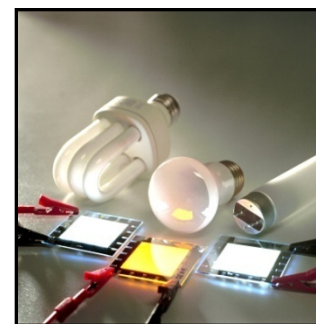# Numerical methods for the simulation of organic and anorganic semiconductor devices

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ECMI 2016, Santiago de Compostela, June 14, 2016

Beautiful Galicia region

(Punta Nariga)

Motivation for the work

- 30 years of experience in simulations in the electronics industry
  - Semiconductor device simulation
  - Electronic circuit simulation
  - Electromagnetics
- Models for organic devices (OLED) very similar to the models for 'normal' semiconductor devices
- **Our mathematical knowledge can be transferred to the OLED area!**
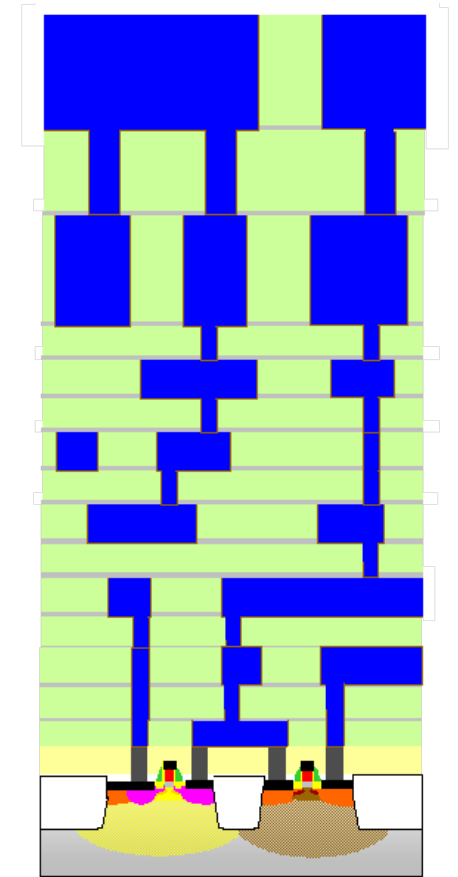
(Courtesy of NXP Semiconductors)

Survey of numerical methods for (anorganic) semiconductor devices

The drift-diffusion model

$$-\nabla \bullet (\varepsilon \nabla \psi) = q(p - n + D)$$

Poisson

$$q\frac{\partial p}{\partial t} = -\nabla \bullet J_p - qR$$

Cont.eqn. holes

$$q\frac{\partial n}{\partial t} = \nabla \bullet J_n - qR$$

Cont.eqn. electrons

Constitutive relations for current densities

$$J_p = -kT\mu_p \nabla p - q\mu_p p \nabla \psi$$

$$J_n = kT\mu_n \nabla n - q\mu_n n \nabla \psi$$

Model parameters

- *For realistic simulations, it is extremely important to have accurate models for the model parameters:*
  - *Mobility of holes and electrons*
  - *Recombination/generation*

$$r_{SRH} = \frac{n \cdot p - n_i^2}{\tau_p \cdot (n + n_i) + \tau_n \cdot (p + n_i)}$$

Singularly perturbed character of constitutive equations

The first-order differential equation involving current density is singularly perturbed:

$$\frac{kT}{qE_{max}}\nabla n - \frac{\nabla \psi}{E_{max}}n = \frac{J_n}{\mu_n n E_{max}}$$

Small when E large

O(1)

▸ **Special discretisation scheme needed: Scharfetter-Gummel scheme**

The Scharfetter-Gummel scheme is based on physical insight. It is related to the rule for adding resistances:

$$\frac{1}{R_{total}} = \sum_i \frac{1}{R_i}$$

Maths derivation of S-G scheme

Consider: $-(a(x)u'(x))' = 0$ Then: $a(x)u'(x) = C$

Hence

$$u(x_{i+1}) = u(x_i) + C\int_{x_i}^{x_{i+1}} (a(s))^{-1} ds$$

This can be rewritten as

$$H(a;[x_i, x_{i+1}])\frac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i} = C$$

where H is the harmonic average:

$$H(a;[x_i, x_{i+1}]) = \left[\frac{1}{x_{i+1} - x_i} \int_{x_i}^{x_{i+1}} (a(s))^{-1} ds \right]^{-1}$$

Some striking observations

<u>Striking fact:</u> S-G is the same as the well-known exponentially fitted scheme developed by Il'in! This follows from:

$$H(e^{-q(s)};[x_i,x_{i+1}]) = \frac{q(x_{i+1}) - q(x_i)}{e^{-q(x_{i+1})} - e^{-q(x_i)}}$$

**<u>Even more striking:</u> both schemes were published in 1969!**

Relation to multigrid

▸ Consider the following discrete scheme for a 2nd order SP equation:

$$-\varepsilon \sigma_i^h \frac{u_{i+1}^h - 2u_i^h + u_{i-1}^h}{h^2} + a\frac{u_{i+1}^h - u_{i-1}^h}{2h} = f_i$$

▸ Write down the same discretised equation of a fine grid, with spacing h/2:

$$-\varepsilon \sigma_i^{h/2} \frac{u_{i+1/2}^{h/2} - 2u_i^{h/2} + u_{i-1/2}^{h/2}}{(h/2)^2} + a\frac{u_{i+1/2}^{h/2} - u_{i-1/2}^{h/2}}{2.(h/2)} = f_i$$

▸ Eliminating the fine points leads to an alternative discrete scheme on coarse grid
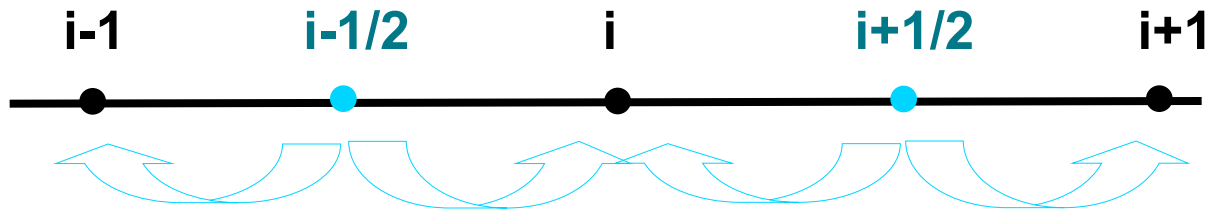
▸ Assuming that <u>fine grid</u> solution and <u>coarse grid</u> solution coincide at coarse grid points leads to a **functional relation** between σ_i^h and $\sigma_i^{h/2}$
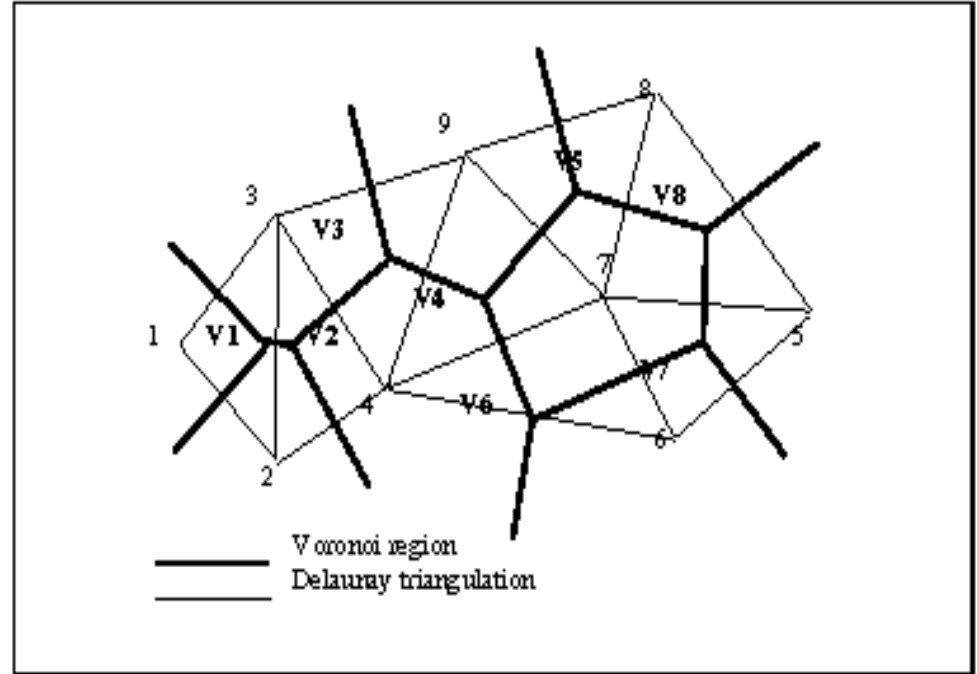
➡ **Il'in/Scharfetter-Gummel!**

Finite volume method

We developed software for arbitrary semiconductor devices using:
- finite volume method
- exponentially fitted expressions for current densities
- Delaunay triangulations with Voronoi polygons

Voronoi region
Delaunay triangulation

- **provably positive carrier concentrations and maximum principles due to Delaunay properties (homogeneous problems)**
- **special quadrature needed to guarantee stable solutions (inhom.)**
- **current conservation guaranteed by virtue of finite volume method**

Mimetic discretisation methods are crucial!

