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Simulation of Organic Thin Film Transistors for Gas Sensing Application

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  - Uniform distribution of traps
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- Conclusion

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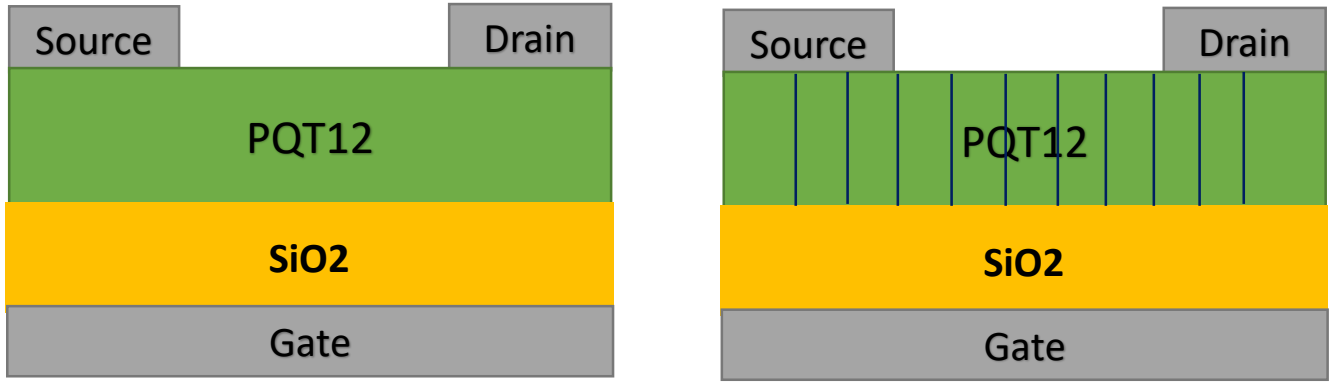
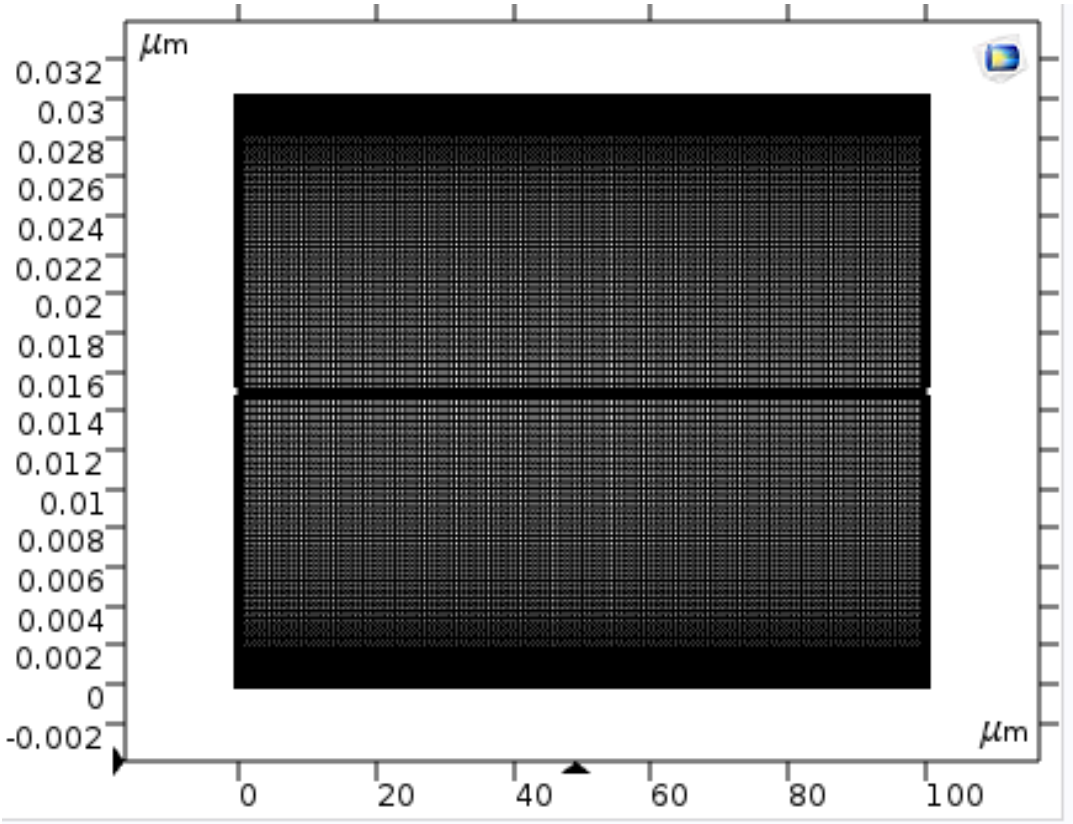
Device Simulation

