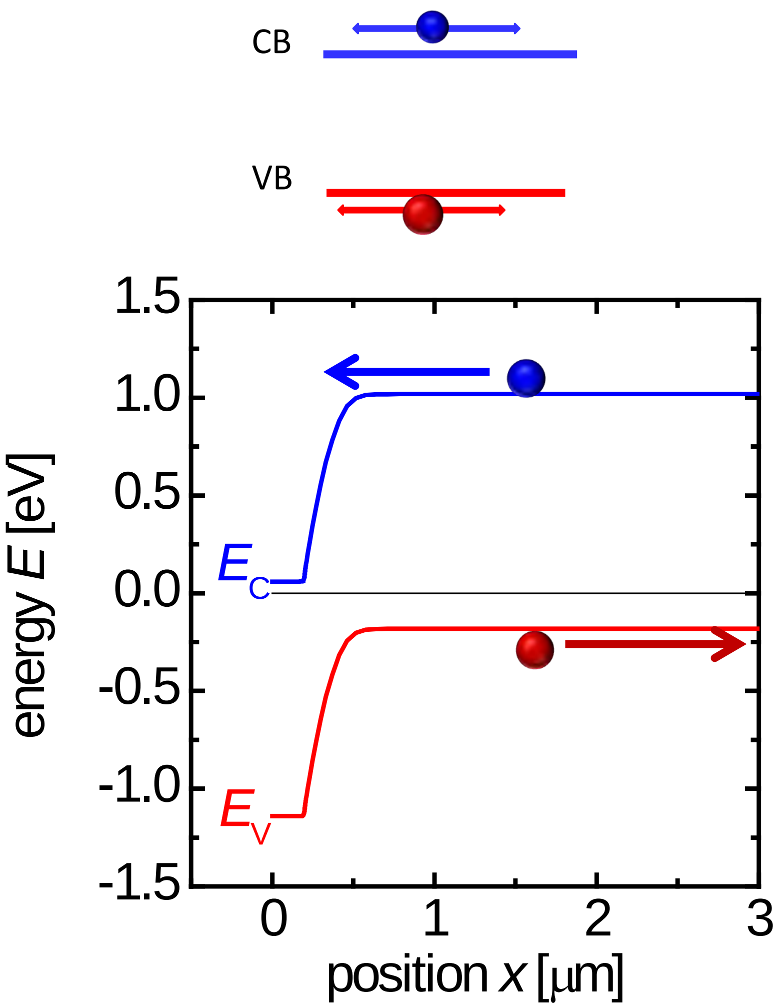


$$J_n = eD_n \frac{dn}{dx} + en\mu_n F$$

Band transport: D_n, μ_n are constant

Hopping: D_n, μ_n are *n* dependent

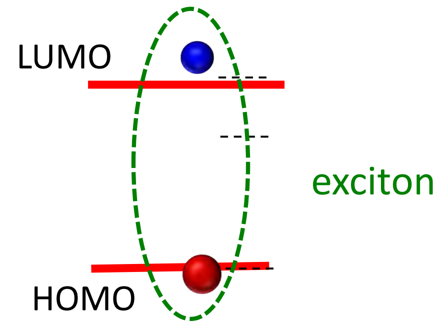
Photocurrent generation in inorganic vs. organic solar cells

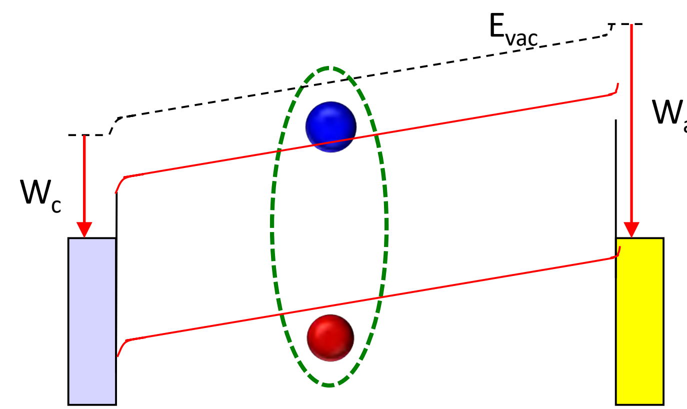


e.g. using a pn-junction

$$G(E,x) = L(E,x)$$

inorganic | organic



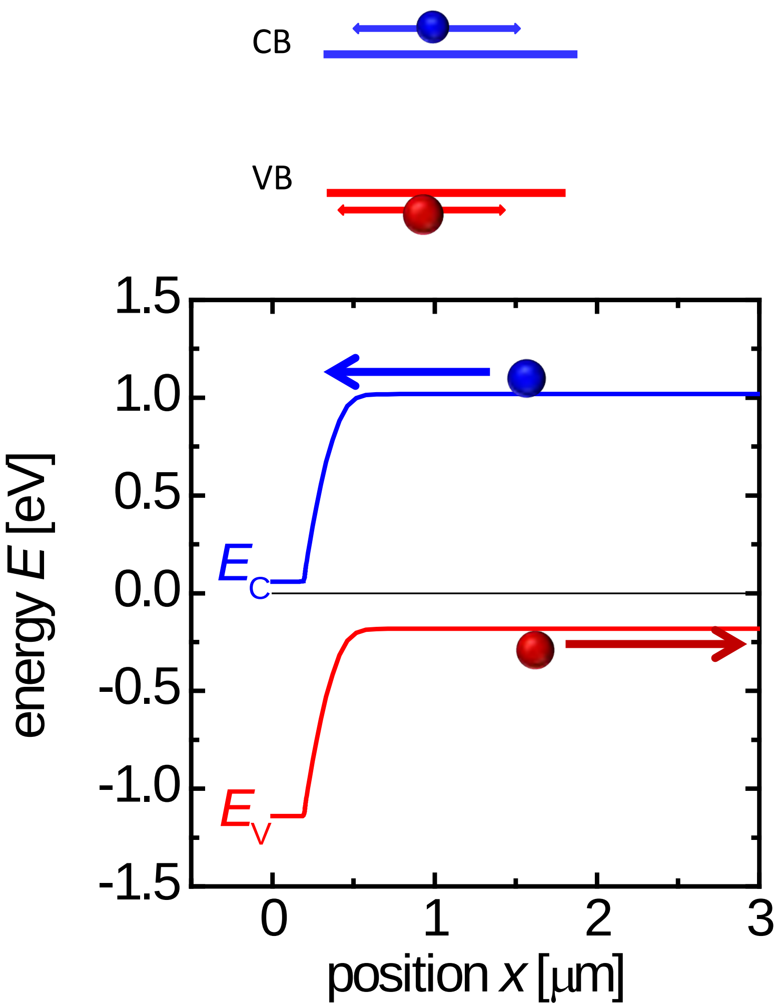


e.g. using a MIM junction

$$G(E,x) = P_{cs} L(E,x)$$

$$P_{cs} \ll 1$$

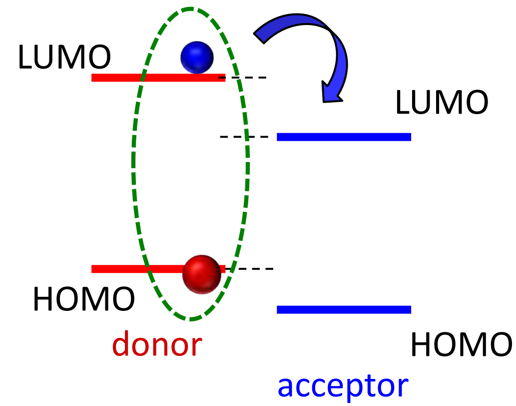
Photocurrent generation in inorganic vs. organic solar cells