Nonlinear solution techniques: Correction transformation

▸ **Based on previous observations, we developed a new method: CT**

▸ **Idea simple: use nonlinear variable transformation, and perform Newton's method in new variable** $e^{40x} - 1 = 0 \rightarrow y - 1 = 0$

▸ **Let u be original variable, and problem to be solved:** $F(u) = 0$

▸ **Define new variable v=v(u), u=u(v):** $0 = F(u(v)) \equiv G(v)$

▸ **Then:** $\nabla_u F(u) = \nabla_v G(v(u)) \nabla_u v(u)$ **so that**

$$dv^k = \nabla_u v(u^k) du^k$$

CT algorithm

1. **Choose initial guess u^0, and set $k=0$**

2. **Evaluate du^k by solving linear system**   ← **Linear system in u**

3. **Transform correction to dv^k**

4. **Construct $v^{k+1}=v^k+dv^k$**   ← **Nonlinear system in v**

5. **Solve $v(u^{k+1})=v^{k+1}$ for u^{k+1}**

6. **No convergence, go to 2. Otherwise stop.**

Transformed correction $Du^{k+1}=u^{k+1}-u^k$

- *Method very effective for the extremely nonlinear device problems*

- *Additional advantage: different variables can be used for solution of linear and nonlinear systems (condition number of linear systems!)*

# Alternative solution method

▸ **Drawback of Newton's method:**
  – **Properties of off-diagonal blocks unknown**

$$\begin{pmatrix} \partial F_{\psi}/\partial \psi & \partial F_{\psi}/\partial p & \partial F_{\psi}/\partial n \\ \partial F_{p}/\partial \psi & \partial F_{p}/\partial p & \partial F_{p}/\partial n \\ \partial F_{n}/\partial \psi & \partial F_{n}/\partial p & \partial F_{n}/\partial n \end{pmatrix}$$

▸ **Much more attractive: nonlinear block Gauss-Seidel**
  – **Diagonal block of Poisson equation symmetric positive definite (CG!)**
  – **Diagonal blocks of 2nd and 3rd equation positive definite**

▸ **Known as Gummel's method**
  – **Based on fixed point algorithm, also used to prove existence of solutions**
  – **Many versions, only 1 based on mathematical theory**

Convergence of Gummel's method can be quite slow
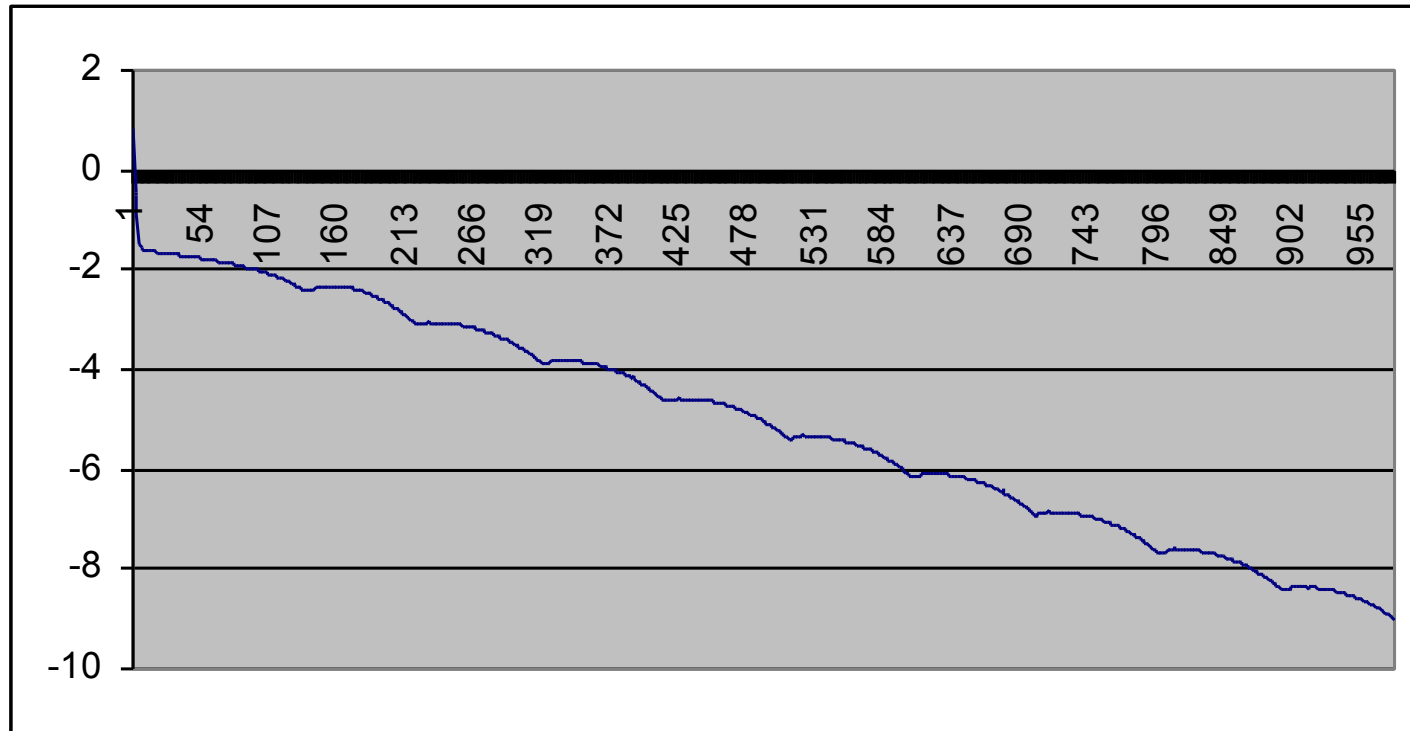
# Idea: vector extrapolation

- **Published in the early '90s**

- **Survey paper by Sidi, Ford and Smith (1986), book by Brezinski & Redivo Zaglia**

- **Extensive work by Avram Sidi on**
  - **Minimal polynomial extrapolation (MPE)**
  - **Reduced rank extrapolation (RRE)**

- **Both MPE and RRE:**
  - **Matrix free**
  - **Only need to know action of operator**
  - **For linear problems equivalent to CG resp. GMRES**

$$\psi^k \longrightarrow \phi_p^k \longrightarrow \phi_n^k \longrightarrow \psi^{k+1}$$

F
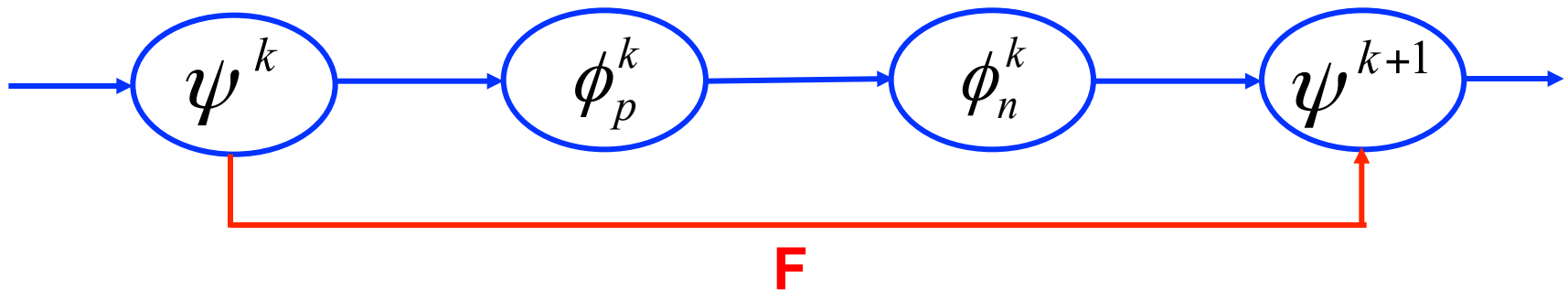
Convergence of vector extrapolation for LDDMOS transistor

