Multi-dimensional Numerical Modeling of Organic Thin Film Transistors

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Team

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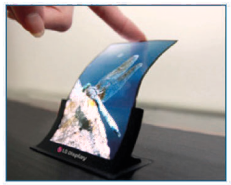
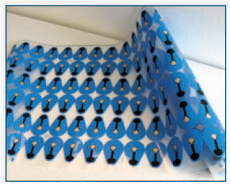
Organic Electronics

Integrated Smart Systems (ISS)

OLED Lighting



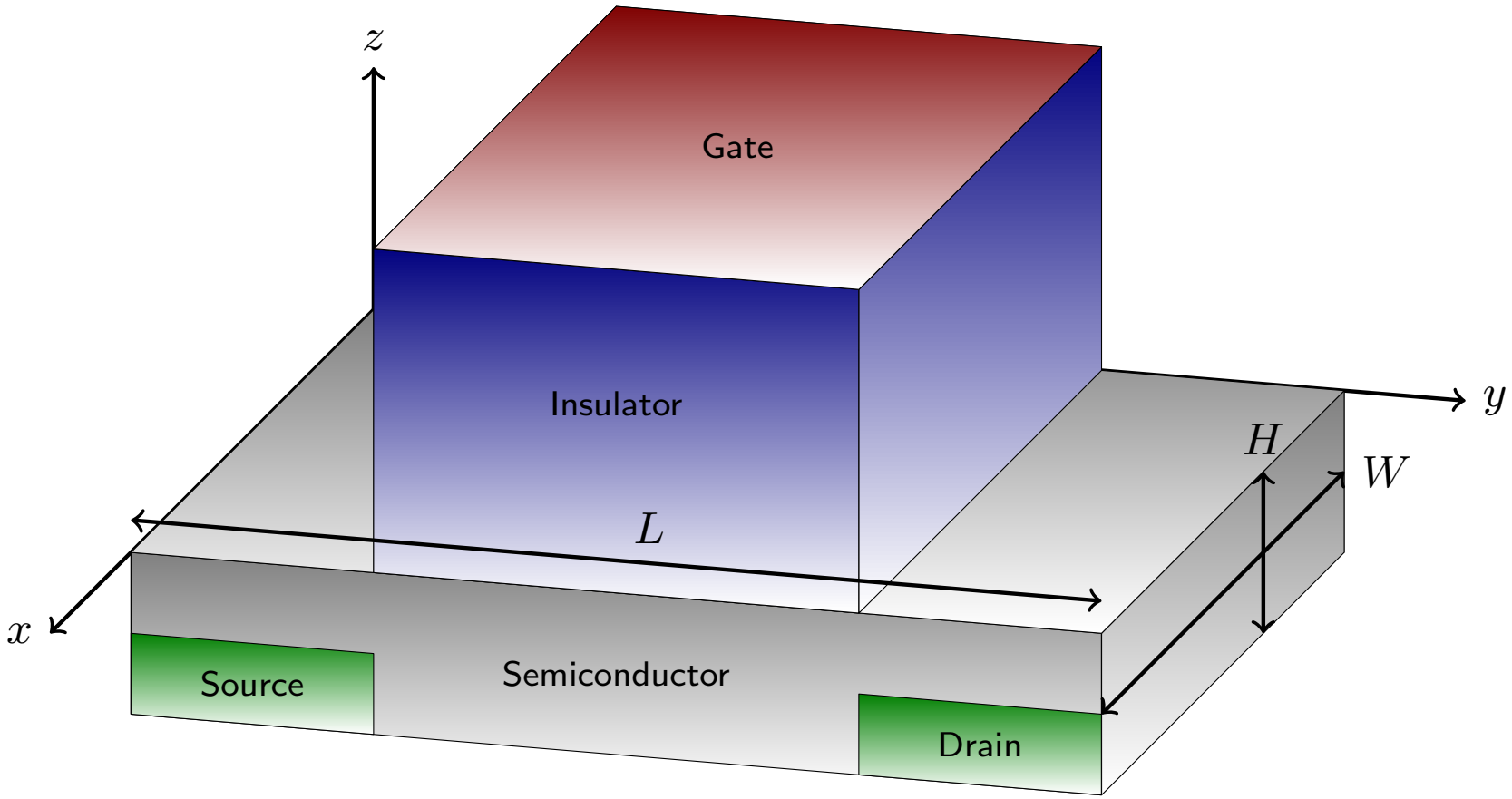
Flexible Displays and OLED



Organic Photovoltaic

Electronics & Components

OTFTs (Organic Thin Film Transistors)



Drift-Diffusion equations

$$
\begin{cases}
-\nabla \cdot (\varepsilon \nabla \varphi) + q(n-p) = 0, & \text{in } \Omega, \\
\dfrac{\partial n}{\partial t} - \dfrac{1}{q}\nabla \cdot \mathbf{J}_n = G_{np}(n,p,X), & \text{in } \Omega_{semic}, \\
\dfrac{\partial p}{\partial t} + \dfrac{1}{q}\nabla \cdot \mathbf{J}_p = G_{np}(n,p,X), & \text{in } \Omega_{semic}, \\
\dfrac{\partial X}{\partial t} + \nabla \cdot \mathbf{J}_X = G_X(n,p,X), & \text{in } \Omega_{semic},
\end{cases}
$$

where

$$
\begin{aligned}
\mathbf{J}_n &= -q\left(\mu_n n \nabla \varphi - D_n \nabla n\right), \\
\mathbf{J}_p &= -q\left(\mu_p p \nabla \varphi + D_p \nabla p\right), \\
\mathbf{J}_X &= -\left(D_X \nabla X\right).
\end{aligned}
$$

Disordered materials:

$$
\begin{aligned}
\mu_n &= \mu_n(n, \nabla \varphi), \\
\mu_p &= \mu_p(p, \nabla \varphi).
\end{aligned}
$$

Aims

- Extend transient 1D simulator to the 2D/3D case, implementing **accurate physical models** (mobility coefficients and boundary conditions);