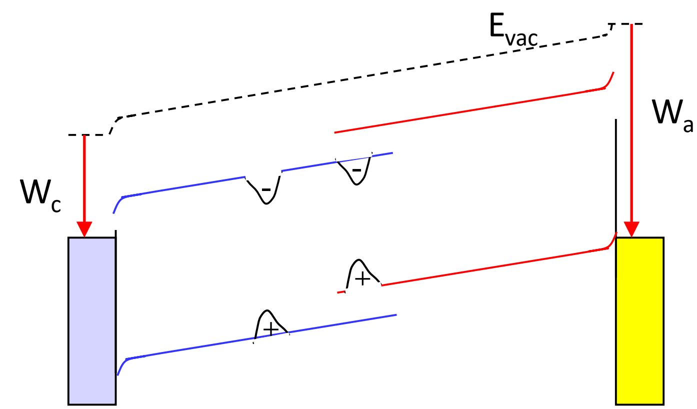


e.g. using a pn-junction

inorganic

organic

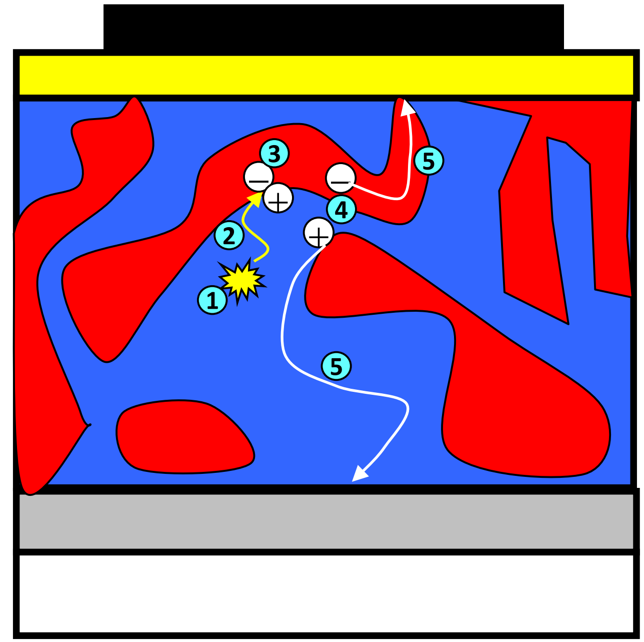




using a planar or bulk heterojunction

$$G(E,x) = P_{cs} L(E,x)$$
$$P_{cs} < \sim 1$$

Key steps in OPV device function



1. Photon absorption

2. Exciton diffusion

Exciton decay

3. Exciton dissociation ⇨ geminate charge pair

⇨ e.g. triplets

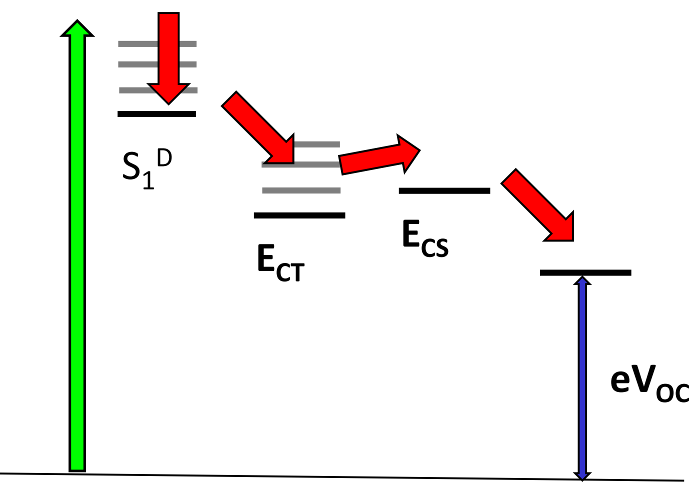
4. Geminate charge pair separation

Geminate recombination

5. Charge transport to contacts

Non-geminate recombination

Current generation



Processes captured with a device scale model

1. Photon absorption

2. Exciton diffusion

Exciton decay

3. Exciton dissociation ⇨ geminate charge pair

⇨ e.g. triplets

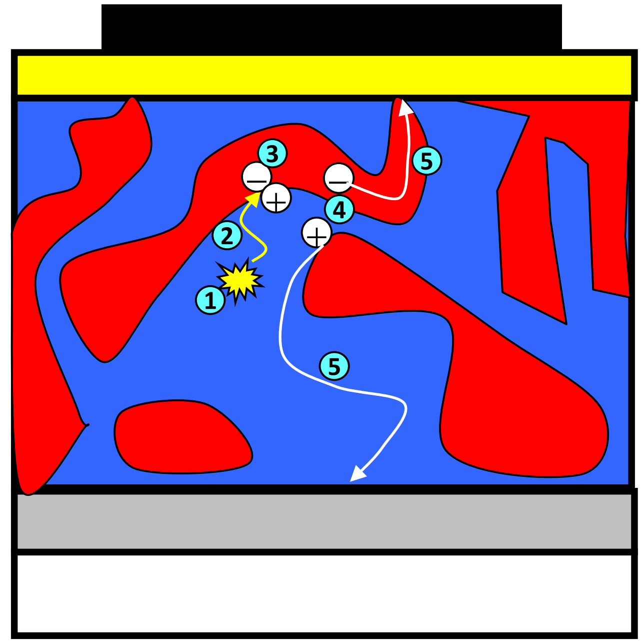
4. Geminate charge pair separation

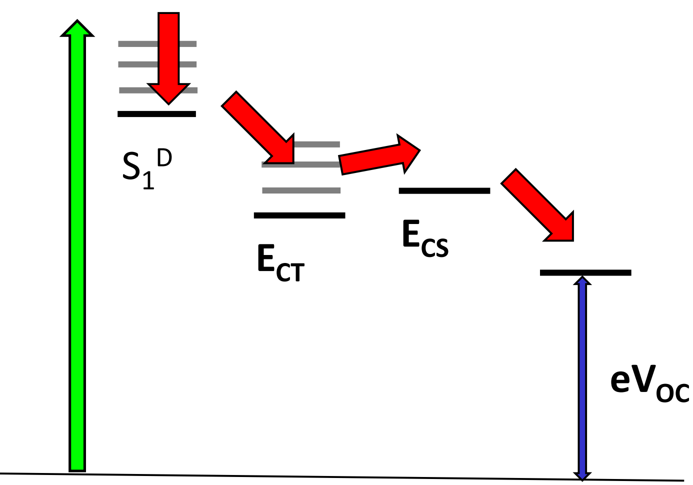
Geminate recombination

5. Charge transport to contacts

Non-geminate recombination

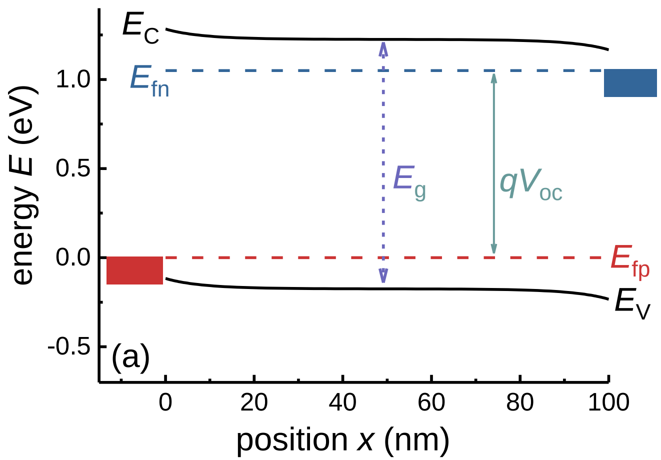
Current generation



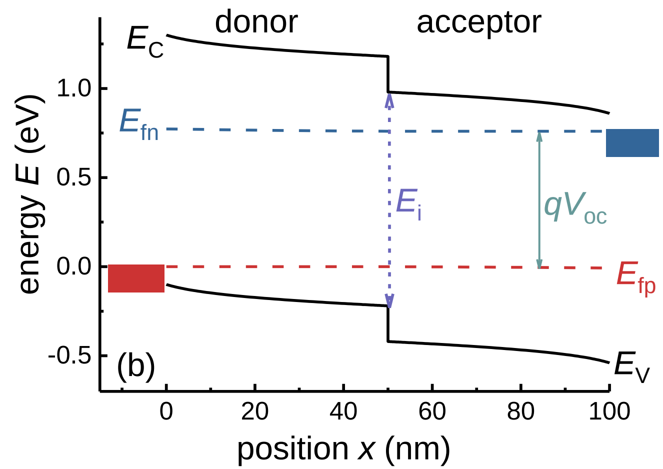


Dealing with the bulk heterojunction: Effective medium

Homojunction (MIM structure)



Planar heterojunction

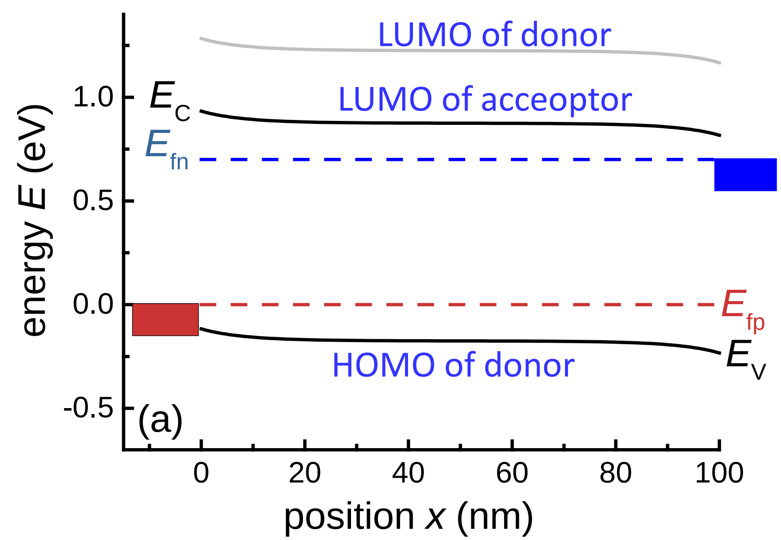


DOI: 10.1016/j.trechm.2019.01.010

- Active layer is an effective semiconductor medium with conduction band energy at LUMO of acceptor and valence band at HOMO of donor

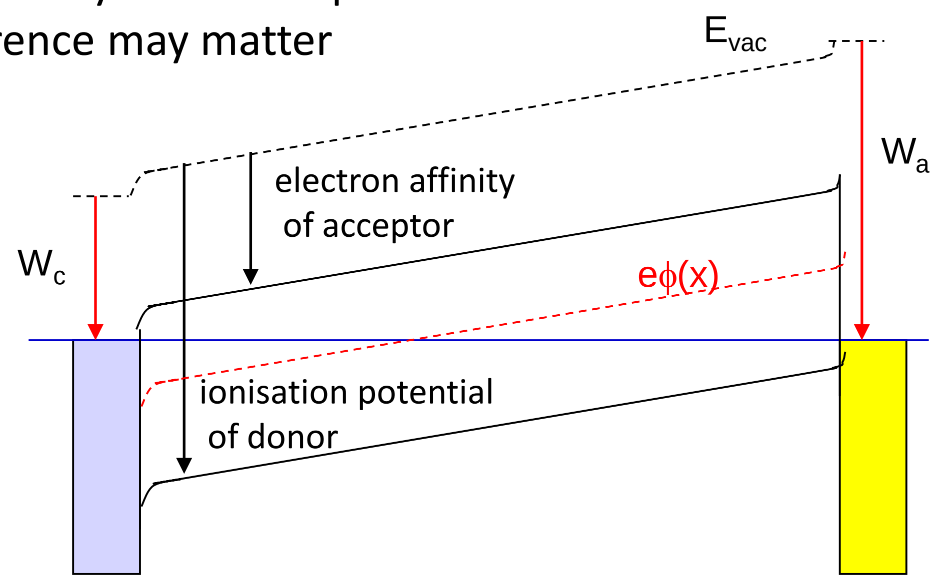
- Charge dynamics and electrostatics within active layer described by same coupled partial differential equations and boundary conditions… except coefficients may not be constant!

Bulk heterojunction



Device Physics of Organic Solar Cell: What's different?

Semiconductor layer is thin: optical interference may matter



Material not (intentionally) doped

(so rely on electrodes for photocurrent direction)

Material is energetically disordered: DoS extends into gap

$$-\frac{1}{e}\frac{dJ_n}{dx} = G - R$$

$$J_n = eD_n\frac{dn}{dx} + en\mu_n F$$

$$\frac{dF}{dx} = \frac{e\rho(x)}{\epsilon_0\epsilon_r}$$

Generation is not well understood

Lifetime, mobility and diffusion are not constant

ε_r is small (3-4)

Outline

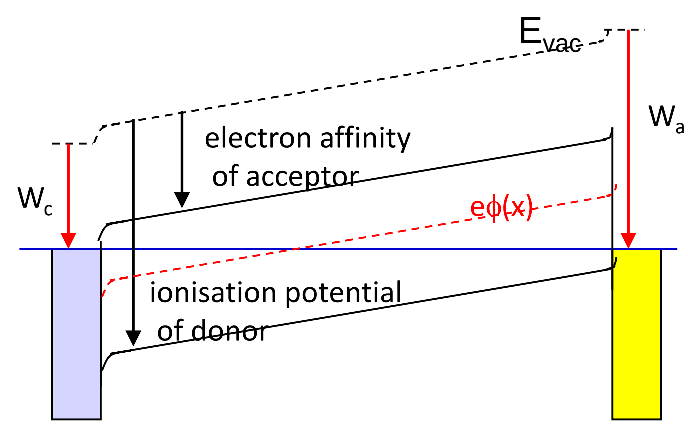
- Basics of solar cell device modelling
- What is different about organic solar cells
- **Device modelling approaches to OPV**
- Case studies: steady state models
- Transient device modelling

Common approach to OPV device physics

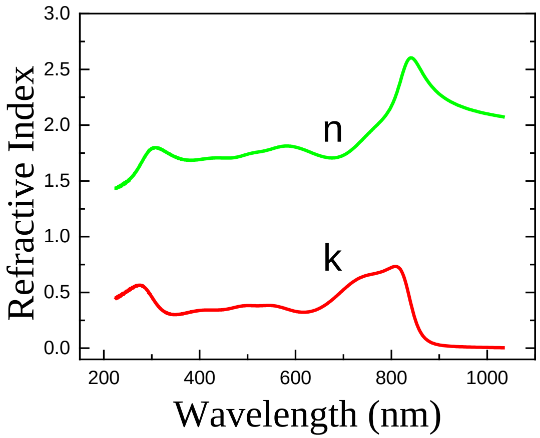
- Use **effective medium** for photoactive layer,
- **Undoped** /lightly doped active layer, metallic electrodes, doped interlayers possible
- Parabolic density of states in conduction and valence bands, possibly with discrete deep **traps** and / **or tail states**
- **Quasi thermal equilibrium** assumed (commonly)
- Transfer matrix, Beer Lambert or uniform generation
- Empirical formula to **relate pair generation to photon absorption** (often P_{cs} = 1)
- Only charge carriers above band edges are mobile; makes average mobility dependent on total charge density
- Uniform free carrier (or "band") mobility
- **Shockley Read Hall recombination** statistics (distinguishing trapped and free carriers) and recombination at electrode interfaces

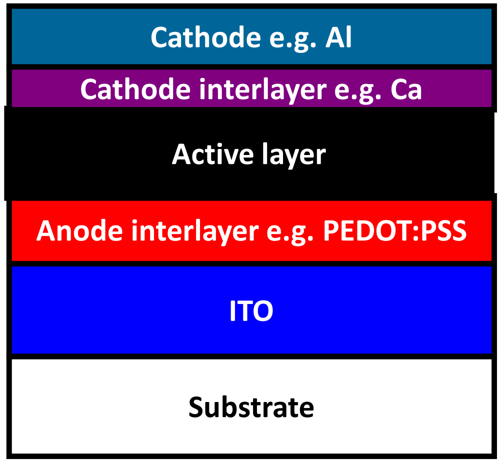
Implement DE solver in MATLAB or other code;
Use commercial software

(most simulations in this talk done with ASA)



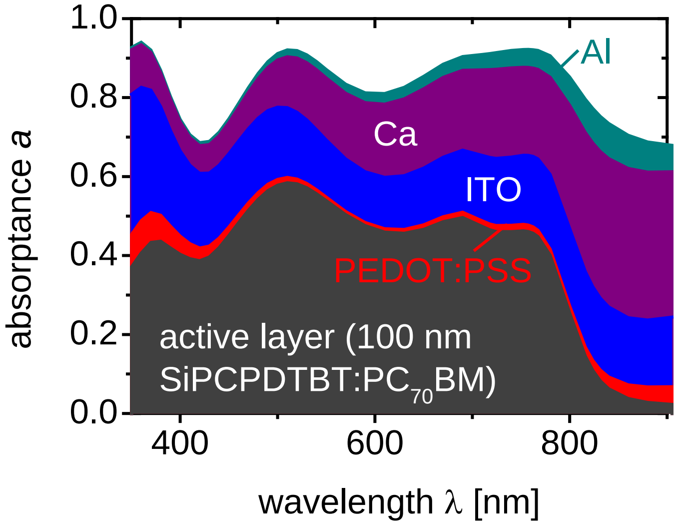
Device simulation input: Optical absorption





