Simulation of Gaussian Traps in Organic Semiconductor Devices

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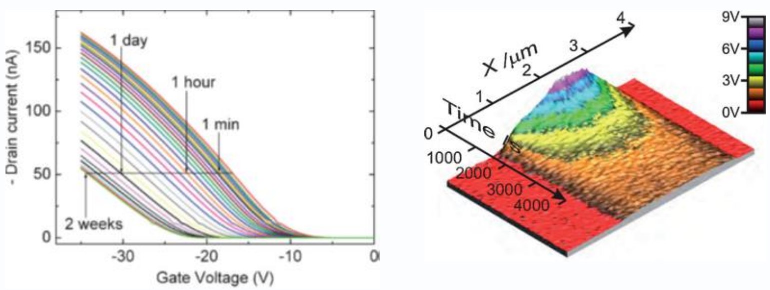
Main Content

1. Traps in Organic Semiconductor Devices

Origin to Form Traps

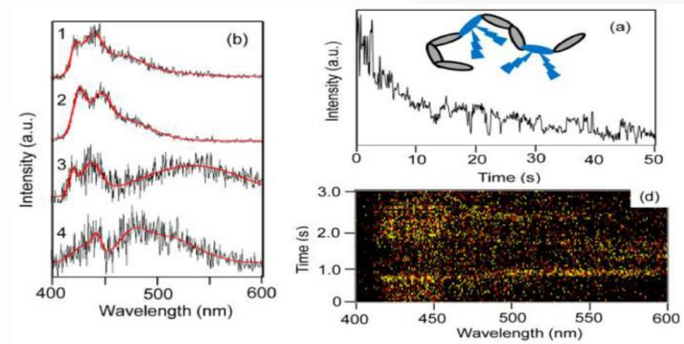
Chemical Impurities, Structure defects, Discontinuous at interface, Environment factors：Oxygen, Moisture、Radiation