Voltage	Gummel	RRE(1)	RRE(2)	RRE(5)
1	159	149	130	70
2	220	210	153	105
3	197	124	110	92
4	131	101	103	94
5	130	85	98	86

Behaviour of RRE(5)
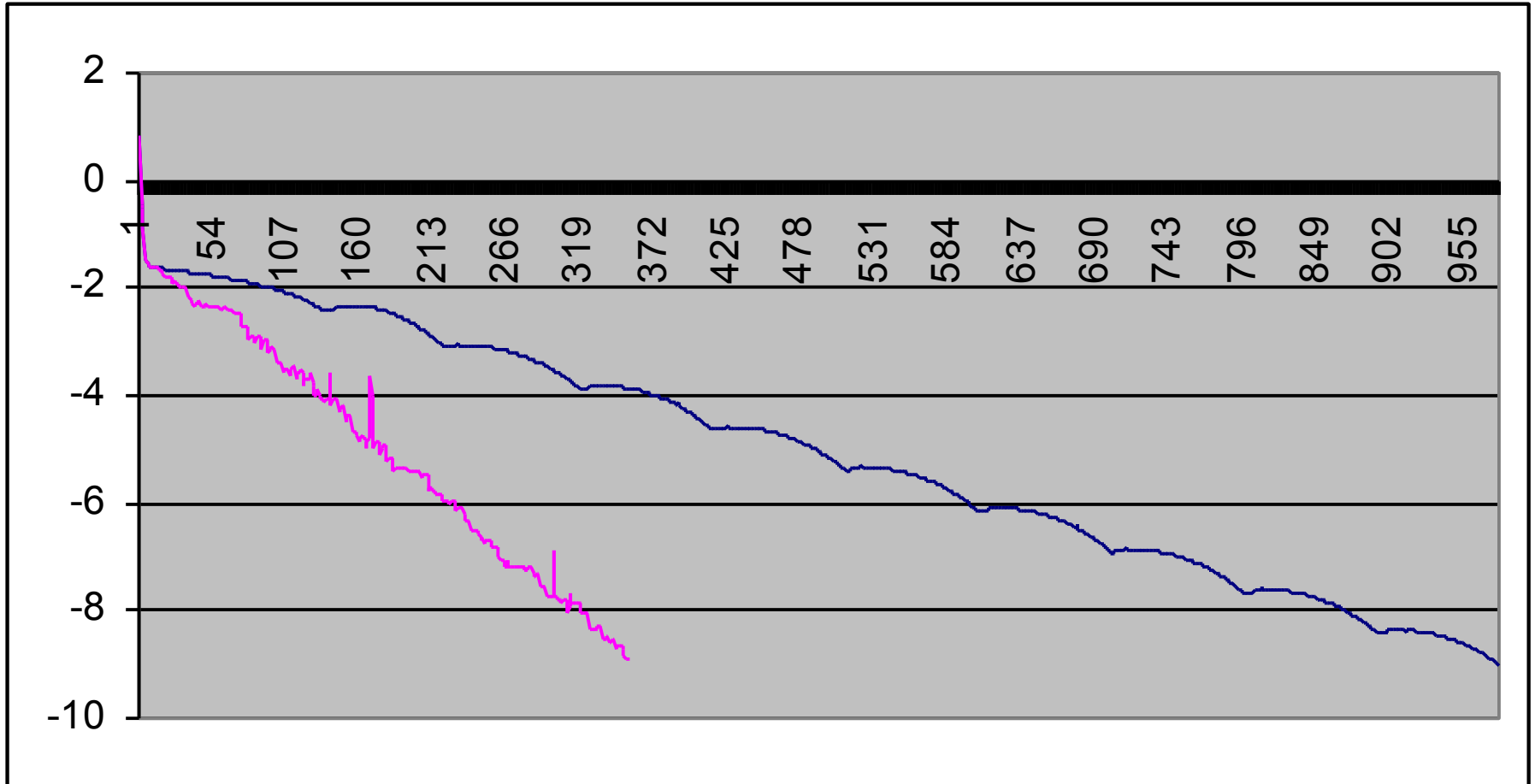
Remarks

▸ **Semiconductor device simulation using the drift-diffusion model is a very mature field, by virtue of numerical analysis**

▸ **Discretisation and solution require very sophisticated algorithms**
 – **Singularly perturbed**
 – **Rapidly varying solutions (range: $0-10^{20}$)**
 – **Extremely nonlinear**

▸ **Different story for extended models, such as the Hydrodynamic Model and others**

▸ **Surprisingly, all of the methods developed can be readily applied to a new field that is becoming very important in industry: OLED simulation (OLED = organic LED)**

HE SHOUTED OUT ABOUT SOME NEW INVENTION & THEN THAT THING HIT HIM!

DeepFat '09
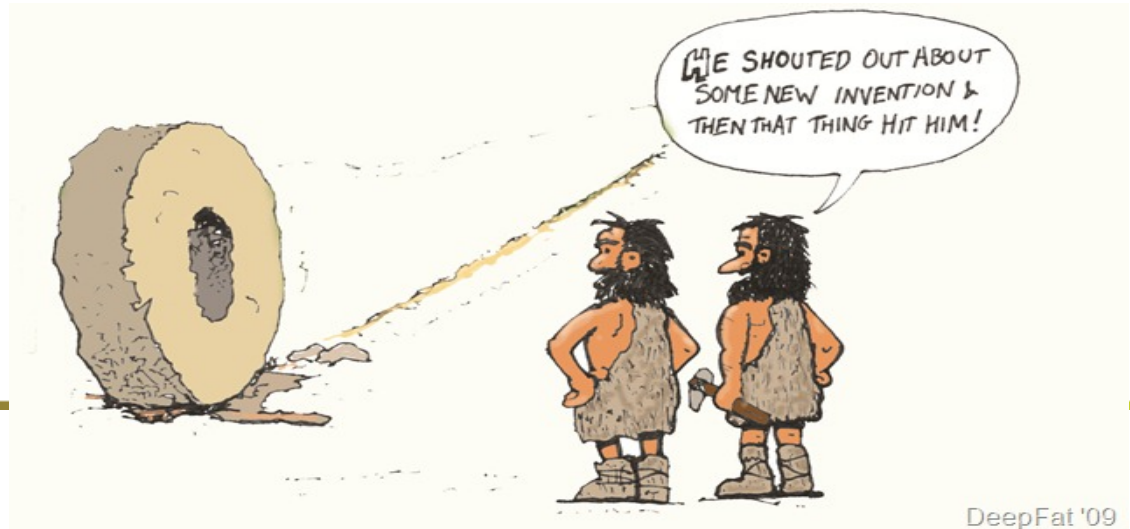
Short recap about OLEDs

About OLED
organic light-emitting diode

Windows that light-up at dark
It is true, this could be possible with OLED. This is because organic light emitting diodes can be transparent. A window could act as a normal window at day, but at night it can be used as a light resource. This vision can replace the boring old bulb in the middle of every room. It is getting even better: nearly every surface can become a lighting source. It does not matter if it's curved or flat - OLED sheets are flexible and ultra-flat.

OLED television
OLED TVs can already be bought, OLED has high potential to make it in common tv screens in the future. Why? The answer is simple: Organic LED are ultra-flat, very bright and consume less power. OLEDs can even become cheaper to produce than traditional LCDs. Right now, the opposite is the case, but it's theoretically possible.