- Layer thicknesses comparable to wavelength of light so use optical model

Transfer Matrix Model

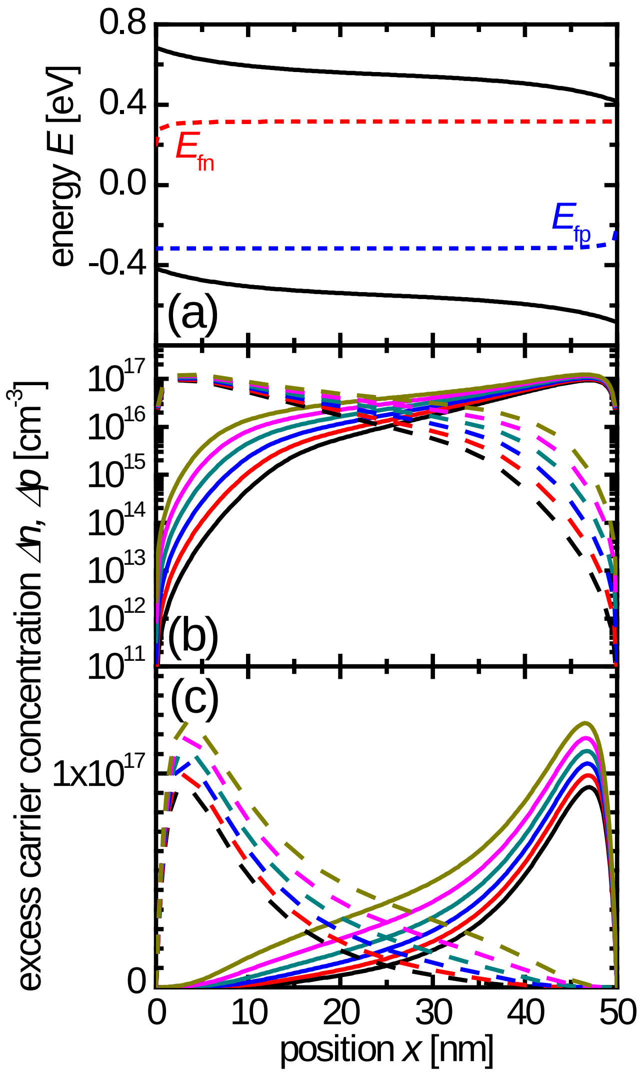


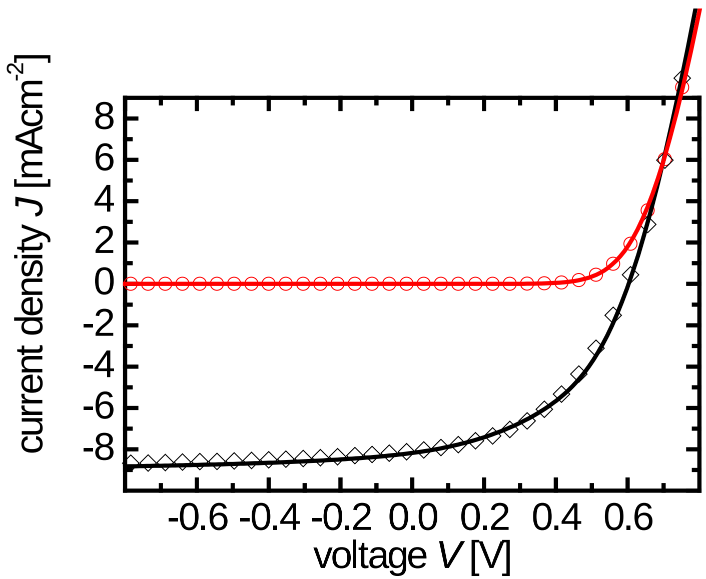
- Tune layer thicknesses to maximise absorbance *A* in the active layer

T. Kirchartz and J Nelson, Top. Curr. Chem. (2013)

Pettersson et al., J. Appl.Phys. 86, 487 (1999); Moule et al., J. Appl. Phys. 100, 094503 (2006);

Device simulation output:
Band profiles, charge density and J-V curves



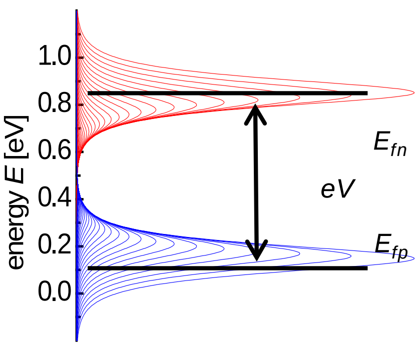


- Spatial variation of n and p mean that zero-dimensional models of recombination are often not accurate

Device simulation output: Tail state filling and ideality factor

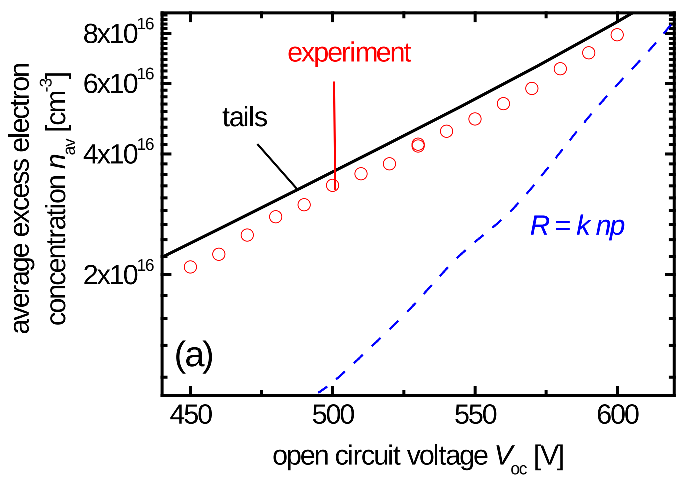
- Band tails can be represented as exponential or Gaussian functions
- Shockley Read Hall recombination via tails (free to trapped charges)
- Charge carrier density as a function of Voc strongly reflects the role of tail states
- Ideality factor indicates recombination mechanism (free to trapped charge)

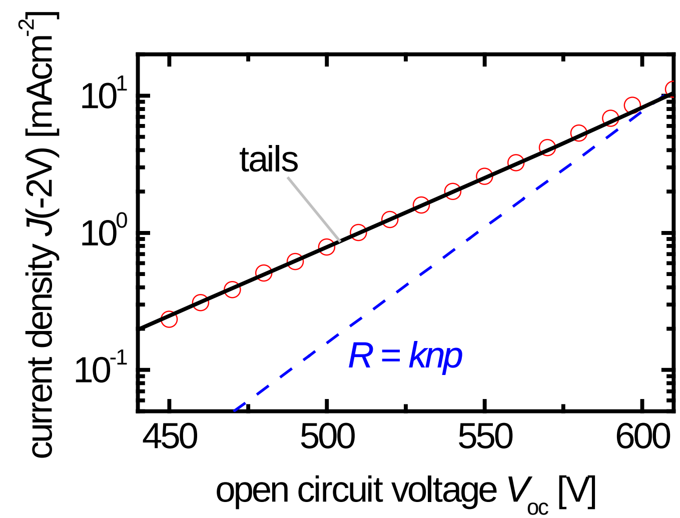
T. Kirchartz et al, Phys. Rev. B (2011)



$$DOS \propto \exp\left(\frac{E}{E_{ch}}\right)$$

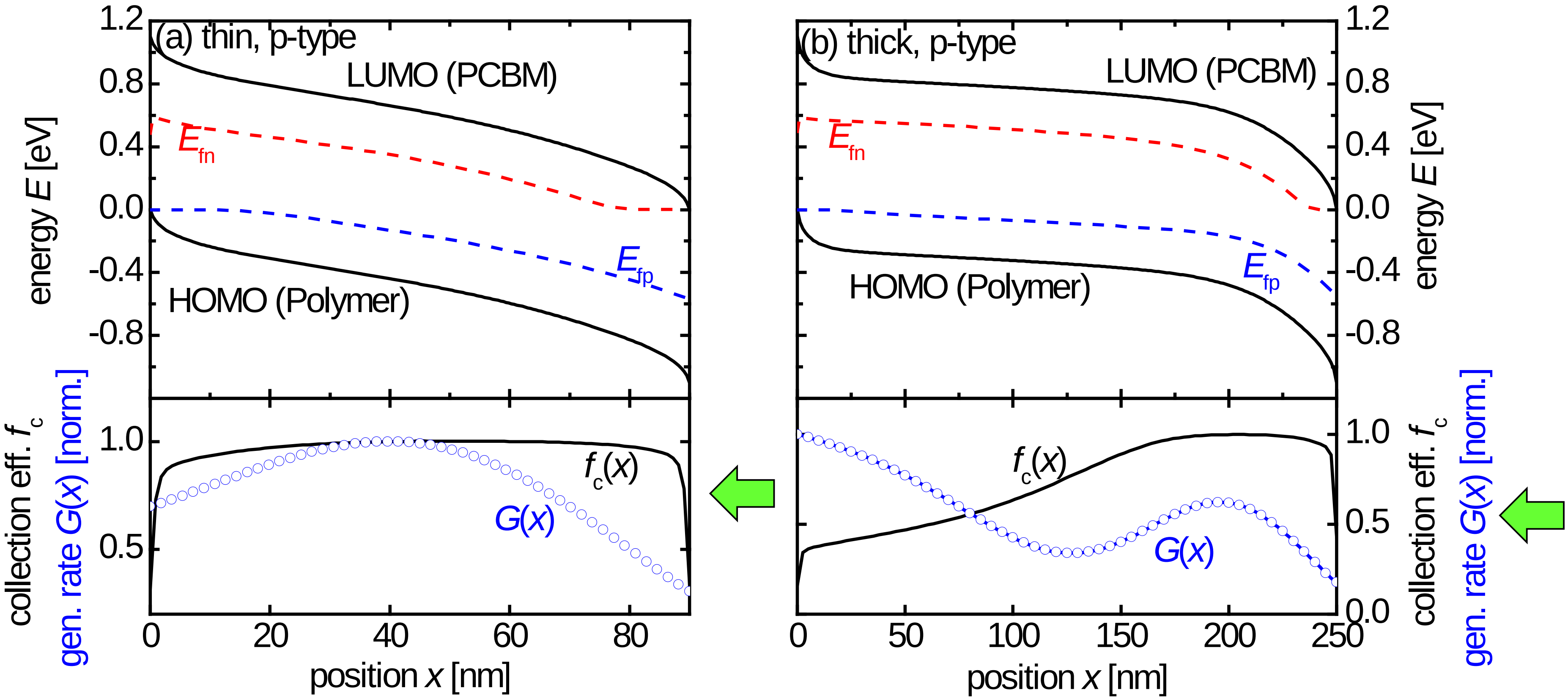
$$n \propto \exp\left(\frac{eV}{2E_{ch}}\right)$$





$$R = kn_{\mathrm{f}}\, p_{\mathrm{t}} = kn_0\, p_0 \exp\left(\frac{qV}{2kT} + \frac{qV}{2E_{\mathrm{ch}}}\right)$$

Device simulation : Generation and recombination profiles



Efficient charge carrier collection needs a high built-in electric field!