Influence:
Degradation of electrical performance



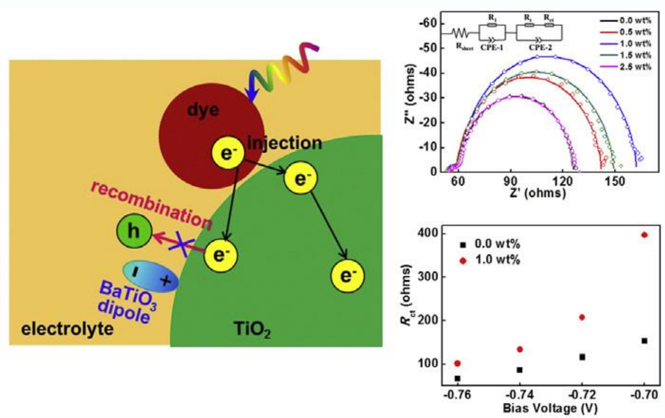
Advanced Materials 2009, 21, 3859-3873

Influence:
Degradation of optical performance



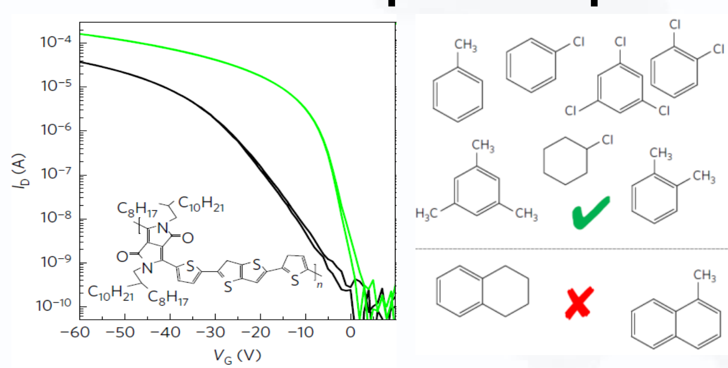
J. Phys. Chem. C 2018, 122, 8137−8146

Exploit: Dye Sensitized solar cells



Journal of Power Sources 350 (2017) 35e40

Optimize:
Small molecular pre- occupation



Nat Mater 2017 Vol. 16 Issue 3 Pages 356-362

2. Conventional Method to Deal Traps

Density of State for Donor-like Traps in Organic Semiconductor

1、Unique site

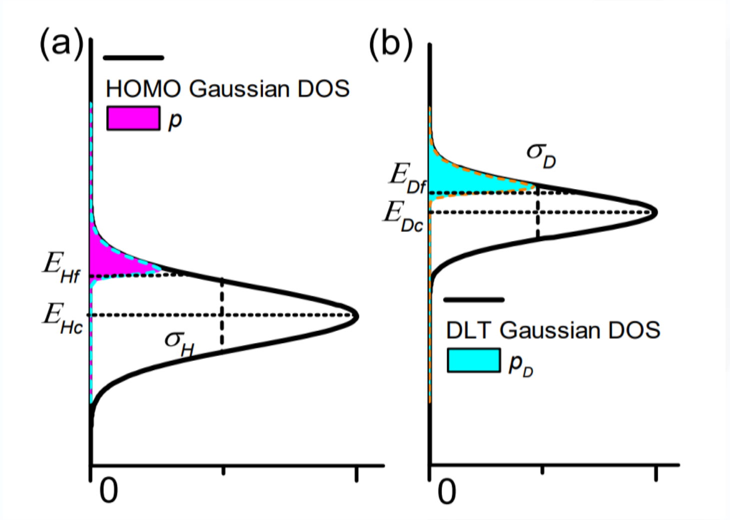
$$E = C$$

2、Exponent distribution

$$g = N_{t_0} \exp\left(\frac{E - E_t}{k_B T_t}\right)$$

3、Gaussian distribution

$$g = \frac{N_T}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(E - E_c)^2}{2\sigma^2}\right)$$



HOMOs　　Donor-like Traps

Complementary Gaussian Fermi Integral

Holes: $$p = \int_{-\infty}^{\infty} g_H(E_H, E_{Hc}, \sigma_H)(1 - f(E_H, E_f))dE_H$$

Traps: $$p_D = \int_{-\infty}^{\infty} g_D(E_D, E_{Dc}, \sigma_D)(1 - f(E_D, E_{Df}))dE_D$$

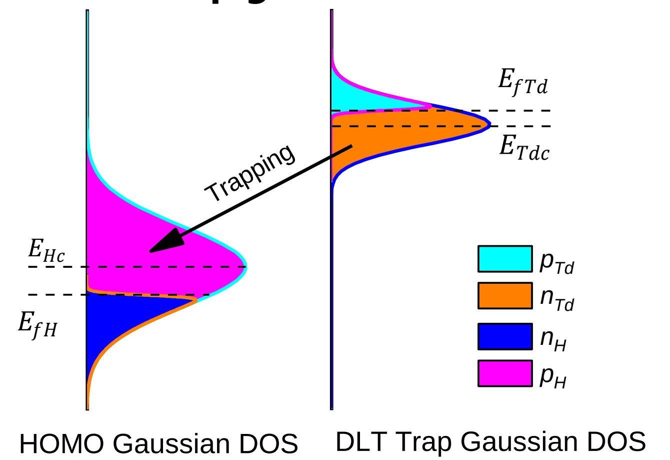
3. Models for the Donor Like Traps

Progress for trap generation and combination

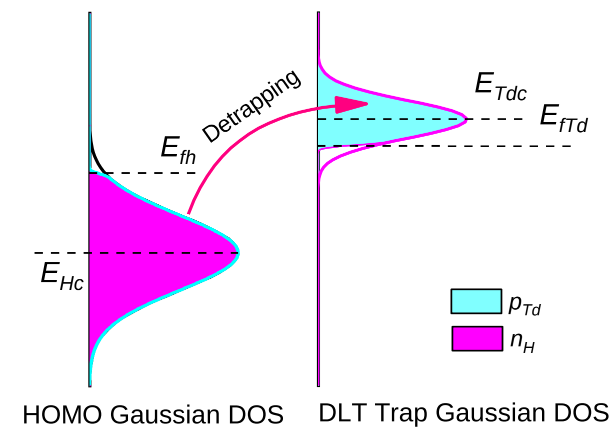
Miller-Abrahams rate equation

$$v_{ij} = v_0 \exp\left(-2\frac{R_{ij}}{a_i} - \frac{\boxed{E_j - E_i + |E_j - E_i|}}{2k_BT}\right)$$