OLEDs for lighting applications

White light

luminous efficacy [lm/W]

fluorescent

White LED

White OLED

incandescent

Year
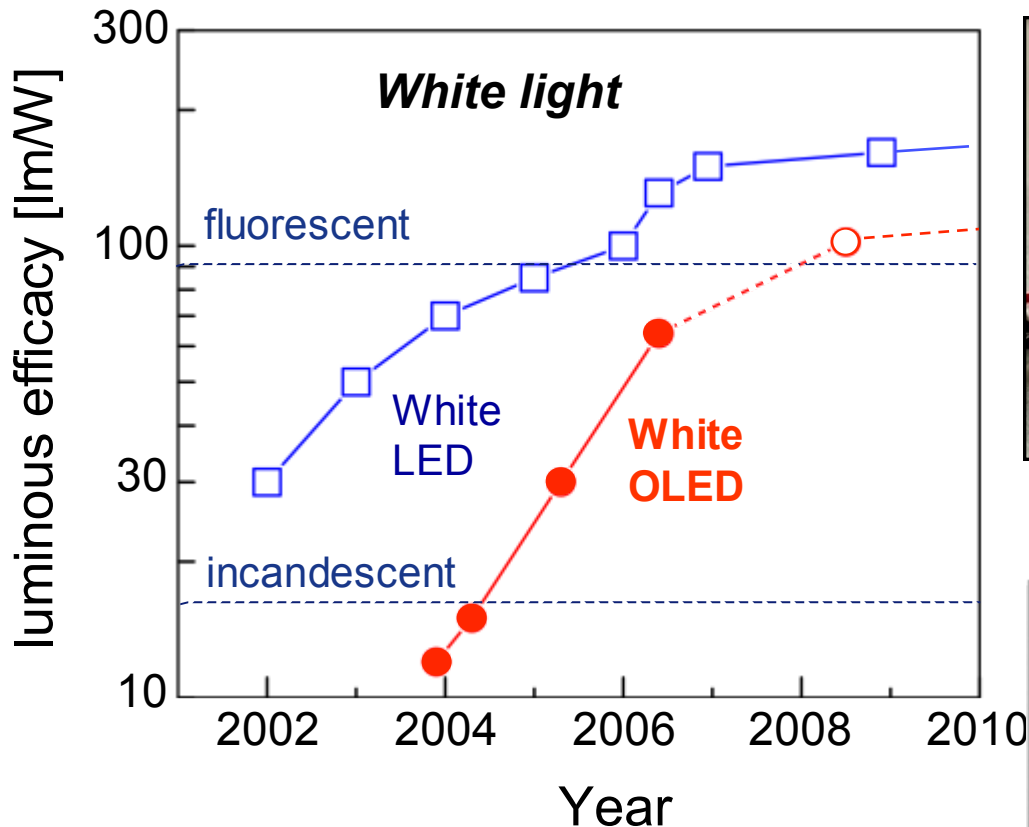
Large annual increase of the luminous efficacy of OLEDs.
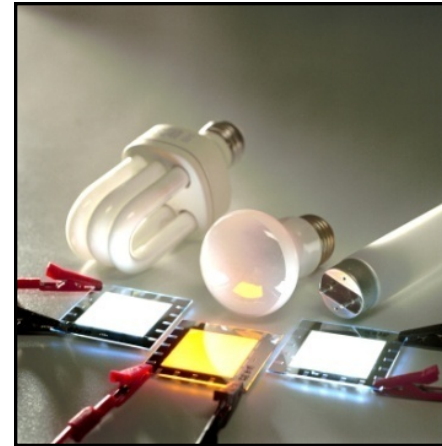
Efficient, ultra thin, flexible, transparent, color tunable.

*First products (Philips Lumiblade).*

Create with Lumiblade

www.lumiblade.com

OLED characteristics

- In OLEDs, use is made of organic semiconductors, based on small molecules or polymers, that have a disordered structure
  - Recent theoretical studies have indicated that disorder can give rise to lamentary current threads. However, the full consequences of disorder on relevant processes and device performance are not fully understood.

- Light is generated as a result of radiative recombination of electrons and holes in an organic semiconductor layer.

- The organic materials used in OLEDs are amorphous semiconductors, within which the electrons and holes move by "hopping" between neighbour molecules, of which the energy levels are randomly distributed.

OLED behaviour

- An organic light-emitting diode basically consists of one or more thin (10 -100 nm) organic semiconductor layers sandwiched in between two electrodes on top of a transparent substrate
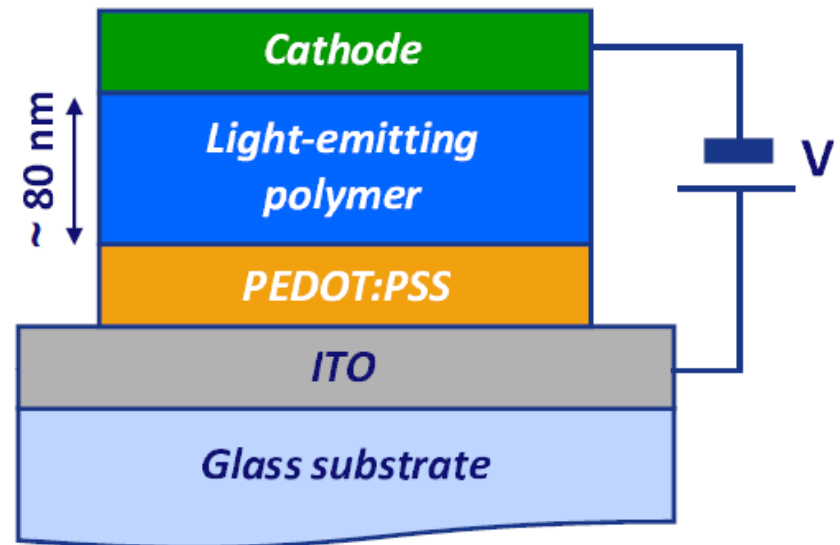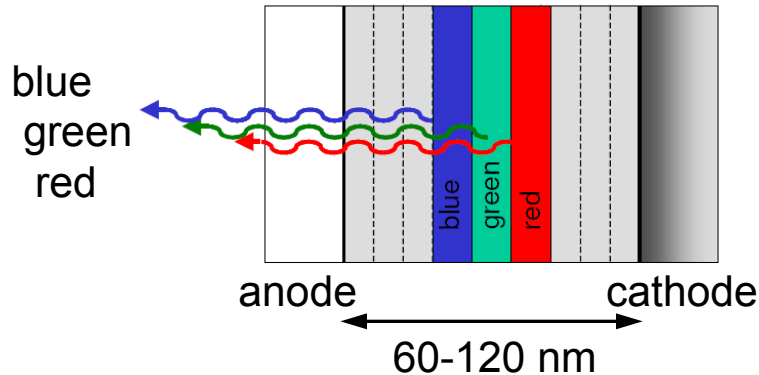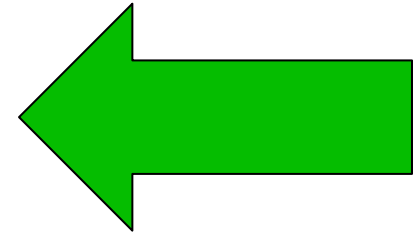
OLED behaviour (2)

- When a bias voltage V is applied that is larger than the built-in voltage, holes are injected into the light-emitting polymer layer from the transparent bottom electrode and electrons are injected from the cathode.
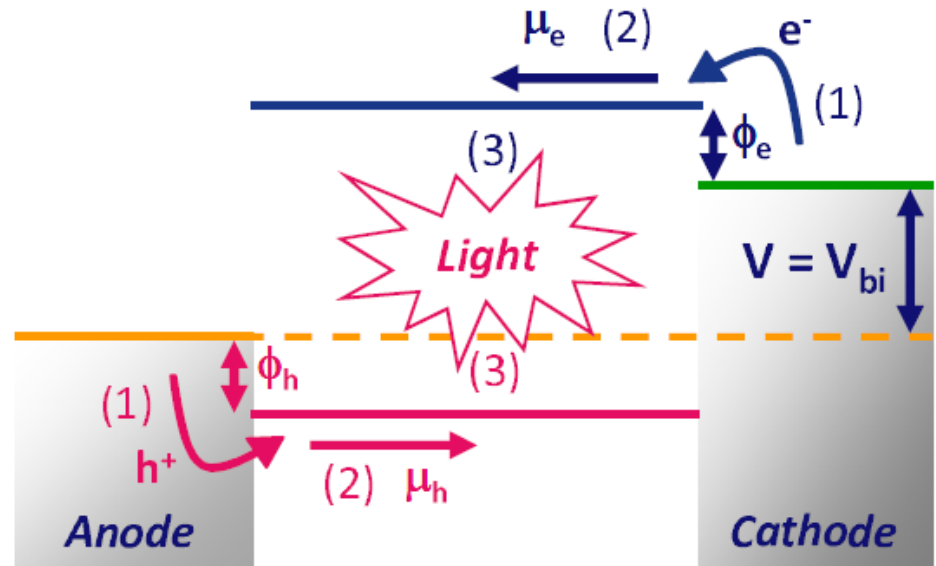
OLED device modeling needed