Simulated device dimensions

- 100 μm long gold S/D electrodes
- 400μm polysilicon gate electrode
- The gate oxide is a 300 nm thick SiO2
- 200μm channel length



(a) (b)



(c)

Fig.1 (a) Uniform distribution of traps and defects, (b) Channel divided in to multiple grains, (c) COMSOL Mesh structure

Table 1 Summary of material parameters used in both simulation approaches

	PQT12	PQTS12
Band gap	2 eV	1.8eV
Affinity	3.1 eV	3.2 eV
Permittivity	3	3
Trap density	$7.1x10^{15}cm^{-3}$	$1.2x10^{16}cm^{-3}$
Polymer thickness	100 nm	100 nm
Oxide thickness and permittivity	300 nm, 3	300 nm, 3
S,D Gold thickness and wf	50 nm, 5.1 eV	50 nm, 5.1 eV
Gate, n-poly-Si thickness and wf	50 nm, 4.15 eV	50 nm, 4.15 eV
Channel length	2 mm	2 mm
Channel width	11 mm	11 mm
Interface charge	$1.2x10^{11}$ cm^{-2}	$2x10^{10}$ cm^{-2}

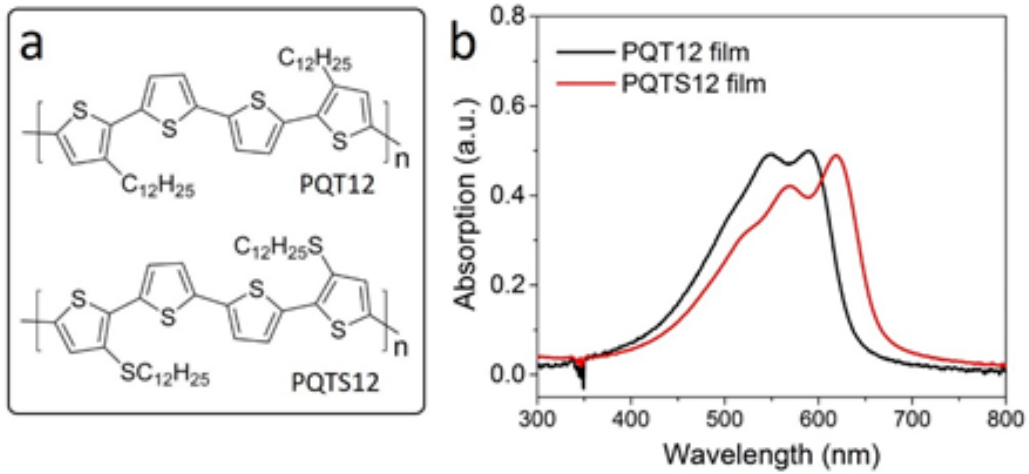


Fig.2 Chemical structure and absorption spectrum

Computational Methods:

COMSOL **Semiconductor Module** is used to solve Poisson and Continuity equations:

$$-\nabla\cdot(\varepsilon\nabla V) = q(p - n + N_D^+ - N_A^-)$$

$$\frac{\partial n}{\partial t} = -\frac{1}{q}J_n - U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}J_p - U_p$$