Trap generation



Trap combination



$$k_T = \iint_{-\infty}^{\infty} v_{DH} g_D(E_D) f(E_D, E_{Df}) g_H(E_H)(1 - f(E_H, E_{Hf})) dE_D dE_H$$

$$k_T = v_{DH} n_D p$$

$$k_D = \iint_{-\infty}^{\infty} v_{HD} g_H(E_H) f(E_H, E_{Hf}) g_D(E_D)(1 - f(E_D, E_{Df})) dE_H dE_D$$

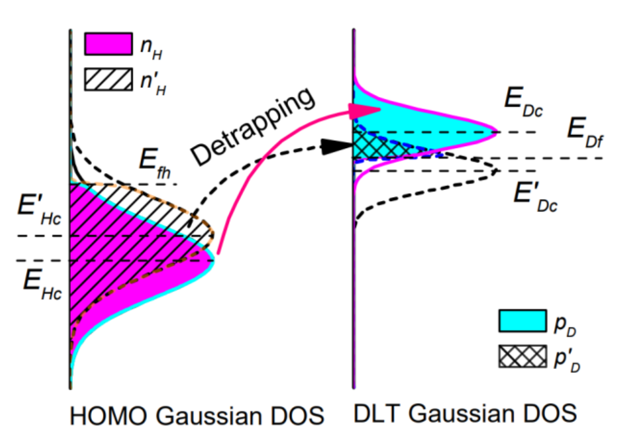
Energy Barrier ➡ Hard to Solve

Chen, Q.S.; Sanchez, J. E.; Lin, D.; Lei, Y.; Zhu, G., Analytical model for donor like Gaussian traps in organic thin-film transistor. Organic Electronics 2022, 103, 106464.

3. Models for the Donor Like Traps

Combination rate $$k_D = \iint_{-\infty}^{\infty} v_{HD0} \exp\left(-\frac{E_D - E_H}{k_B T}\right) g_H(E_H)$$
$$f(E_H, E_{Hf}) g_D(E_D)(1 - f(E_D, E_{Df})) dE_H dE_D$$

Simplify the calculation



HOMOs Center $$E'_{Hc} = E_{Hc} + \frac{\sigma_H^2}{k_B T}$$

Effective Center for Traps $$E'_{Dc} = E_{Dc} - \frac{\sigma_D^2}{k_B T}$$

Effective electrons for HOMOs: $$n'_H = \int_{-\infty}^{\infty} g_H(E_H, E'_{Hc}, \sigma_H) f(E_H, E_{Hf}) dE_H$$

Effective Density of Traps: $$p'_D = \int_{-\infty}^{\infty} g_D(E_D, E'_{Dc}, \sigma_D)(1 - f(E_D, E_{Df})) dE_D$$

Combination rate $$k_D = c_E v_{DH0} n'_H p'_D$$

Generate Rate $$k_T = v_{DH} n_D p$$

Coefficient $$c_E = \exp\left(\frac{\sigma_H^2 + \sigma_D^2}{2k_B^2 T^2} + \frac{E_{Hc} - E_{Dc}}{k_B T}\right)$$