Typical structures of state-of-the-art OLEDs

blue
green
red

anode   cathode

60-120 nm

anode   cathode

150-200 nm
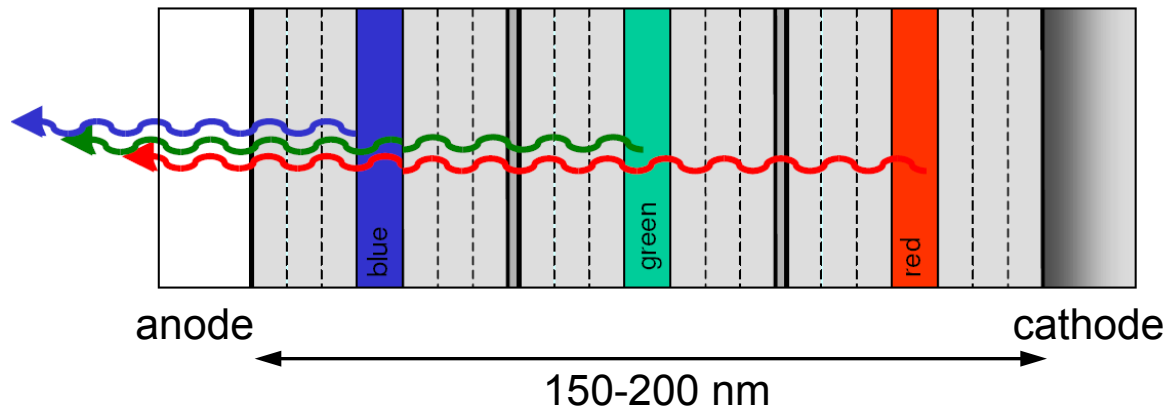
OLEDs have today **complex layer structures**.

Rational and fast OLED design no longer possible without an experimentally validated model. **Not yet available.**

OLED modeling

Understanding OLED's

- Understanding the functioning of OLEDs is for many reasons quite challenging, especially due to the disordered nature of the active organic materials.

- The disorder in the active organic materials in OLEDs originates from an irregular packing of the molecules, which are deposited either from solution, e.g. via spin-coating, or via evaporation techniques.

- For polymers the disorder also originates from the distribution of chain lengths (polydispersity) and twists, kinks or defects in the polymer chains.

- This disorder strongly affects the local HOMO and LUMO energies in such materials, and the local energy gap.

- In the end, this leads to *energetic disorder.*
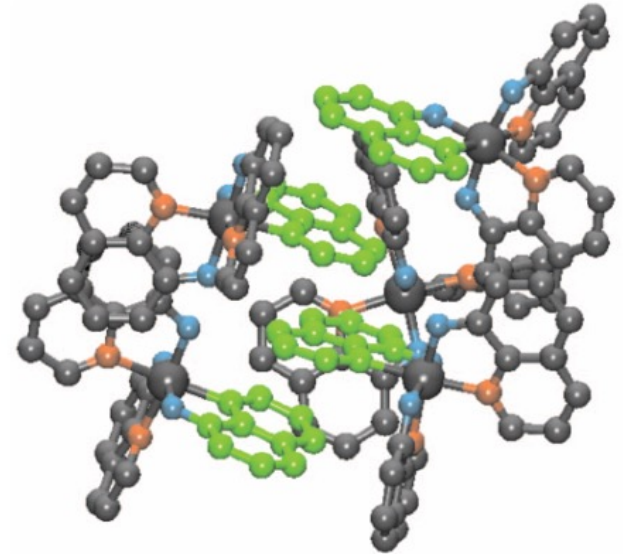
OLED device modelling – approach chosen

Calculation **light outcoupling**

Calculation **exciton** diffusion and radiative decay

Calculation **current density and recombination profile**

Calculation **mobility** in disordered materials

Calculation jump rates between two molecules

Calculation amorphous structure

Advanced Experimentally Validated Integrated OLED Model

EU-project AEVIOM, 9 partners
www.aeviom.eu

1. **3D-supercomputer calculations**, including energetic disorder, but neglecting molecular details.

2. 3D$\rightarrow$1D "translation".

3. **Experimental validation**.

4. Fast **commercial software**.

5. Research and business **applications**

Systematic study of transport physics
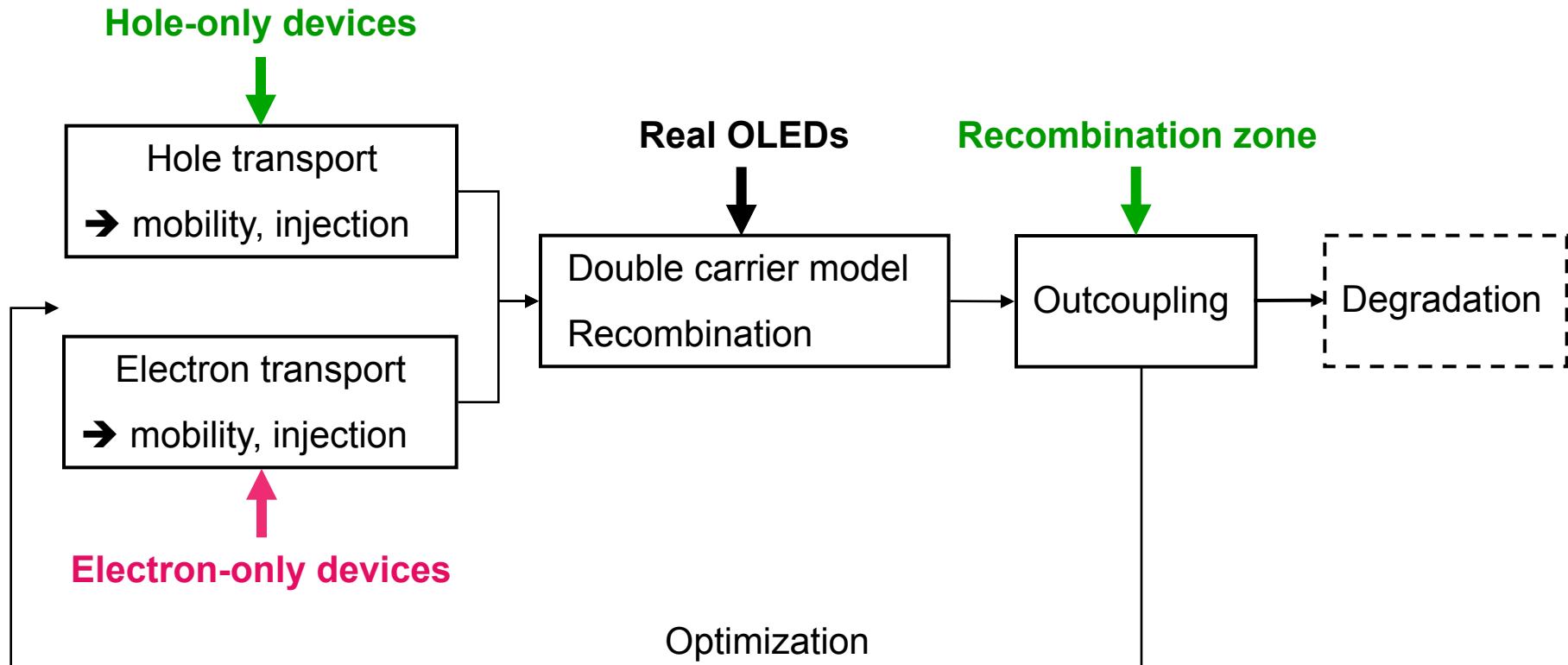
"First generation" OLED models

Smith et al. (1996), Blom (1997), Campbell Scott (1999), Staudigel (1999), Zuppiroli et al. (2002).

- Current density **laterally uniform** (pseudo-1D model).