Exponential Trap distribution

$$g_{TA}(E) = n_{TA}\exp[\frac{E - E_C}{w_{TA}}]$$

$$g_{TD}(E) = n_{TD}\exp[\frac{E_V - E}{w_{TD}}]$$

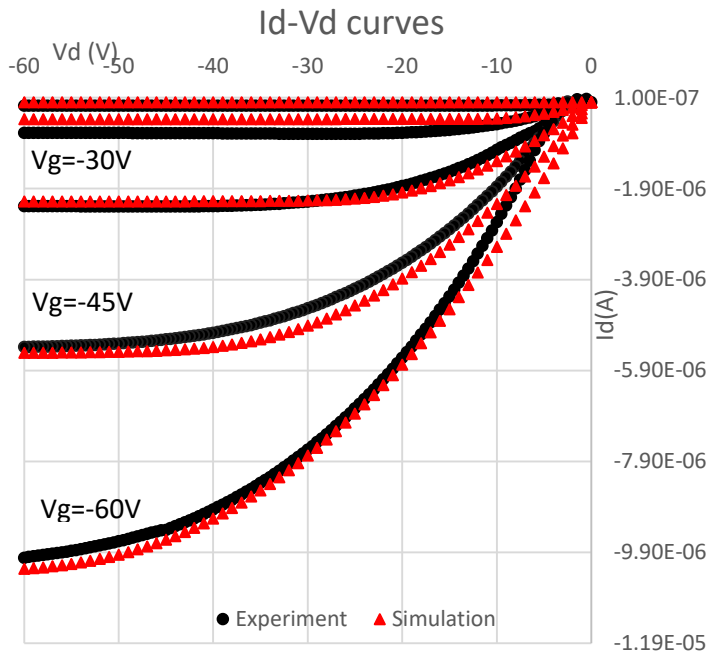
Gaussian Trap distribution

$$g_{GA}(E) = n_{GA}\exp\left[-\left(\frac{E_{GA} - E}{w_{GA}}\right)^2\right]$$

$$g_{GD}(E) = n_{GD}\exp\left[-\left(\frac{E - E_{GD}}{w_{GD}}\right)^2\right]$$

Results

(A) Device simulation

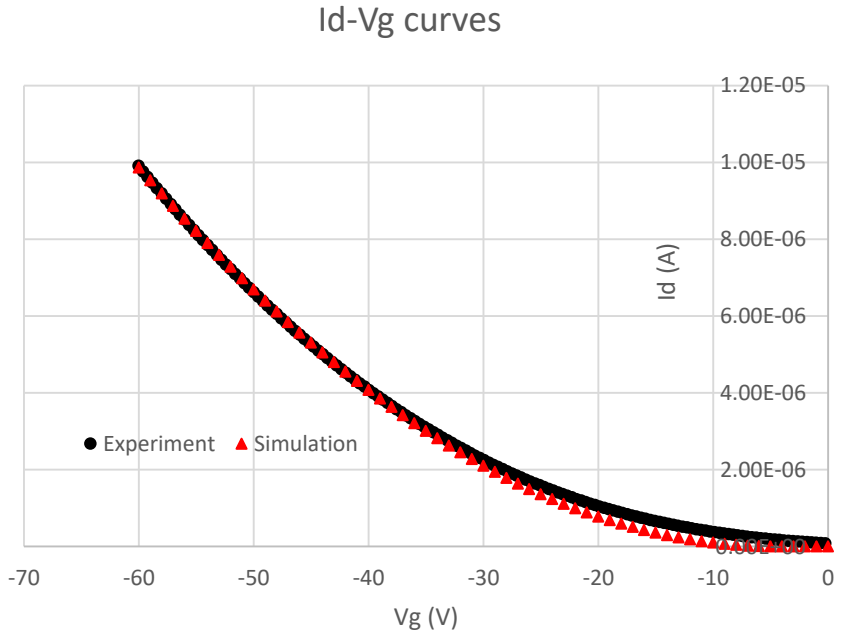


(a)