- extreme aspect ratios $\longrightarrow$ **anisotropy** $\longrightarrow$ numerical challenges:
  - mesh adaptativity;
  - discrete maximum principle;
- coupling with **heat diffusion** and **electromagnetic radiation**;
- **model validation** by comparison with experimental data.

References

Publications

F. Maddalena, C. de Falco, M. Caironi, D. Natali, Assessing the width of gaussian density of states in organic semiconductors, Organic Electronics 17 (0) (2015) 304 – 318.

M. Porro, C. de Falco, M. Verri, G. Lanzani, R. Sacco, Multiscale simulation of organic heterojunction light harvesting devices, COMPEL 33 (2014) 1107–1122.

C. de Falco, M. Porro, R. Sacco, M. Verri, Multiscale modeling and simulation of organic solar cells, Computer Methods in Applied Mechanics and Engineering doi:10.1016/j.cma.2012.06.018.

C. de Falco, R. Sacco, M. Verri, Analytical and numerical study of photocurrent transients in organic polymer solar cells, Comput. Methods Appl. Mech. Engrg. 199 (2010) 1722–1732.

Relevant previous theses

P. Africa, Numerical Modeling of Organic Thin Film Transistors, MSc in EngMath, Supervisor C. de Falco, Co-supervisor D.A.N. Natali.

M. Porro, M. Cogliati, Third Generation Solar Cells: Modeling and Simulation, MSc in EngMath, Supervisor R. Sacco, Co-supervisors C. de Falco, M. Verri.

G. Abbati, Trasporto di Carica nei Semiconduttori Organici Amorfi, BSc in EngMath, Supervisor C. de Falco, Co-supervisors D.A.N. Natali, M. Verri.