- Often used **empirical mobility function:**

$$\mu(F,T) = \mu_0(T) \exp\left(\gamma(T)\sqrt{F}\right)$$

Poole-Frenkel field (F) dependence

$$\mu_0(T) = \mu^* \exp\left(-\frac{\Delta}{k_B T}\right)$$

Polaron hopping
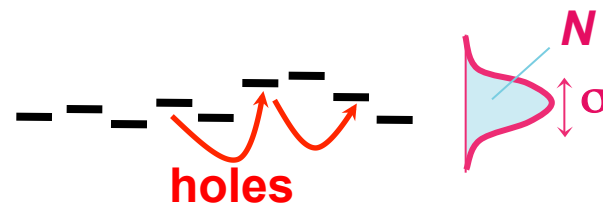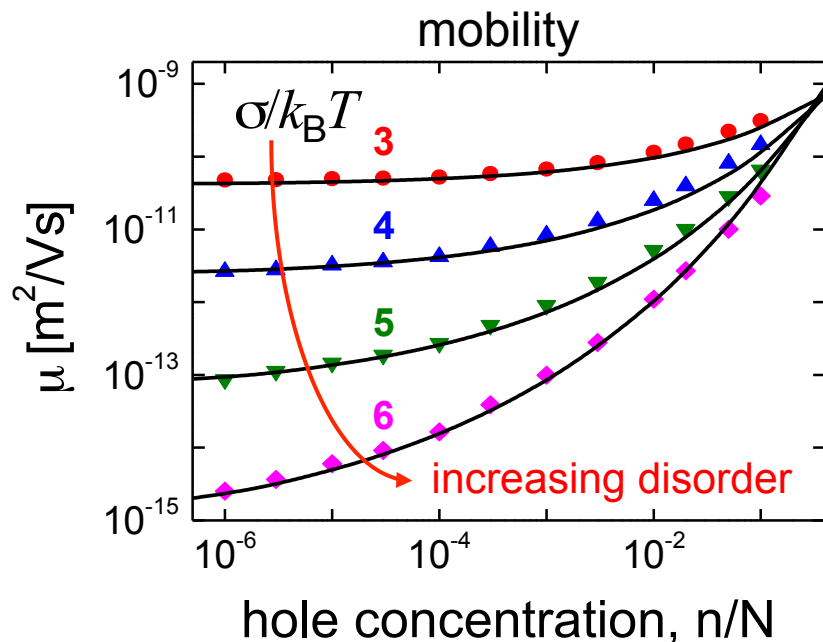(Δ related to the polaron binding energy)

$$\mu_0(T) = \mu^* \exp\left[-C\left(\frac{\sigma}{k_B T}\right)^2\right]$$

Gaussian Disorder Model (Bässler, 1993)
(σ is the width of the density of states; $C \approx 0.44$)

Intensive debate about the validity:
disorder or polarons, injection, PF factor?

Central concept in 1D-models: mobility

mobility

σ/k_BT

3
4
5
6

increasing disorder

μ [m^2/Vs]

hole concentration, n/N

holes

N

σ

Disorder → **strong carrier density dependence of the mobility**.

Type of disorder important, and material dependent:
- Extended Gaussian Disorder Model (**EGDM**) – no spatial correlations
  Pasveer *et al.*, Phys. Rev. Lett. (2005).
- Extended Correlated Disorder Model (**ECDM**) – spatially correlated disorder.
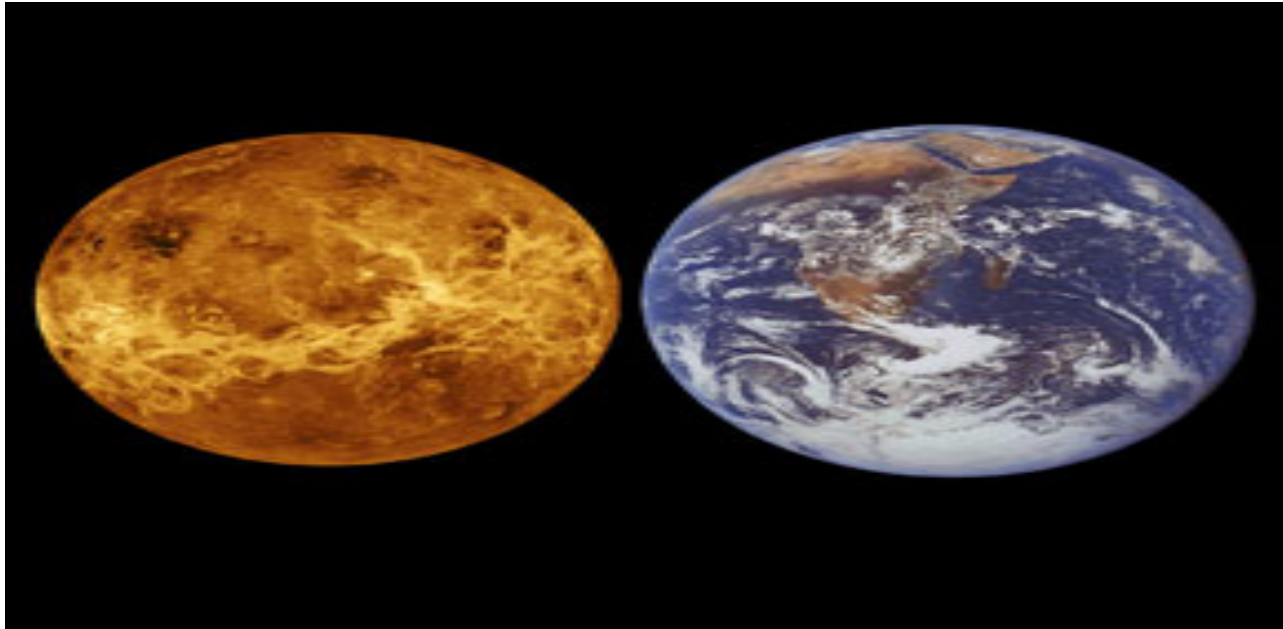 Bouhassoune *et al.,* Organ. Electr. (2009).

Blue OLEDs: model versus experiment

current

20 °C

T = - 60 °C

light emission
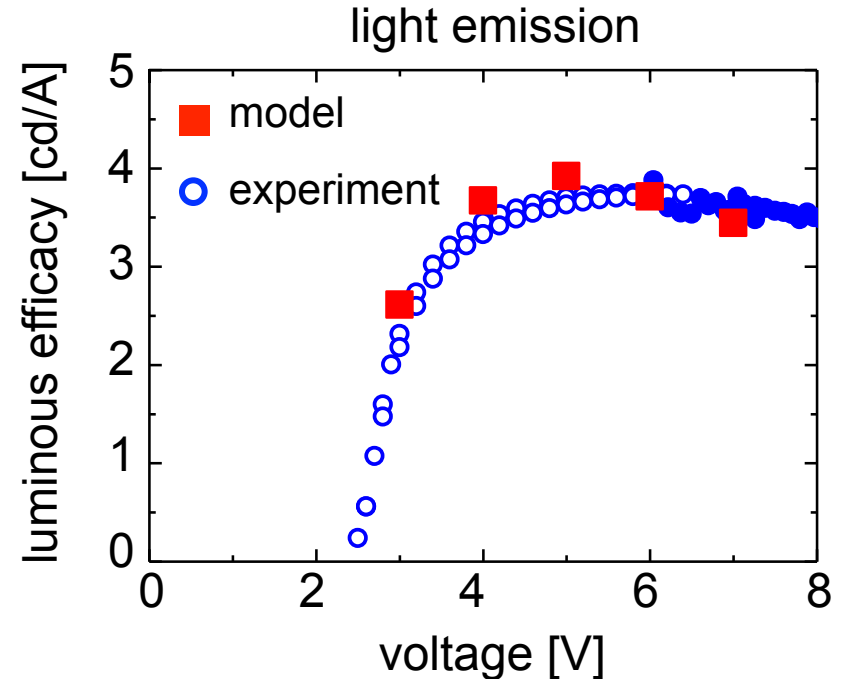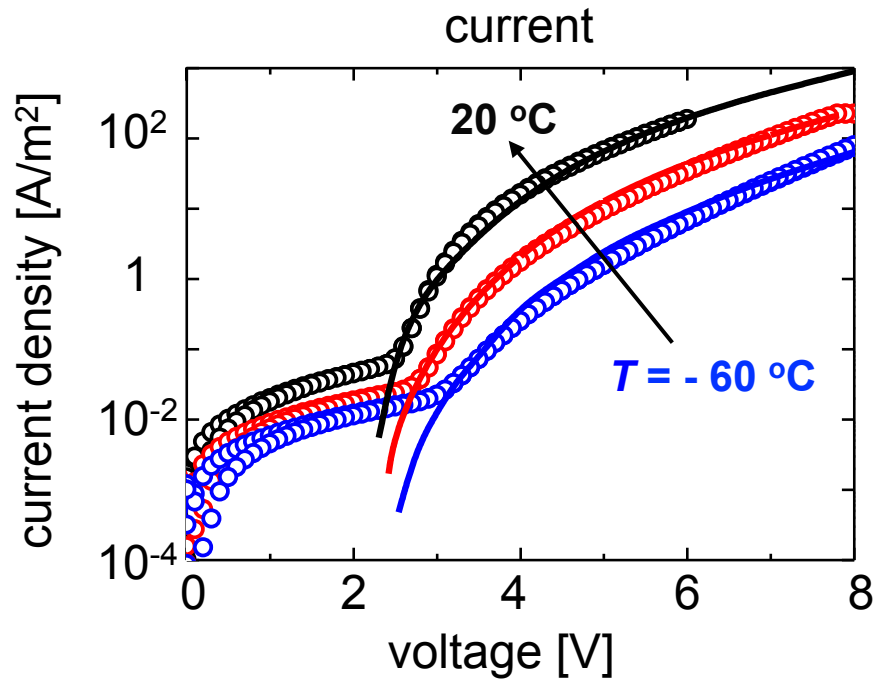
- model
- experiment