T. Kirchartz et al. J. Phys. Chem. Lett. 3, 3470 (2012)

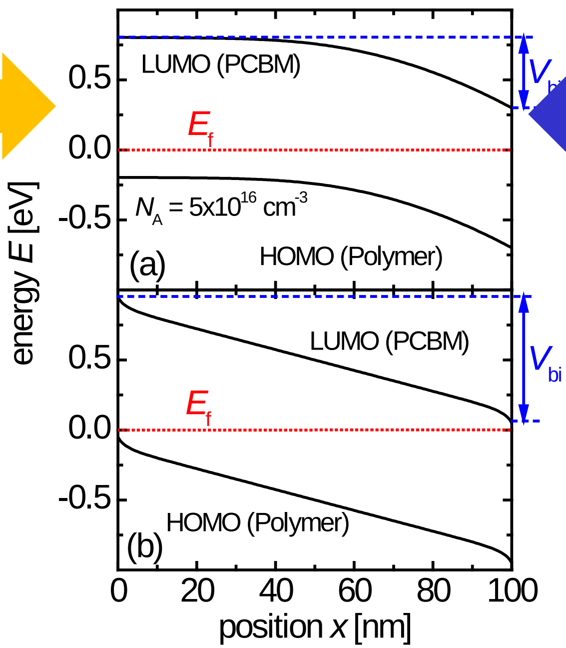
How should things change to account for spin?

- Use **effective medium** for photoactive layer,
- **Undoped** /lightly doped active layer, metallic electrodes, doped interlayers possible
  - Spin dependent injection?
- Parabolic density of states in conduction and valence bands, possibly with discrete deep **traps** and / **or tail states**
- **Quasi thermal equilibrium** assumed (commonly)
- Transfer matrix, Beer Lambert or uniform generation
- Empirical formula to **relate pair generation to photon absorption:**
  - Accounting for ISC, singlet and triplet diffusion to interfaces
  - Accounting for spin dependence of exciton dissociation and charge separation
- Only charge carriers above band edges are mobile; makes average mobility dependent on total charge density
- Uniform free carrier (or "band") mobility
  - Spin dependence of charge transfer and transport
- **Shockley Read Hall recombination** statistics (distinguishing trapped and free carriers) and recombination at electrode interfaces
  - Spin dependence of trapping and detrapping
  - Spin dependence of pair combination
  - Spin dependence of CT state to ground transition

Outline

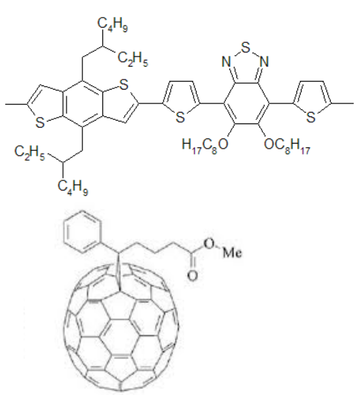
- Basics of solar cell device modelling
- What is different about organic solar cells
- Device modelling approaches to OPV
- **Case studies: steady state models**
- Transient device modelling

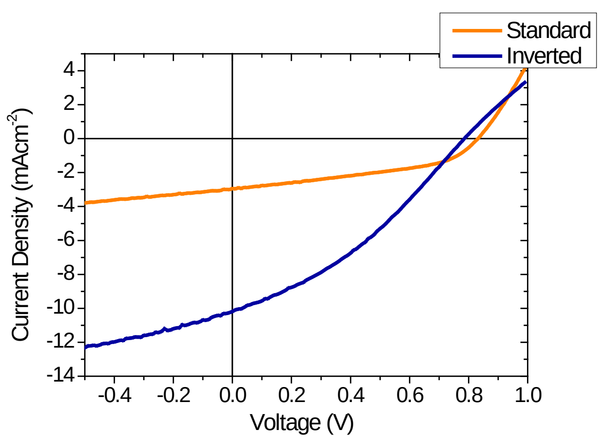
Case study I: Effect of unintentional doping

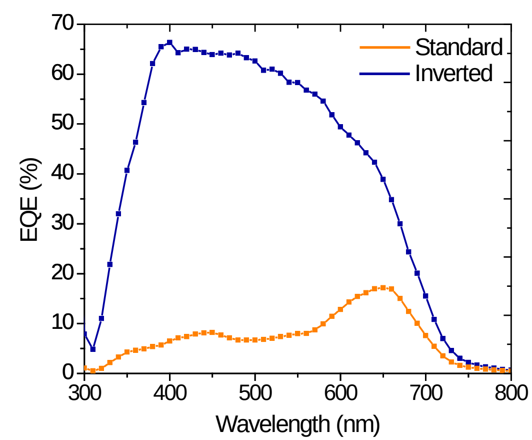


- Equilibrium band profile influenced by doping: doping limits extent of field bearing region
- When mobility is low, field needed for efficient charge collection

- **Example**: polymer:PC70BM solar cells with unintentional p doping of 10^{16} cm^{-3}



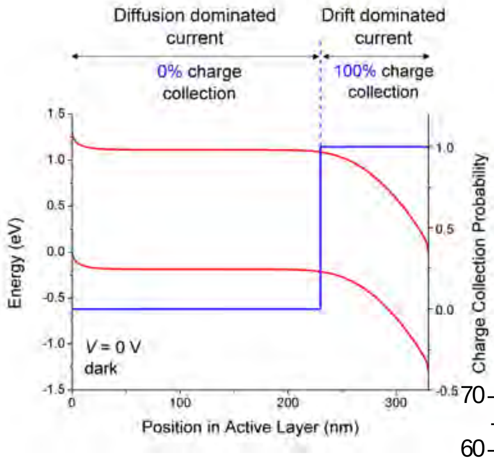




ITO/PEDOT:PSS/OPV-32:$PC_{71}BM$/Ca/Al
ITO/ZnO/OPV-32:$PC_{71}BM$/PEDOT:PSS/Ag

G. Dibb, T. Kirchartz, H. Hoppe, M. Carrasco-Orozco et al., Sci Rep (2014)

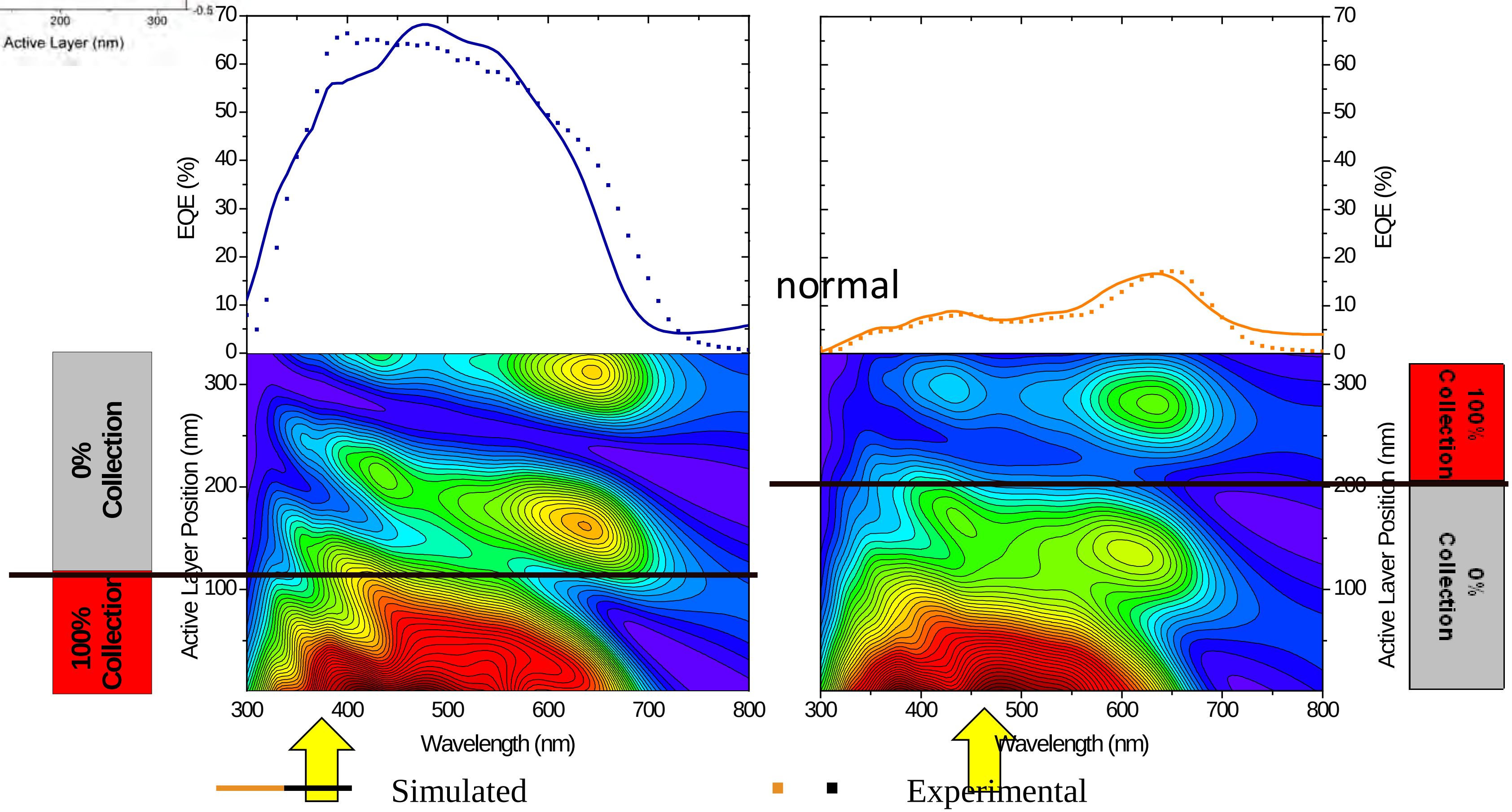
Case study I: Effect of unintentional doping