Expt

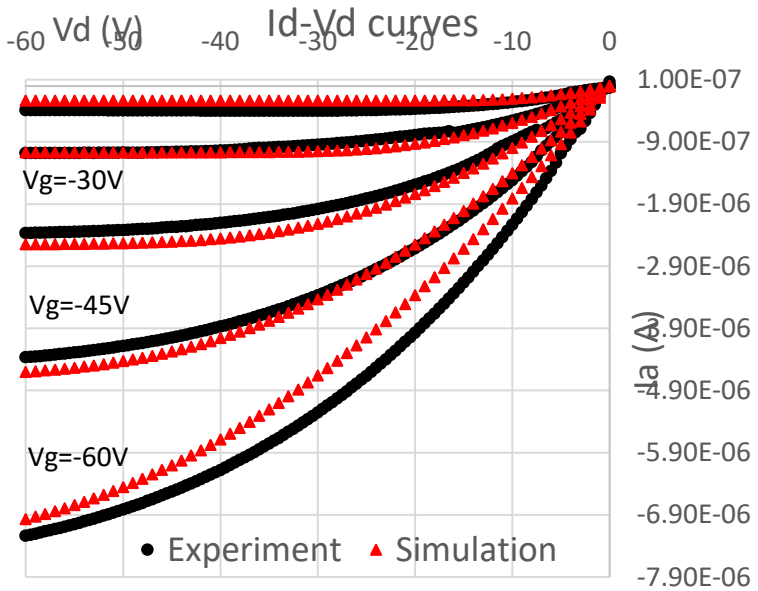
Simulation

PQT12 OTFT



(b)

Fig. 3. (a) Id – Vd curves for different gate voltage
(b) Id – Vg curves

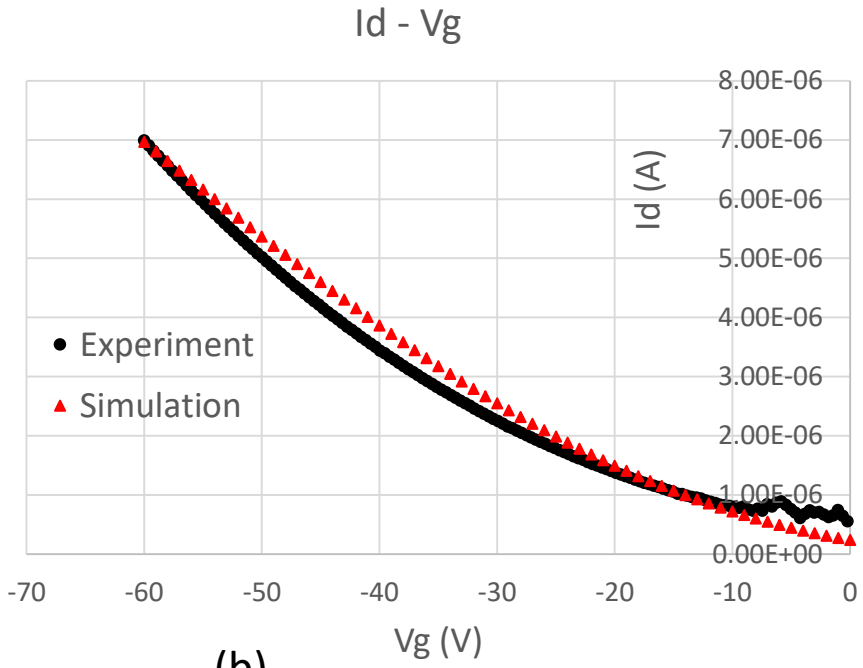


(a)

Expt

Simulation

PQTS12 OTFT



(b)