4. Combined with Finite Volume Method

Poisson Equation

$$-\nabla\cdot(\varepsilon_r\varepsilon_0\nabla\psi)=e\cdot(p-n+p_D)$$

Hole& Electron Continuity Equation

$$\frac{\partial p}{\partial t}=\nabla\cdot(p\mu_p\nabla\psi+D_p\nabla p)+G_p$$

$$\frac{\partial n}{\partial t}=\nabla\cdot(-n\mu_n\nabla\psi+D_n\nabla n)+G_n$$

Conversion from Surface to Bulk Density

$$N_D=\frac{N_{Ds}}{d_D}\exp\left(-\frac{x}{d_D}\right)$$

Net Generate Rate for Traps

$$\frac{\partial p_D}{\partial t}=k_T-k_D$$

Net Generate Rate for Holes

$$G_p=-(k_T-k_D)$$

Net Generate Rate for Electrons

$$G_n=0$$

Mobility of Micro Conductivity

$$\mu_p=\frac{\Gamma}{ep}\exp\left(\frac{E_{Hf}}{k_BT}\right)$$

Simulate Platform

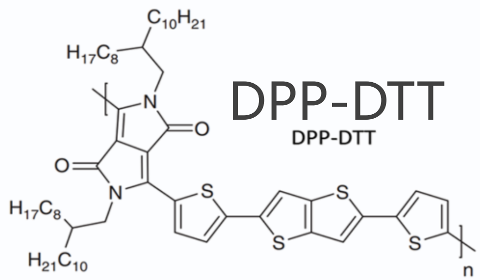
DEVSIM™ TCAD software

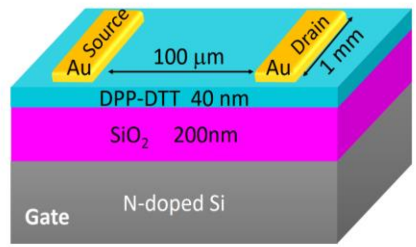
Gmsh

VisIt users.org

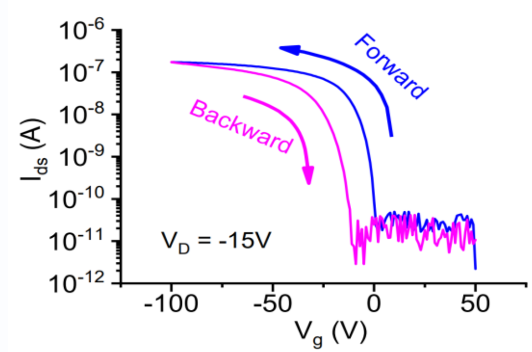
5. Device Verification and Parameters

- Device Fabrication



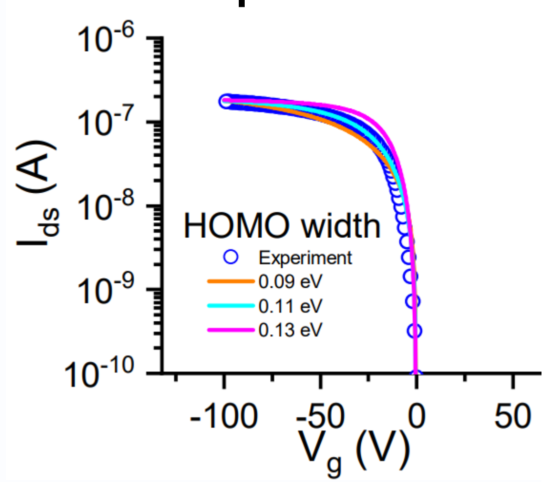


I-V measurement

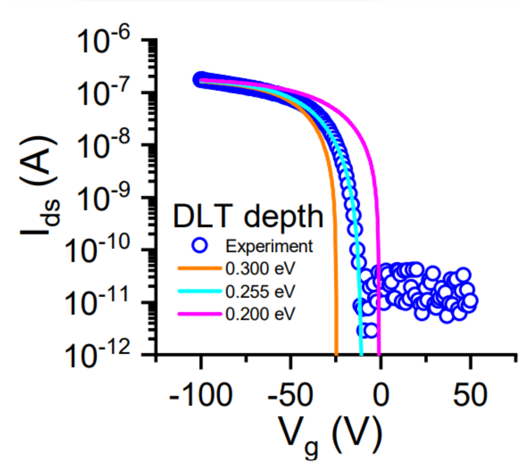


Model	Symbol	Value	Unit
Total density for HOMO (Section 3.6.1)	N_H	1.29×10^{21}	cm^{-3}
HOMO DOS width [1]	σ_H	0.11	eV
HOMO DOS center[80]	E_{Hc}	-5.2	eV
Localization length for HOMO and DLT[91]	a_H, a_D	0.29	nm
LUMO DOS center[80]	E_{Lc}	-3.5	eV
Total density for DLT[74]	N_{Ds}	1.0×10^{13}	cm^{-2}
DLT DOS width[145]	σ_D	0.03	eV
DLT DOS center [1]	E_{Dc}	-4.95	eV
Effective mass for electron and hole[141]	m_e^*, m_h^*	0.097	m_e [2]
Thermionic emission velocity (Eq. 3.37)	υ_n, υ_p	8.64×10^6	cm/s
Trap thickness[73, 145]	d_D	5	nm
Attempt frequency[143]	υ_0	2.31×10^9	s^{-1}
Relative permittivity for DPP-DTT[139, 140]	ε_{r_Semi}	3.5	
Relative permittivity for Insulator SiO_2	$\varepsilon_{r\_SiO_2}$	3.9	
Device temperature (Section 3.5)	T	300	K
DPP-DTT thickness (Section 3.5)		40	nm
Insulator's thickness (Section 3.5)		300	nm
OTFT channel length (Section 3.5)		100	μm
OTFT channel width (Section 3.5)		1	mm