Current-voltage and EQE modelling serve as a diagnostic tool

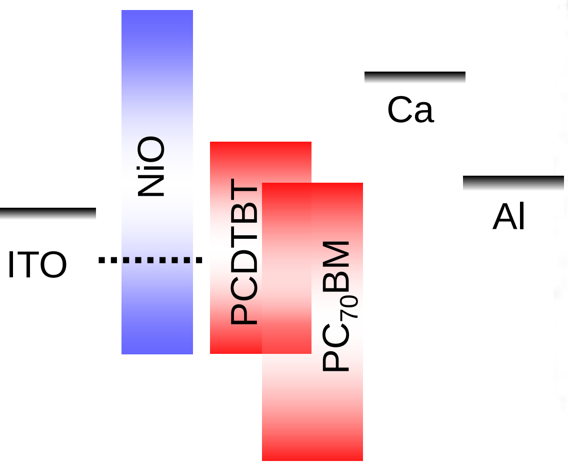
Inverted

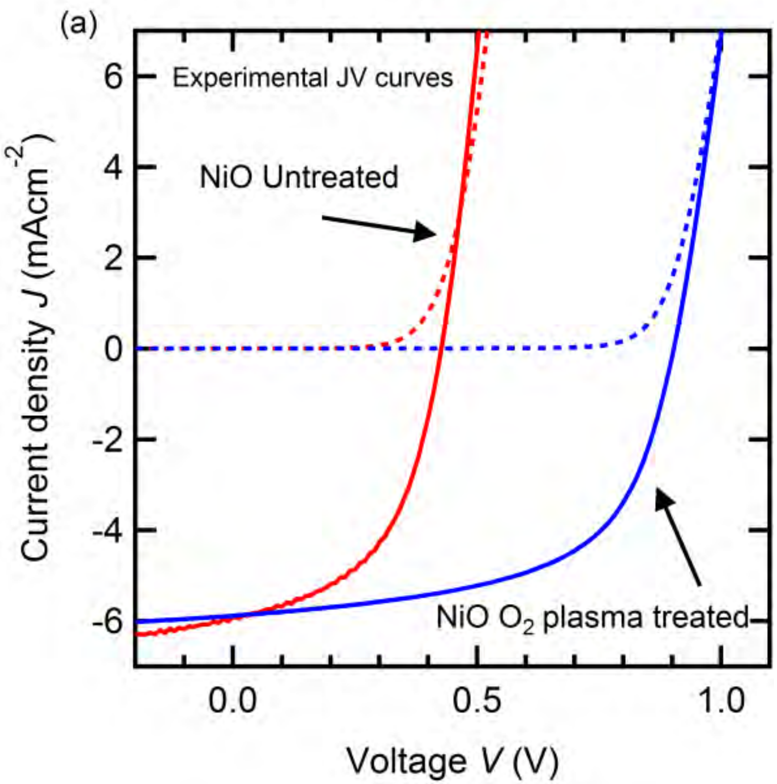
Standard

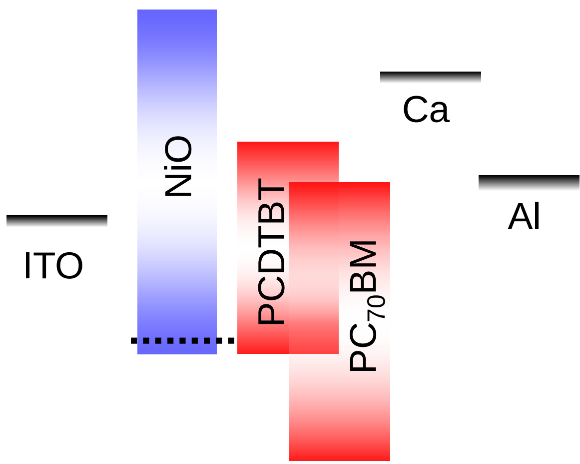


G. Dibb, et al., SciRep 2014

Case study II: electrode band alignment controls surface recombination and Voc



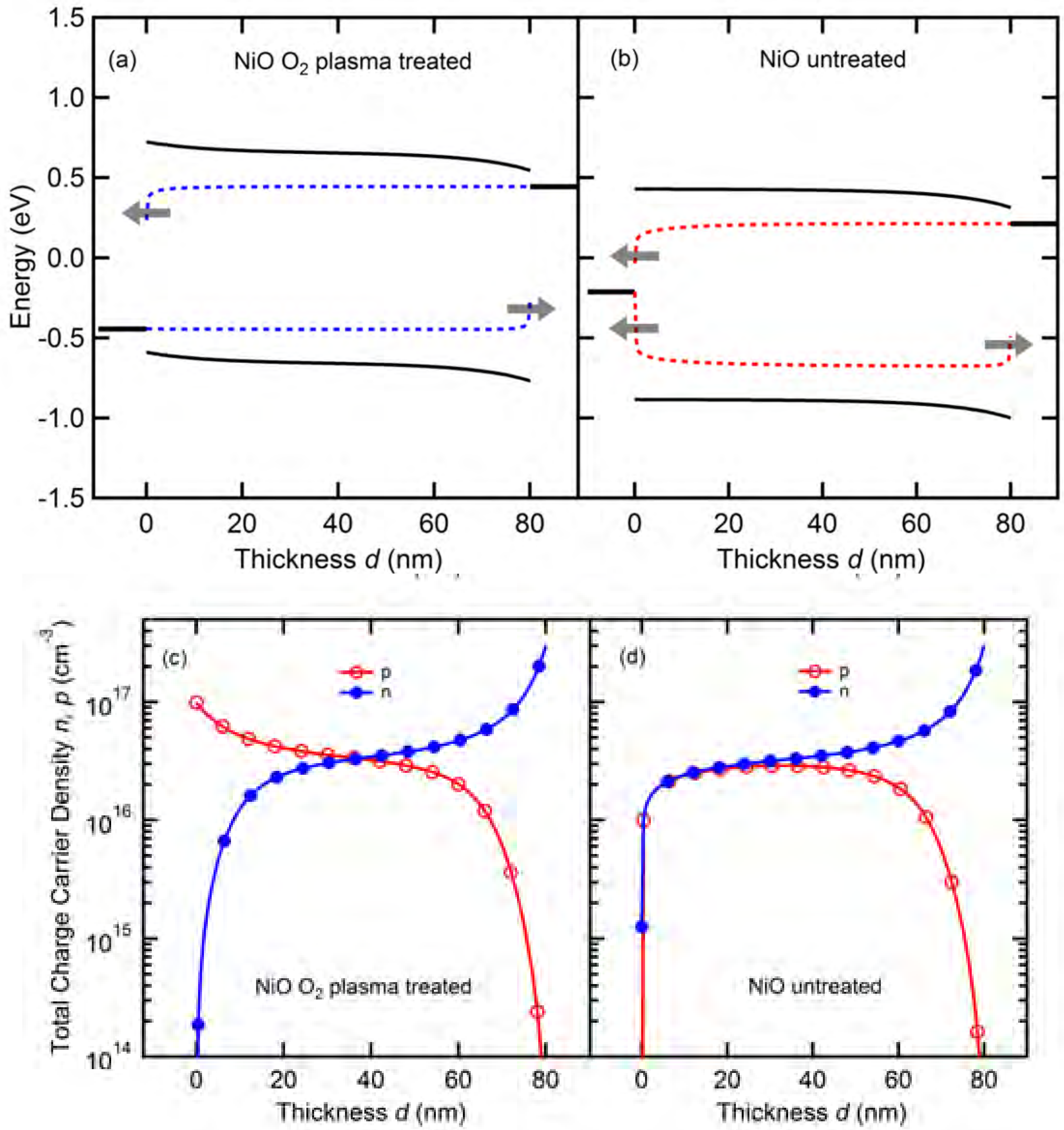




Oxygen plasma treatment of NiO interlayer leads to an increase in the open-circuit voltage

S. Wheeler et al, DOI: 10.1103/PhysRevApplied.4.024020

Case study II : electrode band alignment controls surface recombination and Voc



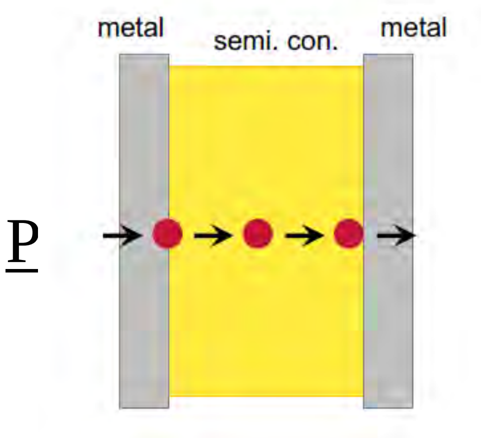
Quasi-Fermi level splitting in the bulk of the active layer largely unchanged

Gradient in the hole quasi Fermi-level at the anode indicates presence of surface recombination

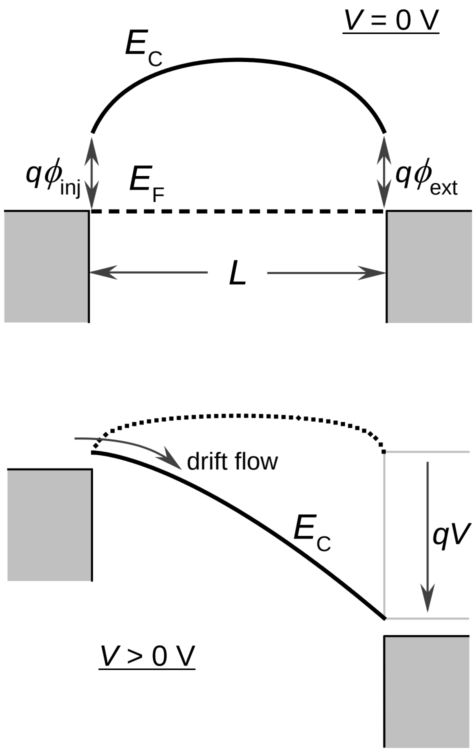
Surface recombination reduces Voc

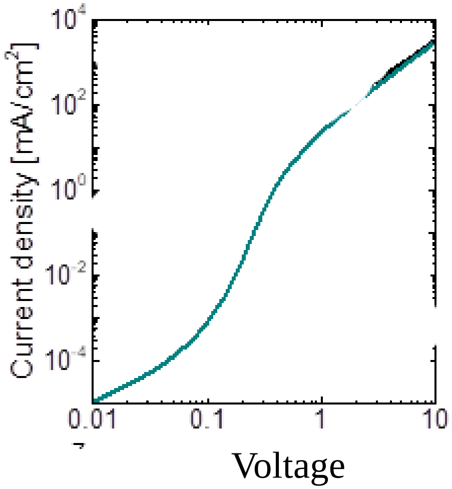
S. Wheeler et al, DOI: 10.1103/PhysRevApplied.4.024020

III: Modelling space-charge-limited current measurements



Space-charge limited current



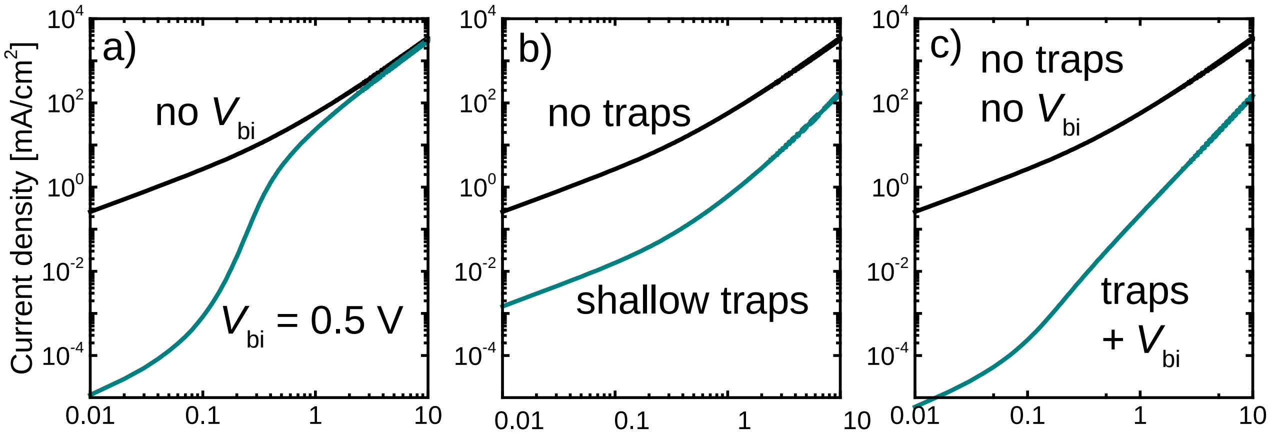


- Simple steady state dark current measurement commonly used to extract mobility
- In absence of traps or barriers, mobility is taken from Mott Gurney law $J = \frac{9}{8}\epsilon_0\epsilon_{r\mu}\frac{V^2}{d^3}$

III: Modelling space-charge-limited current measurements

Mott Gurney law is seldom valid in practical cases. Need a numerical device model

J-V curves

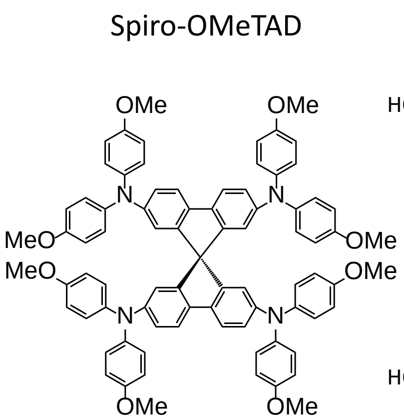


- Solve semiconductor device equations in dark
- Introduce traps and / or tail states, Introduce injection barriers and / or Vbi

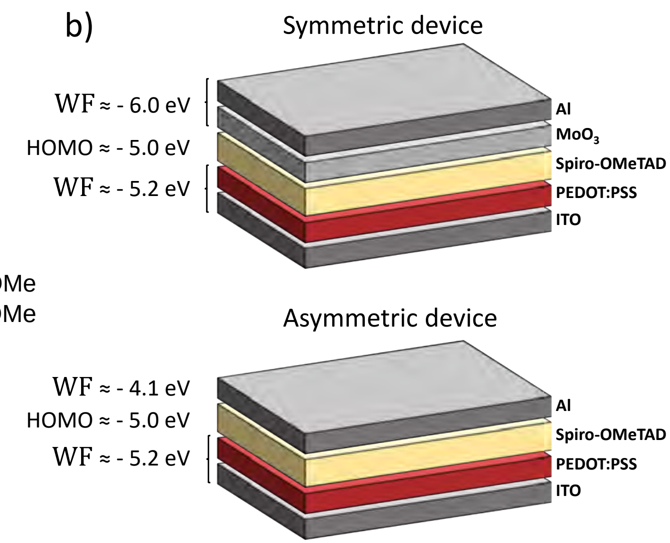
J ason Rohr et al, Phy. Rev. Appl. 10.1103/PhysRevApplied.9.044017