- **No (new) parameters.**
- For the first time: demonstration that **predictive OLED modeling is possible**.

Numerical simulation of OLED devices

Two different worlds

Developers of numerical methods for OLED simulation
•Started all over again
•Did not use the extensive experience available for 'normal' devices
•There are differences, but one should build upon existing knowledge!

Transport model

For OLED simulation, we can use the well known drift-diffusion model that is also used for anorganic ("normal") semiconductors:

$$\nabla \cdot (\epsilon \nabla \psi) = q(n_f + n_t - p_f - p_t)$$

$$\nabla \cdot J_n - q\left(\frac{\partial n}{\partial t}\right) = qR(n_f, p_f),$$

$$\nabla \cdot J_p + q\left(\frac{\partial p}{\partial t}\right) = -qR(n_f, p_f),$$

with the constitutive equations

$$J_n = -qn_f\mu_n \nabla \psi + qD_n \nabla n_f,$$

$$J_p = -qp_f\mu_p \nabla \psi - qD_p \nabla p_f.$$

Mobility and R much different for organic structures!!!

CA SA

TU/e

Mobility for organic semiconductors

In the EGDM model, the mobility may be expressed as a product of a density-dependent and field-dependent function:

$$\mu(T, p_f, F) = \mu_0(T) g_1(p_f, T) g_2(F, T)$$

These functions are nonlinear and strongly increase with larger values of the disorder parameter.

It is also accepted that a different form of the Einstein relation is needed to relate mobility and diffusivity:

$$D = \frac{kT}{q} \mu(T, p_f, F) g_3(p_f, T)$$

Carrier dependent mobility is not encountered in anorganic devices!

Validity of numerical methods???

CA SA

TU/e

Mathematical analysis

- Poisson equation is elliptic and also singularly perturbed, the small parameter corresponding to the Debye length of the device
- The constitutive relations for the current densities can be viewed as first order equations for the carrier concentrations, and are singularly perturbed

$$-qn_f\mu_n \nabla \psi + qD_n \nabla n_f = J_n$$

$$-qp_f\mu_p \nabla \psi - qD_p \nabla p_f = J_p$$

- In this case, the small parameter depends on the inverse of the electric field
- Carrier concentrations are positive: can we prove this for the OLED models?

Mathematical analysis (2)

- For the anorganic case, Markowich and Mock have set up a theory to prove existence of solutions, requiring monotonicity for mobility and recombination
- The proof makes use of fixed point theorems:
  - Start from a given electric potential
  - Solve for hole concentration using new potential and old electron concentration
  - Solve for electron concentration using new potential and new hole concentration
  - Determine a new potential from the new concentrations
  - The mapping defined maps the "old" potential to the "new" potential
- This process converges under certain assumptions
- **A similar result for OLEDs is not available!!!**

Important!

- It is important to set up such mathematical theory
- For semiconductor device simulation, we have derived conditions on the mobilities in order to guarantee solutions
- A model constructed by the electronic engineers did not satisfy these conditions, and also failed to give solutions (monotonicity violated)

Discretisation

- When discretising, meshing is not a problem: rectangular, triangular (Delaunay)

- However, the singularly perturbed character urges us to use exponentially fitted difference schemes that are based on asymptotic expansions

- Such schemes can also be constructed using the method of harmonic averaging

- The schemes are often known as:

  - Il'in difference scheme (*mathematics*)

  - Scharfetter-Gummel scheme (*solid state physics*)

Scharfetter-Gummel scheme

$$j_{i+\frac{1}{2}} = -D\frac{\partial n}{\partial x} + vn(x)$$

- Multiply by integrating factor

$$j_{i+\frac{1}{2}}e^{-v(x-x_i)/D} = \left(-D\frac{\partial n}{\partial x} + vn\right)e^{-v(x-x_i)/D},$$

$$= -D\frac{\partial}{\partial x}\left(ne^{-v(x-x_i)/D}\right).$$

- Integrate

$$\int_{x_i}^{x_i+\Delta} j_{i+\frac{1}{2}}e^{-v(x-x_i)/D}\, dx = -D\int_{x_i}^{x_{i+1}} \frac{\partial}{\partial x}\left(ne^{-v(x-x_i)/D}\right)dx,$$

$$j_{i+\frac{1}{2}}\int_0^\Delta e^{-vx'/D}\, dx' = -D\left(ne^{-v(x-x_i)/D}\right)\Big|_{x_i}^{x_{i+1}},$$

$$j_{i+\frac{1}{2}}\frac{D}{v}\left(e^{-v\Delta/D} - 1\right) = D\left(n_i - n_{i+1}e^{-v\Delta/D}\right).$$

- Hence

$$j_{i+\frac{1}{2}} = v\frac{n_i - e^{-v\Delta/D}n_{i+1}}{1 - e^{-v\Delta/D}}$$

For OLED model???

- Carrier-dependent mobility can be used in Scharfetter-Gummel scheme
- However: the character of the underlying differential equation has dramatically changed due to carrier dependence of mobility
- Probably, SG is NOT correct for this equation
- **We need a thorough asymptotic analysis of the OLED model equations!**

Nonlinear solution procedures

1. **Full Newton method**
   - Need good initial guess, often based on asymptotic expansions
   - Often divergence due to bad initial guess
   - Matrix properties not known
2. **Sequential method** ("Gummel method", nonlinear block Gauss-Seidel)
   - Converges virtually always (if potential updates suitably restricted)
   - Matrix properties very favourable (only diagonal blocks)
   - Convergence acceleration possible using **Reduced Rank Extrapolation** (this can save many iterations!)
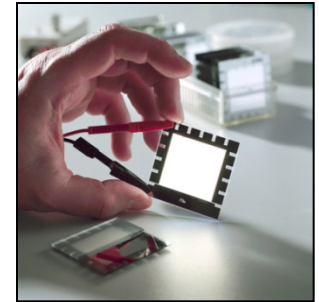   - Mimics behaviour of fixed point mapping