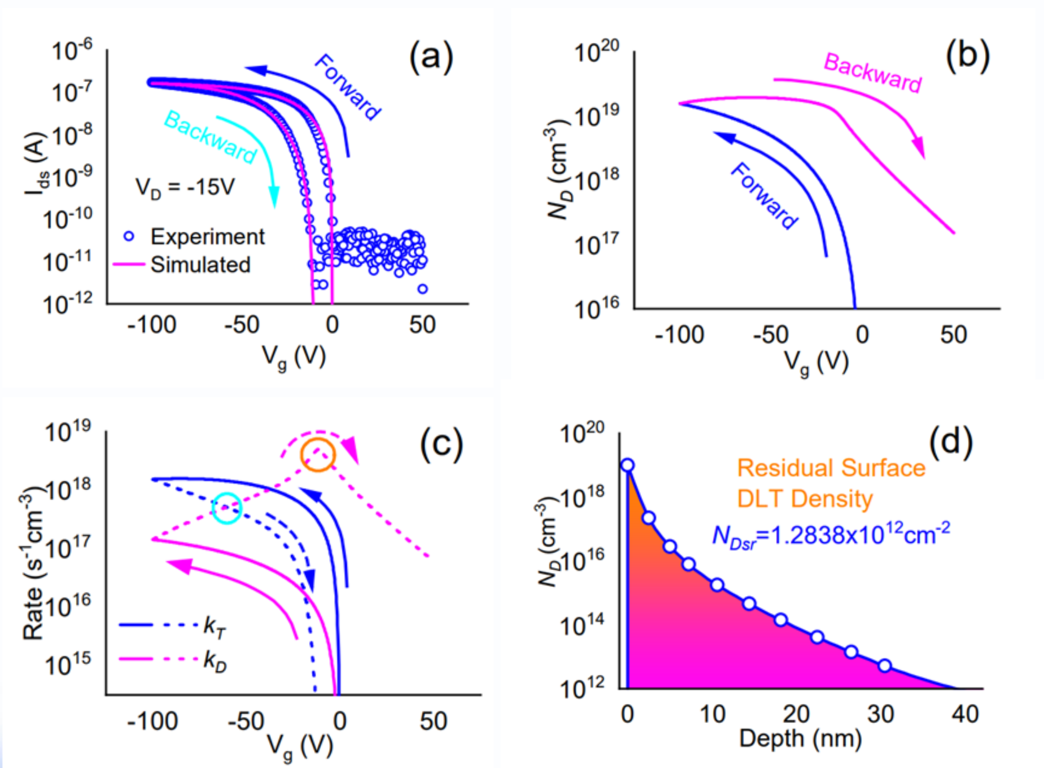
Depth for HOMO



Depth for Traps



6. Experimental Results Analysis



(a) Transfer Curves

On-off ratio 6×10^4

Threshold Voltage:

0 V −12 V

Subthreshold swing:

1.73 V/dec 2.61 V/dec

(b) Trap density Evolution:

Max @ −60.08 V

(c) Generate and Combination rate: Detrapping$_{max}$ @ −12.00 V

(d) Experimental Surface Trap Density

$$N_{Dsr} = \frac{C_i}{e} \times \Delta V_{th}$$

Accurate of Residual Surface Density: $\dfrac{1.2838 \times 10^{12} cm^{-2}}{1.2931 \times 10^{12} cm^{-2}} = 99.283\%$

Other Application Scenario : Acceptor-like Traps, Electroluminescence of OLEDs

This is a noncommercial free project because it has been granted with a Chinese patent [Granted No.: CN 113297818 B]

7. Symbolic TCAD Platform——DEVSIM

DEVSIM™ TCAD software

- Founder： Juan E. Sanchez Email: jsanchez@devsim.com
- Brief Biography:
  - Received the B.S.E.E. degree in 1995 from the University of South Florida, Tampa, and the M.S. and Ph.D. degrees from the University of Florida, Gainesville, in 1997 and 2002, respectively, both in electrical and computer engineering.
  - He has been developing the DEVSIM TCAD simulator since 2008.