III: Modelling SCLC measurements in Spiro-OMeTAD

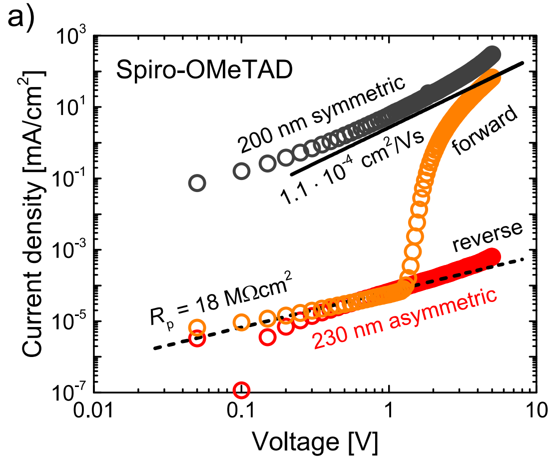
a)



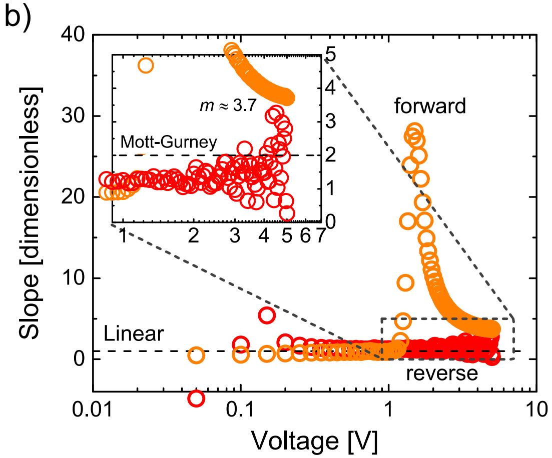
b)



a)



b)



Fit with Mott Gurney ⇨ $\mu_h \approx 1 \times 10^{-4}\ cm^2/Vs$

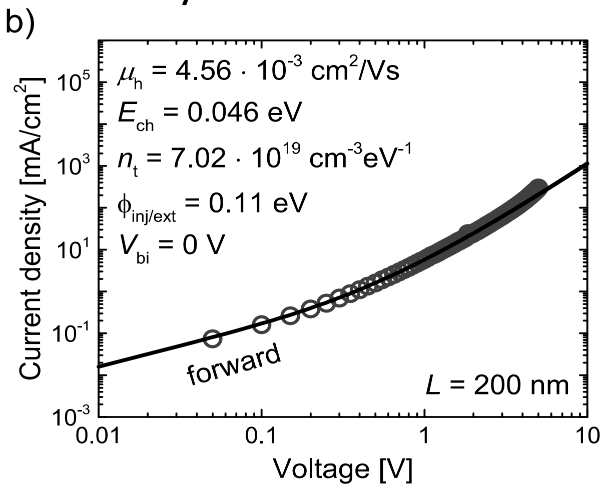
Consistent with previous reports

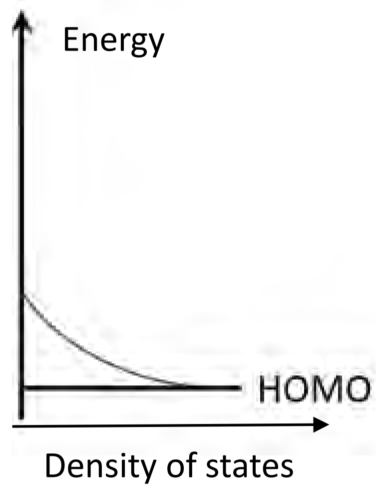
Is it reliable?

J ason Rohr et al, Phy. Rev. Appl. 10.1103/PhysRevApplied.9.044017

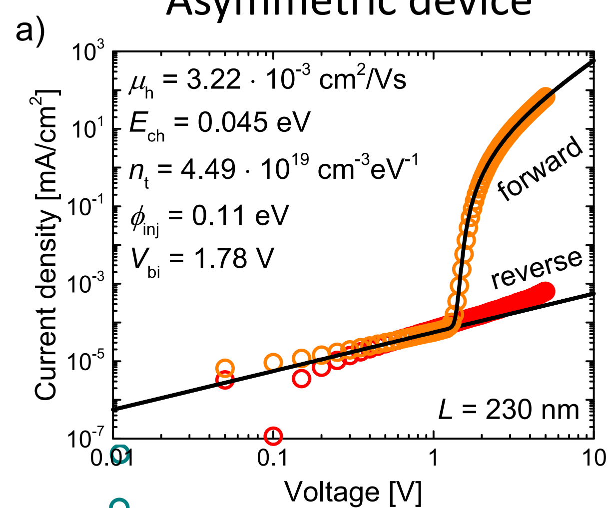
III: Modelling SCLC measurements in Spiro-OMeTAD

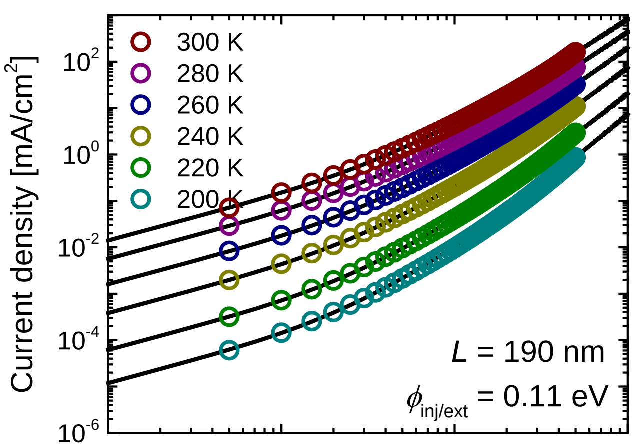
Symmetric device

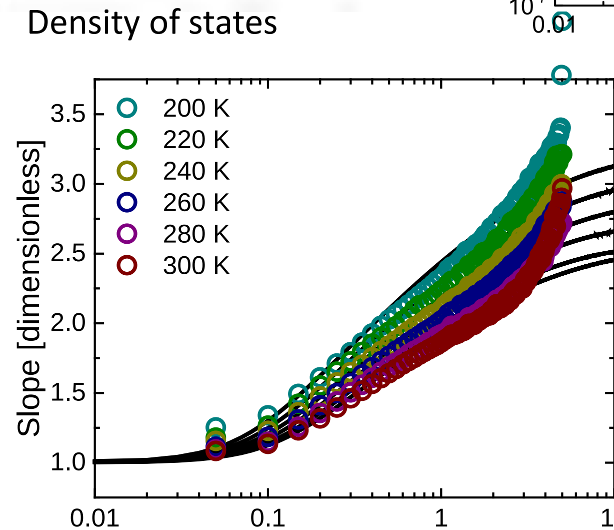




Asymmetric device





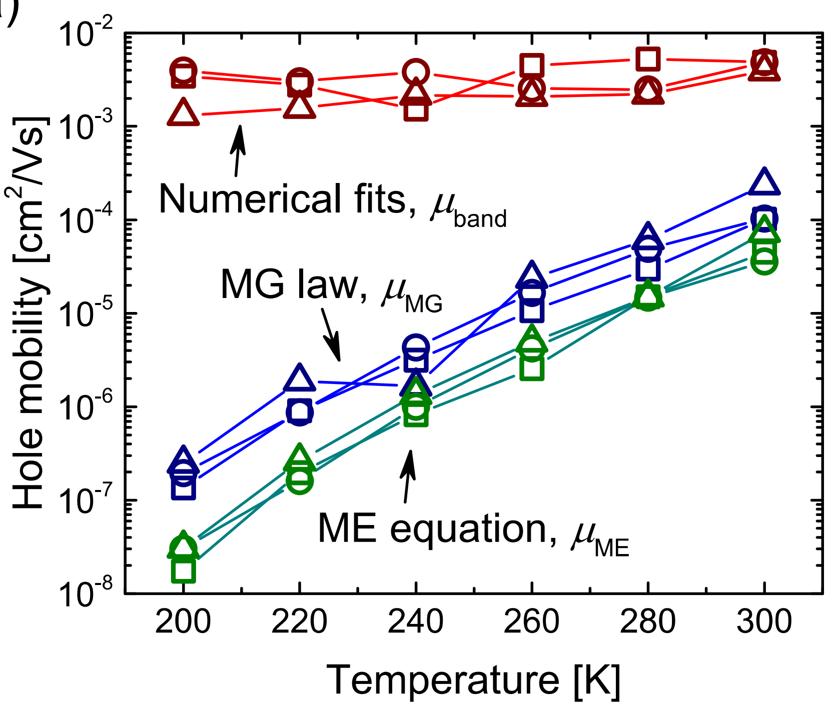


- Fit experimental data with numerical model including exponential tail of states
- Symmetric and asymmetric device data yield very similar models for DoS
- Temperature dependent data fit to same DoS

Jason Rohr et al, Phy. Rev. Appl. 10.1103/PhysRevApplied.9.044017

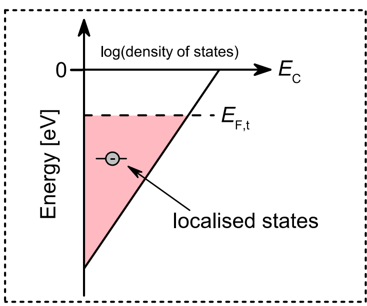
III: Modelling SCLC measurements in Spiro-OMeTAD

a)



- Mott-Gurney law and moving electrode equation yield temperature dependent mobilities. Function of trapping and injection barriers..
- Numerical model yields a temperature independent *band* mobility…
- Validation for the transport model (trapped charge immobile, free charges have constant mobility)

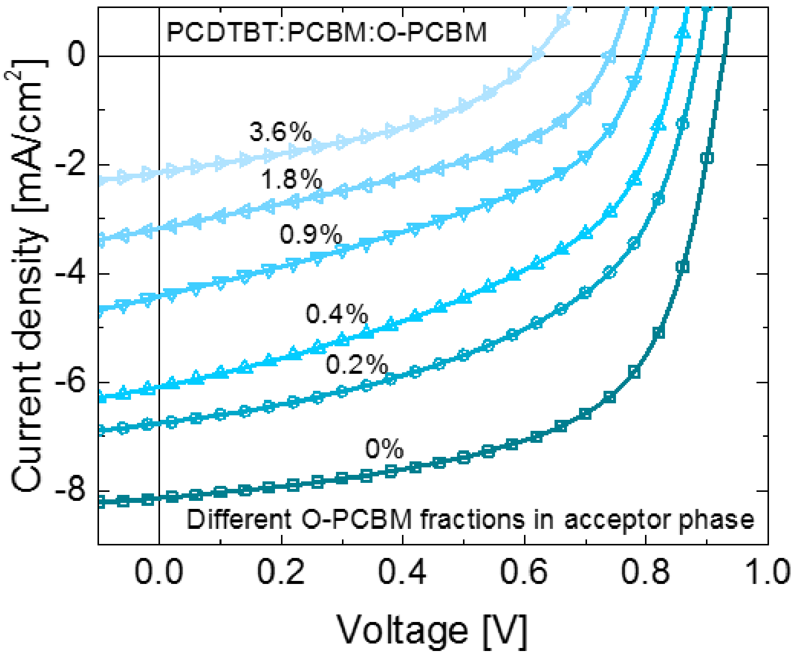
c)

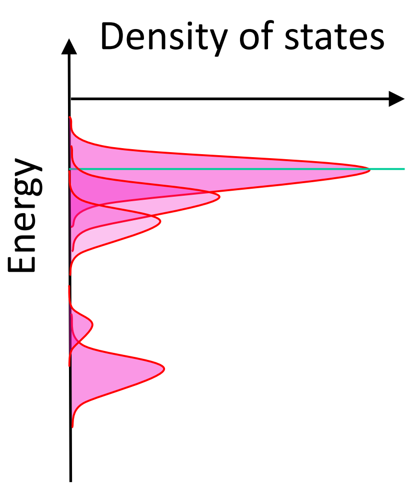


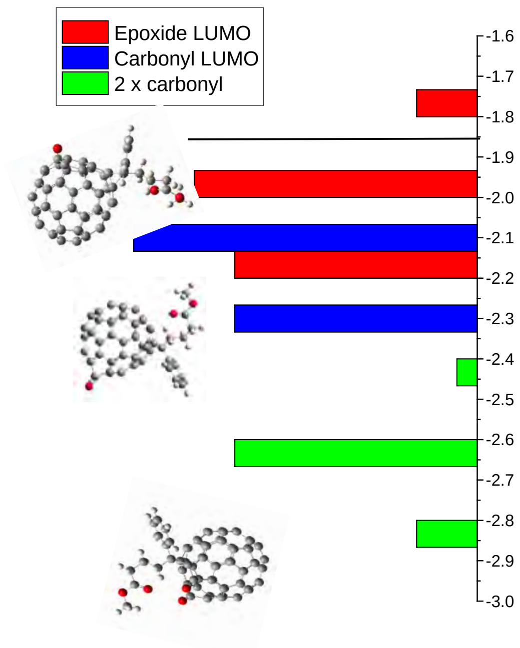
J ason Rohr et al, Phy. Rev. Appl. 10.1103/PhysRevApplied.9.044017

IV: Modelling electrical response of degraded OPV device

- Adding controlled amounts of oxidised fullerene reduces Voc, Jsc and fill factor
- Fullerene oxidation expected to induce **electron traps**
  - Likely to affect mobility, lifetime and density of states
- Can these explain the changes in device performance?