Validation of numerical approach
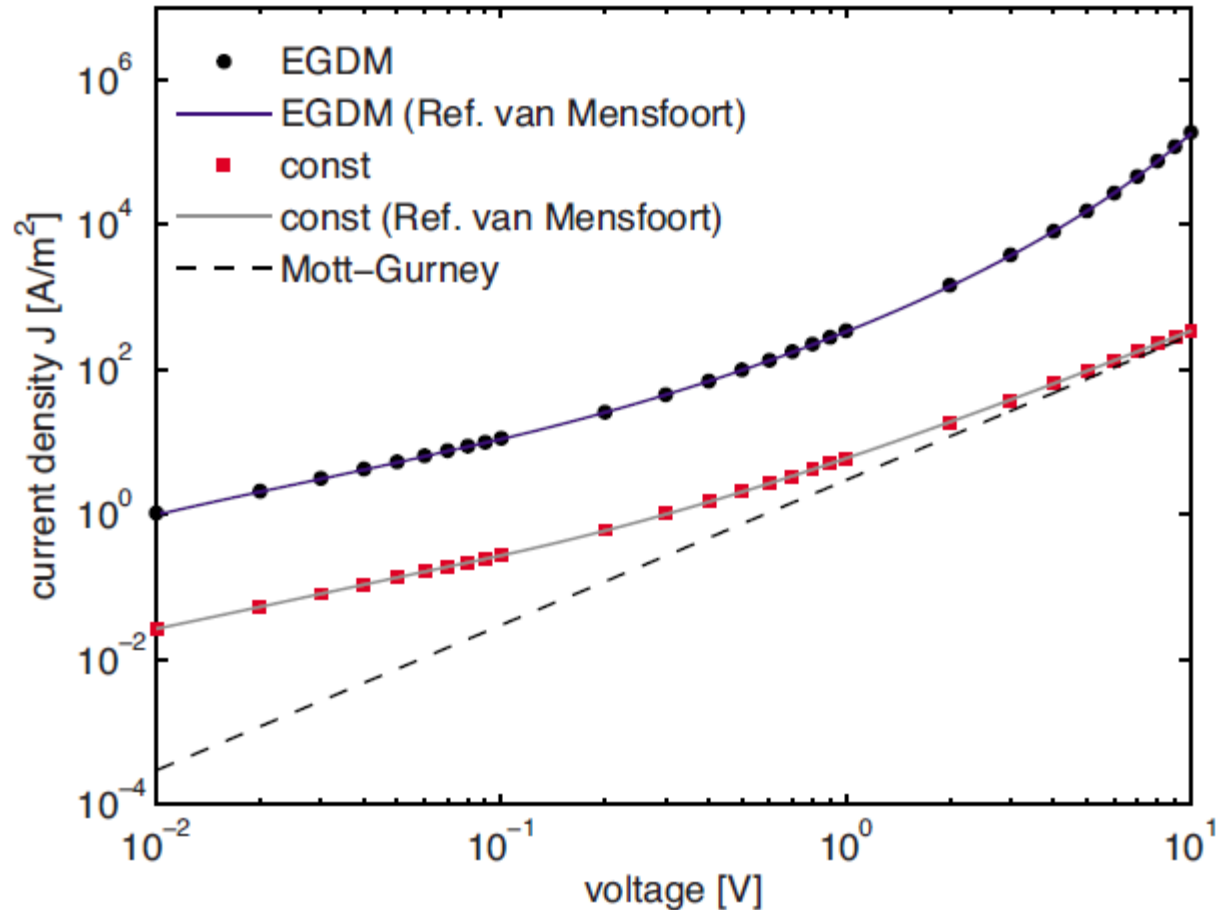
Comparison of Newton & Gummel
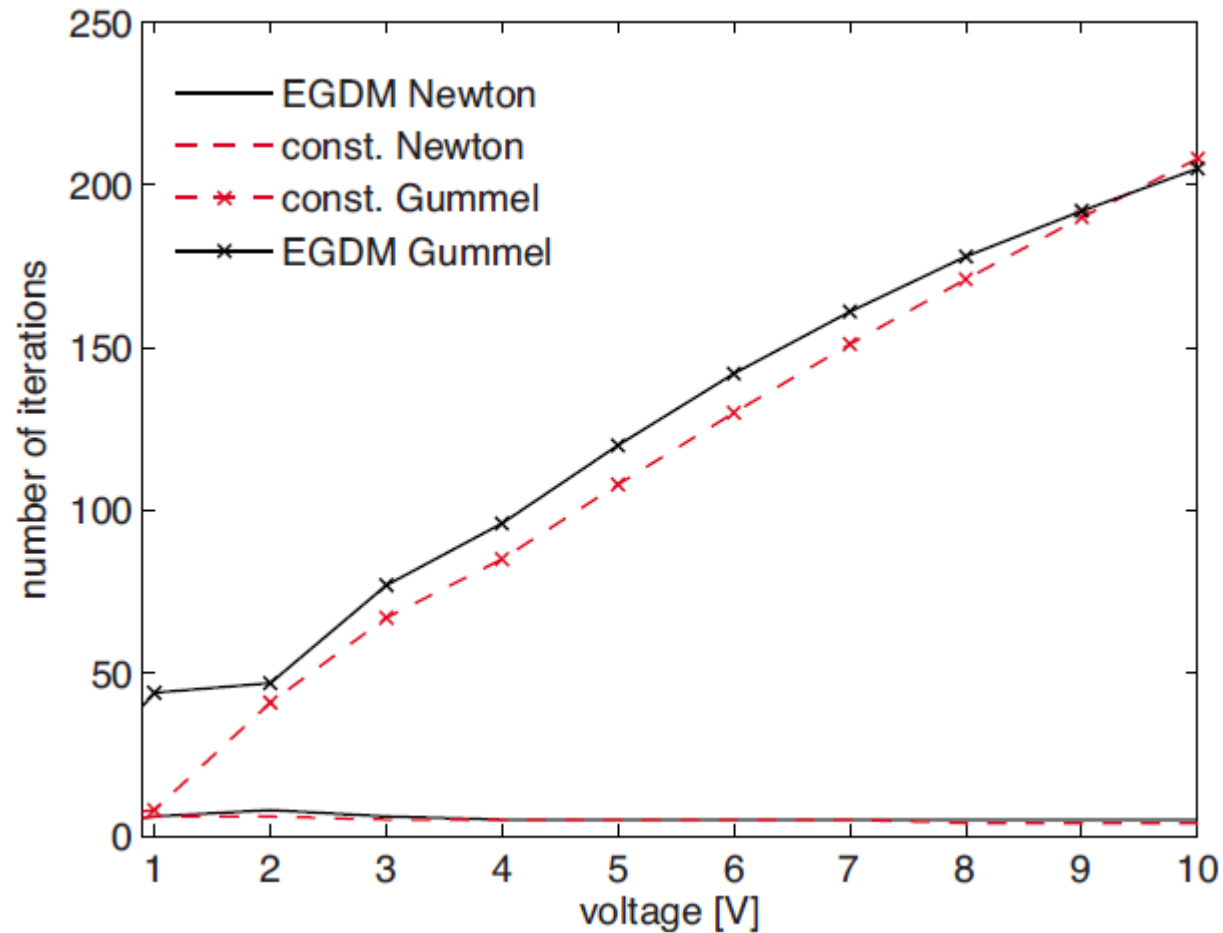
Conclusions

- The **complexity** of white OLEDs requires the availability of an experimentally validated OLED model. Crucial element: **disorder.**

- **First predictive model** developed for single layer OLEDs, consistent with full 3D-modelling.

- **Mathematical analysis** is still lacking, due to the carrier dependence of mobility and the recombination terms

- Numerical methods depend on the mathematical analysis, specific development is needed for an **adapted Scharfetter-Gummel scheme**

Much mathematical work remains to be done…..
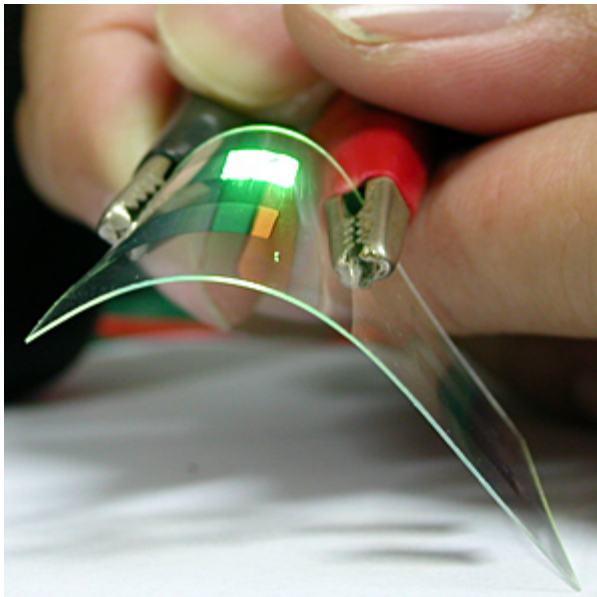
in close collaboration with the physicists/ chemists!

Mathematicians need to be flexible, like OLEDs!

Acknowledgements