Fig. 4. (a) Id – Vd curves for different gate voltage
(b) Id – Vg curves

(B) Analyte Sensitivity simulation

PQT12 OTFT

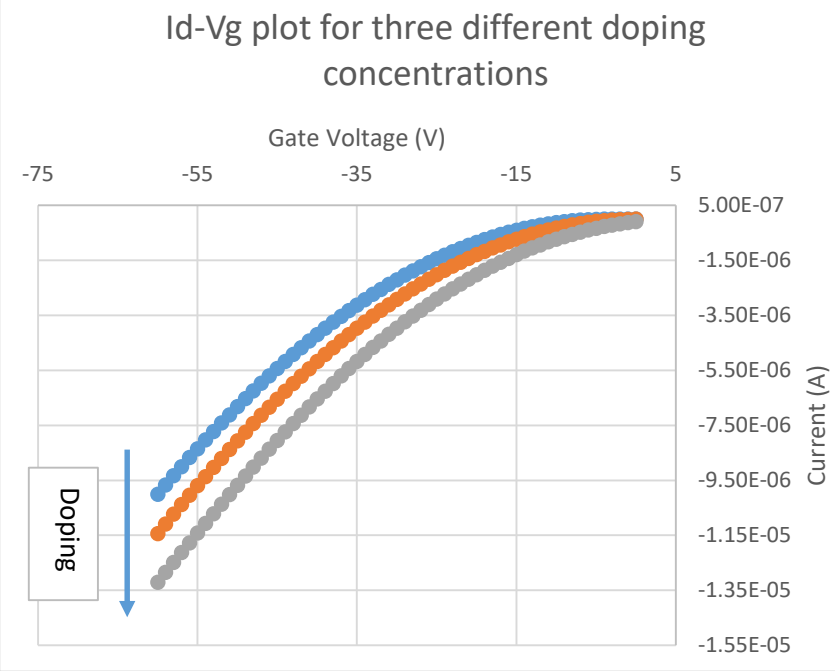


Table 2 Effect of doping on drain current and mobility

Change in doping	Change in drain current	Change in mobility	Comparison with Expt.
0	0	0	No exposure
300%	14.67%	0.27%	5 min exposure at 1ppm (14.0%±2.1%)
680%	31.95%	0.61%	10 min exposure at 1ppm (31.6%±1.6%)

Fig.5 Id – Vg curves for different doping conc.

PQTS12 OTFT

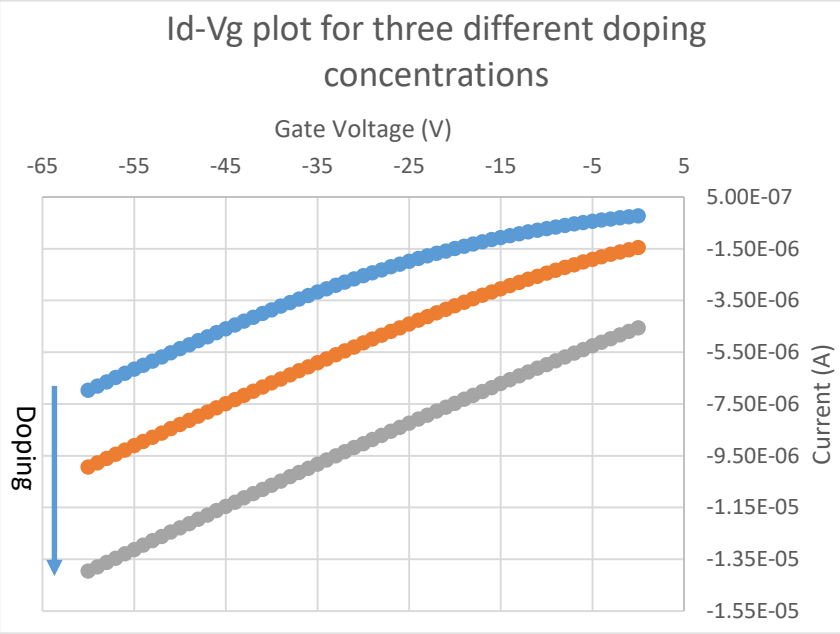


Fig.6 Id – Vg curves for different doping conc.

Table 3 Effect of doping on drain current and mobility

Change in doping	Change in drain current	Change in mobility	Comparison with Expt.
0	0	0	No exposure
143%	42.7%	1.39%	5 min exposure at 1 ppm (42.7%±4.8%)
333%	100.4%	3.26%	10 min exposure at 1 ppm (100.4%±5.2%)

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Conclusion

- Semiconductor Module used to study gas sensing by OTFT
- Interface and bulk traps models used with Gaussian and exponential distribution
- Simulation issues - convergence