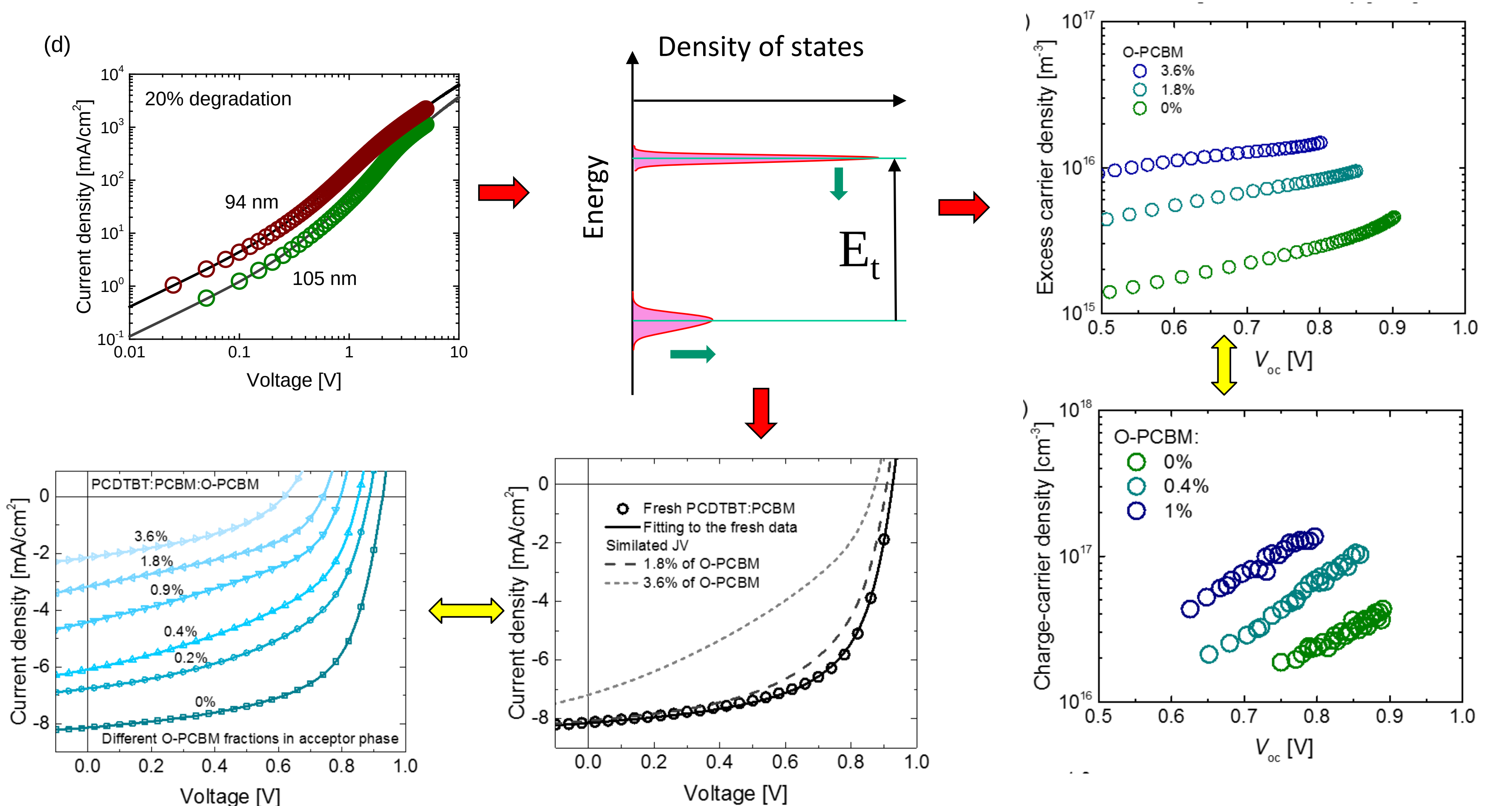




H. K. H. Lee et al, Energy Env. Sci. 2018, DOI: 10.1039/C7EE02983G

IV: Modelling electrical response of degraded OPV device:

- Modelling strategy:
  - SCLC ⇨ Deliver model for the density of states
  - Check against measured density of states from charge extraction
  - Apply to simulate device J-V response



H. K. H. Lee et al, Energy Env. Sci. 2018, DOI: 10.1039/C7EE02983G

Outline

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- **Transient device modelling**

Beyond the simple device model: time resolved response

Driftfusion

An open source MATLAB-based drift diffusion simulation tool for modelling optoelectronic devices with mixed ionic-electronic semi-conductors

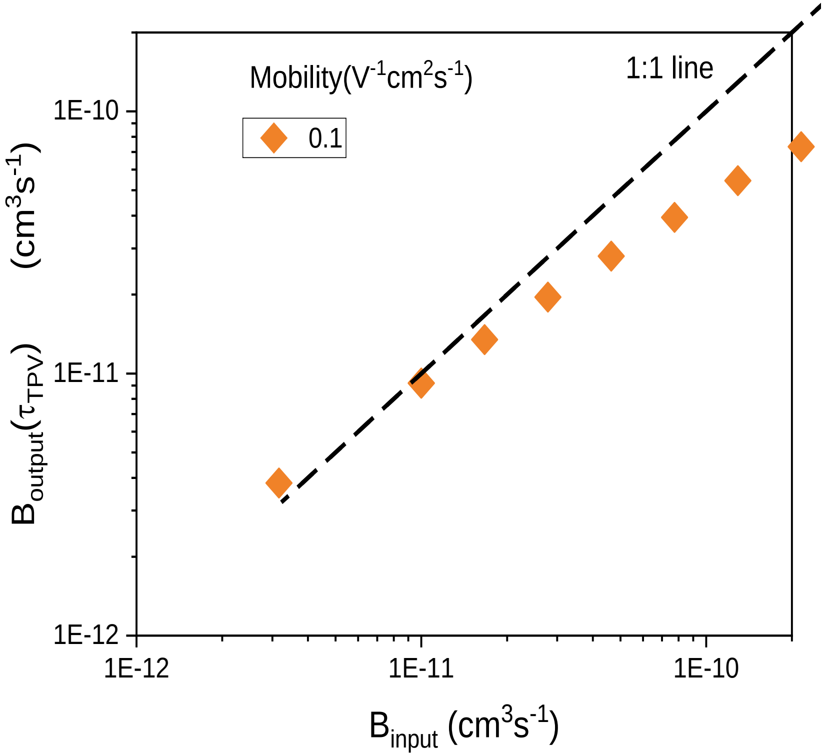
Download and contribute at:https://github.com/barnesgroupICL/Driftfusion

Imperial College London

EPSRC

Engineering and Physical Sciences Research Council

TPV and Recombination rate coefficient correlation



- In the small perturbation approach ($\Delta n \ll n_{Voc}$) :

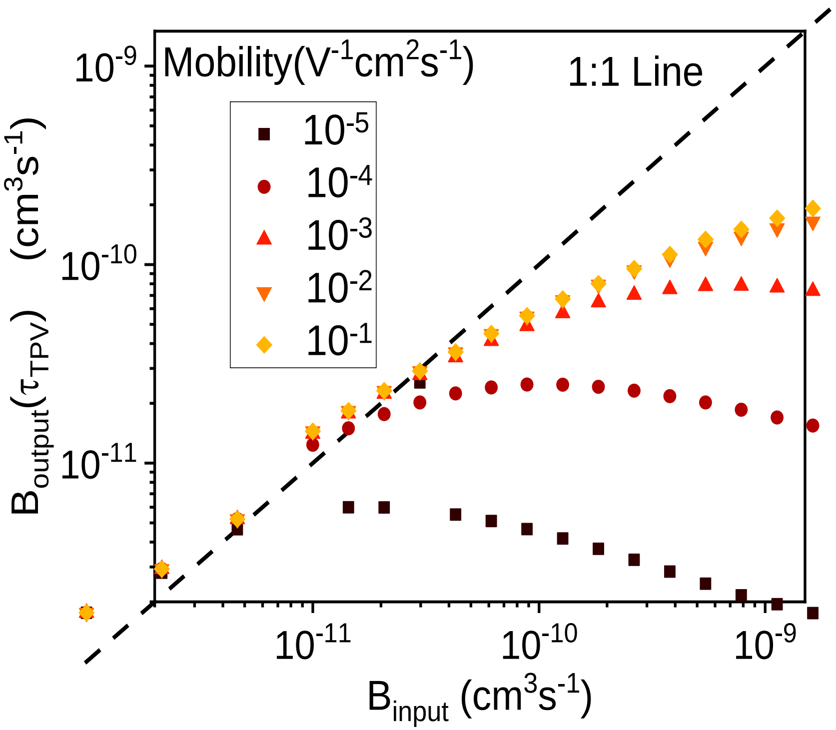
$$B_{\text{output}}(\tau_{\text{TPV}}) = \frac{1}{2\tau_{TPV} n_{V_{oc}}} \sim B_{input} \qquad ?$$

$n_{V_{oc}}$: is the excess charge in the device at open circuit under light intensity.

For High mobility devices and slow recombination the TPV lifetime is as expected

Mohammed Azzouzi, unpublished

TPV and Recombination rate coefficient correlation



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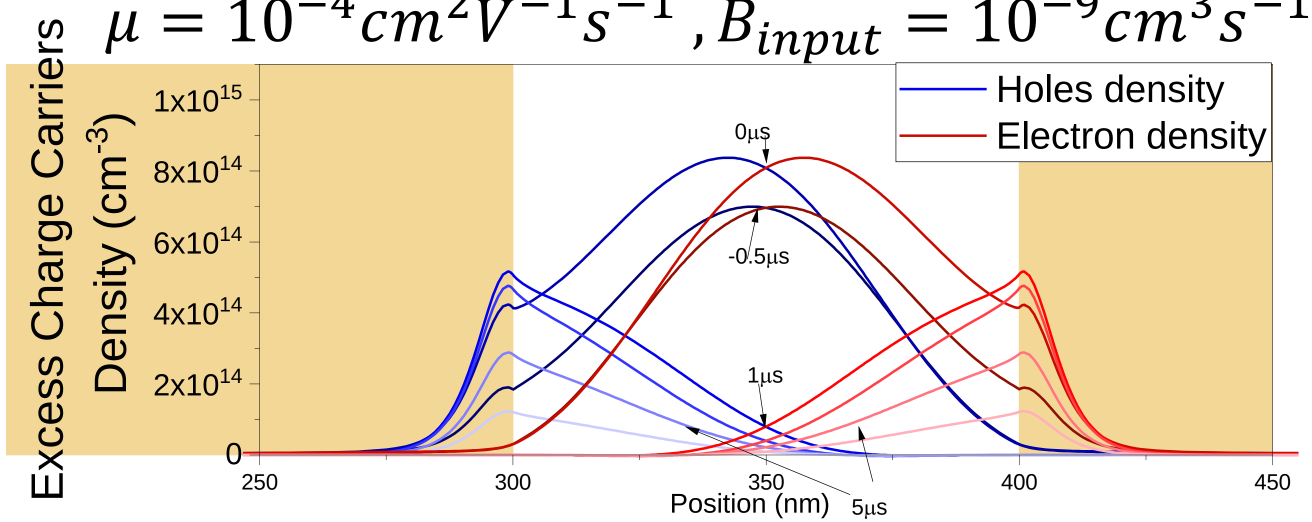
$n_{V_{oc}}$: is the excess charge in the device at open circuit under light intensity.