Main Functions:

1. Simulation of static & dynamic physical field;
2. Simulation the electrical output：I-V、C-V curves;
3. **Traps state simulation;**
4. **Simulation of non-line dielectric: Ferroelectricity**

1. Organic Laser

Character:

Open-source、Symbolic Calculation、Flexible Physical mode deployment、Low cost、Hard to Learn

My Work:

Semiconductor：Organic traps

Ferroelectricity：Miller model、Landau-Ginsburg Model

https://github.com/CQSim/QS-Devsim

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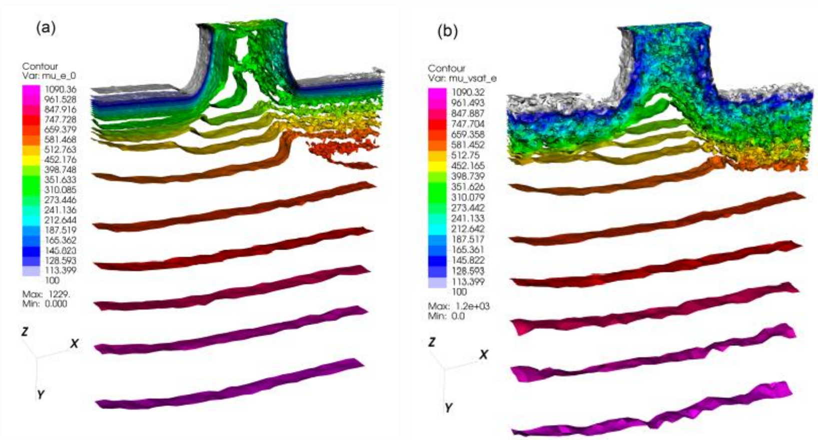
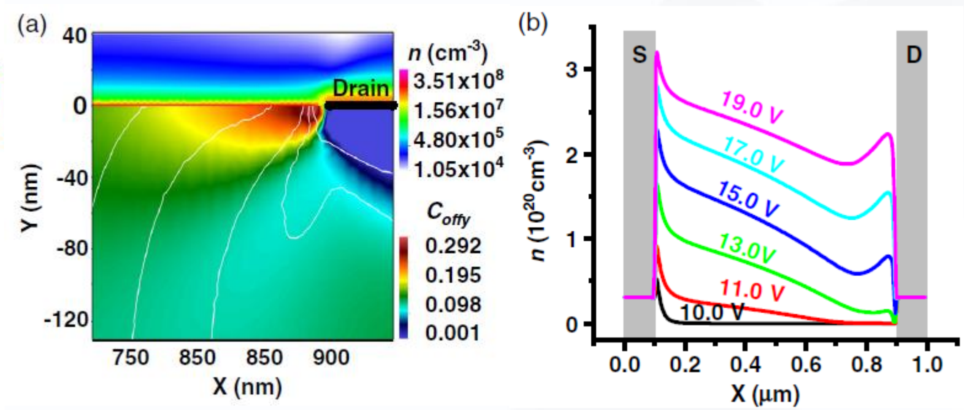
7. Symbolic TCAD Platform——DEVSIM

Achievements of Devsim



IEEE Trans. Electron Devices 2021, 68 (11), 5414



Physica Status Solidi (A) 2021, 218 (22)

1. Chen, Q.S.; Sanchez, J. E.; Lin, D.; Lei, Y.; Zhu, G., Analytical model for donor like Gaussian traps in organic thin-film transistor. Organic Electronics 2022, 103, 106464.
2. Sanchez, J. E.; Chen, Q.S.(co-firstauthors), Element Edge Based Discretization for TCAD Device Simulation. IEEE Trans. Electron Devices 2021, 1-7.
3. Chen, Q.S.; Lin, D.; Wang, Q.; Yang, J.; Sanchez, J. E.; Zhu, G.D., The Impact of Contact Position on the Retention Performance in Thin-Film Ferroelectric Transistors. Physica Status Solidi (A) 2021.
4. J. Lauwaert, "Technology computer aided design based deep level transient spectra: Simulation of high-purity germanium crystals," Journal of Physics D: Applied Physics, 2021, doi: 10.1088/1361-6463/ac34ad.
5. L. Hulbert, "Designing a Simulator for an Electrically-Pumped Organic Laser Diode," Master's Thesis, California Polytechnic State University, San Luis Obispo, CA, 2019, doi: 10.15368/theses.2019.60.

Thanks!