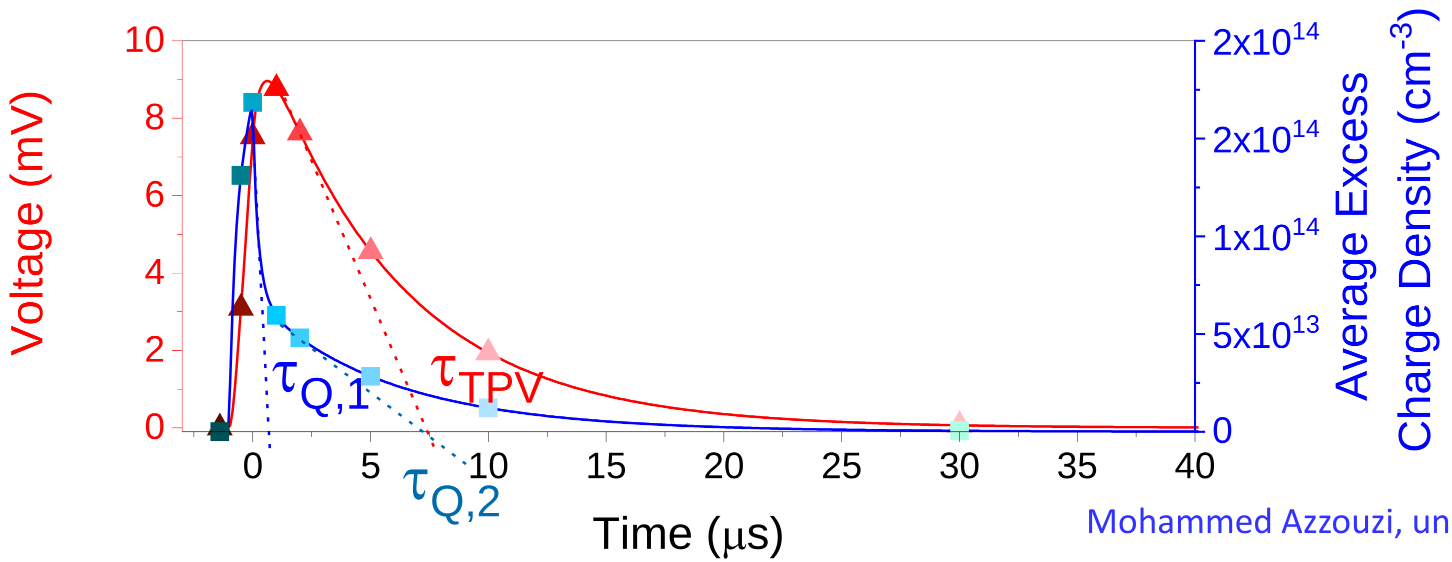
For Low Mobility devices the recombination rates extracted from TPV deviate from the expected value

Mohammed Azzouzi, unpublished

Simulated TPV Decay Differs from charge decay for low mobility or fast recombination

$$\mu = 10^{-4} cm^2 V^{-1} s^{-1}, B_{input} = 10^{-9} cm^3 s^{-1}$$





Mohammed Azzouzi, unpublished

Why is the TPV Decay Different from the charge decay?

$$u = 10^{-4} cm^2 V^{-1} s^{-1}, B_{input} = 10^{-9} cm^3 s^{-1}$$

Mohammed Azzouzi, unpublished

Do we need energy resolved device models?

HOME SCREENSHOTS DOWNLOAD EXAMPLES DONATE DOCUMENTATION

gpvdm

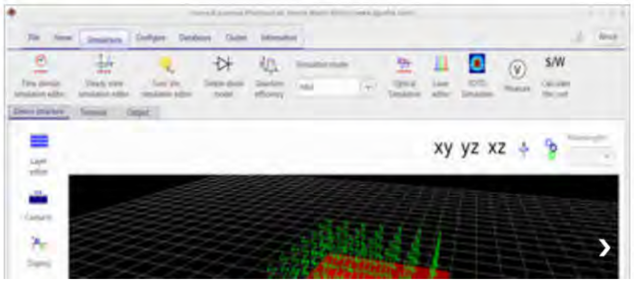
General-purpose Photovoltaic Device Model

DOWNLOAD

Simulate organic/Perovskite, Solar Cells, OFETs, and OLEDs for free!.

gpvdm is a cross-platform opto-electronic device simulation tool. It can simulate **organic solar cells**, OFET, OLEDs, Perovskite solar cells, and many other types of 1st, 2nd and 3rd generation solar cells. It contains both electrical model and optical models to produce accurate and predictive device simulations. The model can simulate the following types of devices out of the box:

- Organic solar cells (OPV devices)
- Perovskite solar cells - devices with mobile ions
- Organic LEDs (OLEDs)
- Organic Field Effect Transistors (OFETs)
- Crystalline silicon solar cells



www.gpvdm.com

Dr Rod MacKenzie, Nottingham University

Beyond the simple device model: energy resolved carriers

Gauss's Law

$$\nabla \epsilon_o \epsilon_r \cdot \nabla \phi = q \cdot (n - p)$$

Current driving terms

$$J_n = q \mu_e n \nabla E_c + q D_n \nabla n$$

$$J_p = q \mu_h p \nabla E_v - q D_p \nabla p$$

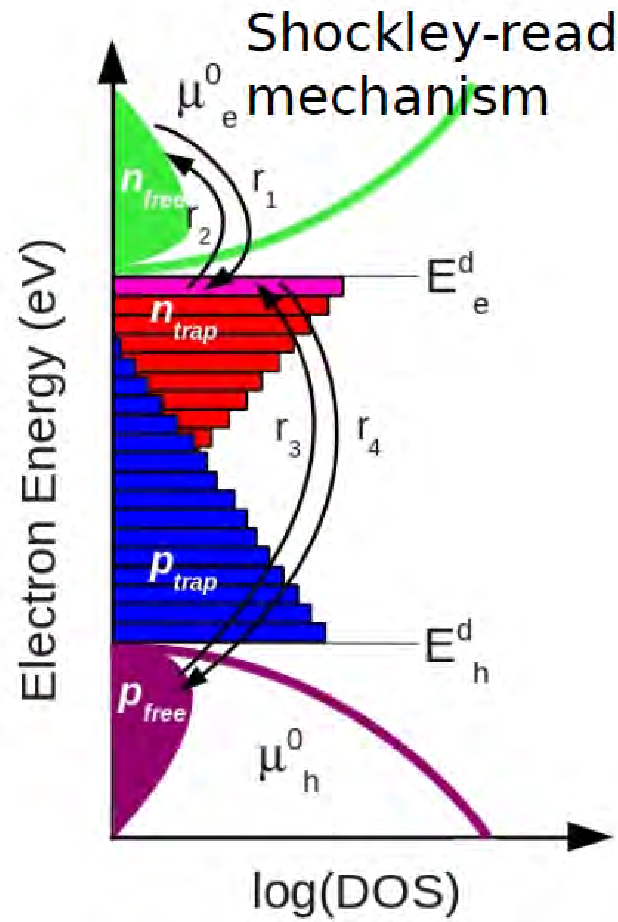
Current continuity equations

Electron continuity

$$\nabla \cdot \boldsymbol{J}_n = q \cdot \left(\sum_0^{n_{band}} (r_1^e - r_2^e) + \sum_0^{p_{band}} (r_3^h - r_4^h) + \frac{\partial n_{free}}{\partial t} \right)$$

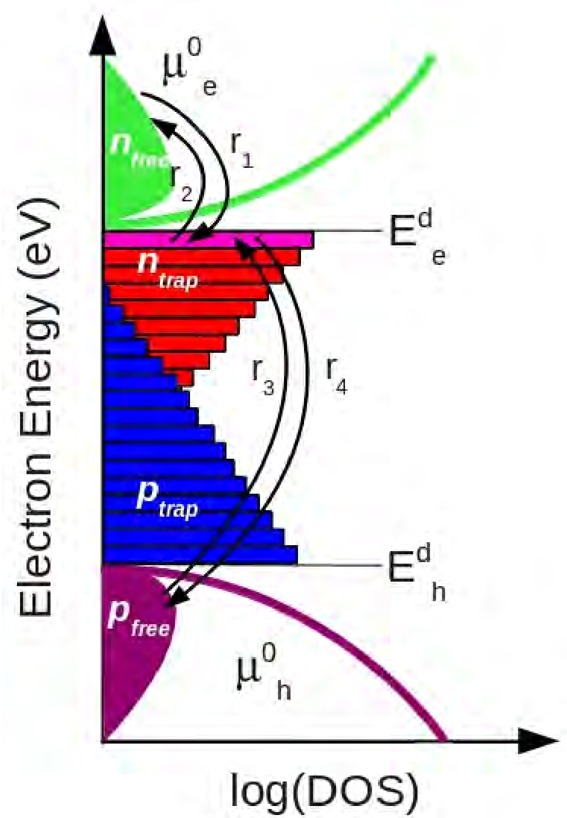
Hole continuity

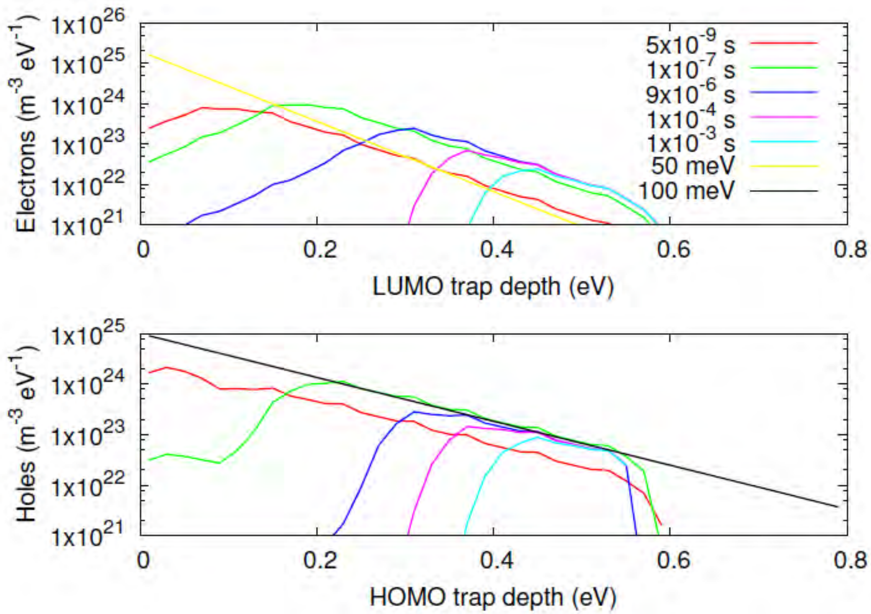
$$\nabla \cdot \boldsymbol{J}_p = -q \cdot \left(\sum_0^{n_{band}} (r_3^e - r_4^e) + \sum_0^{p_{band}} (r_1^h - r_2^h) + \frac{\partial p_{free}}{\partial t} \right)$$



Do we need energy resolved device models?

- Model allows to track the energy distributions of charges during transients
- Thermalisation appears to occur on comparable time scales to charge dynamics
- **Penalty for energetic disorder may be less severe than expected from shape of DoS!**





Rod MacKenzie et al., in review (2012)

Need experimental methods to probe charge energy distribut

Summary

- By making several simplifications (e.g. effective medium) OPV devices are modelled in steady state using traditional semiconductor device model approaches

- Important to include
  - sub-gap states (and recombination involving them)
  - (unintentional) doping
  - Interface barriers
  - Optical interference (sometimes)

- Most models do not include validated physical model for recombination coefficients or charge separation efficiency : these will be important when including spin dependent effects

- Transient models are sometimes necessary to relate observations to underlying physics