COMSOL CONFERENCE
2016 MUNICH

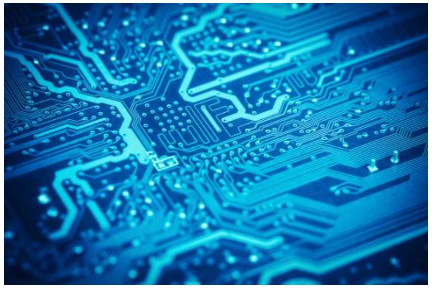
Physical Modeling of Biosensors Based on Organic Electrochemical Transistors

Ph.D. Candidate Shirinskaya Anna
Professors: Gilles Horowitz, Yvan Bonnassieux

Organic Large Area Electronics (OLAE) Group, LPICM (CNRS UMR7647)
Ecole polytechnique, Palaiseau, France

This project receives funding from the European Community's Seventh Framework Program under Grant Agreement n° 607896

Electronic devices

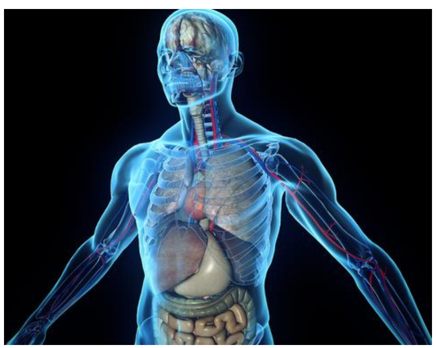


Convergence of biology and electronics

Portable devices

Bioelectronics

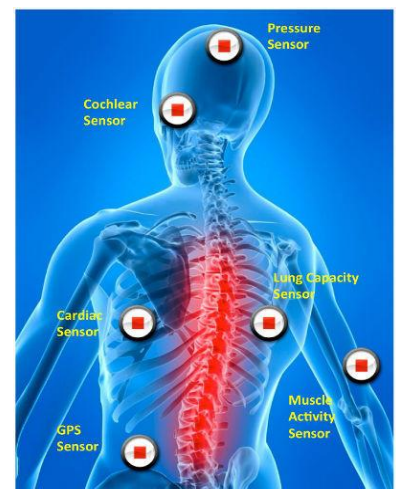
Biosensors



Biological systems

Real time monitoring and diagnostic

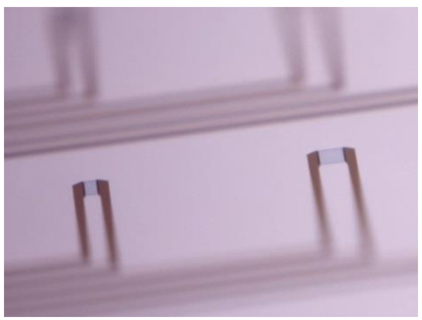
Actuation and therapy

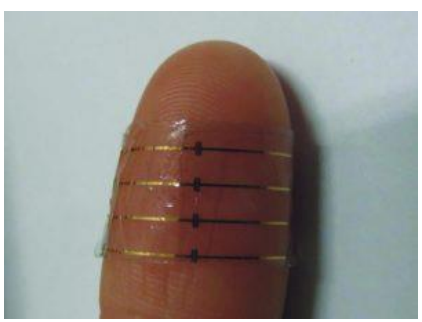


Implantable devices

Biosensors based on Organic Electrochemical Transistor (OECT)

OECT-Conductive polymer based transistor consists of three electrodes (source, drain and gate) and two conducting layers: electrolyte and conducting polymer



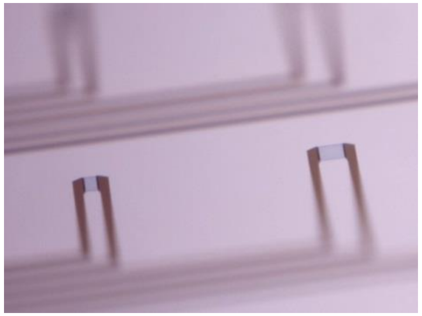


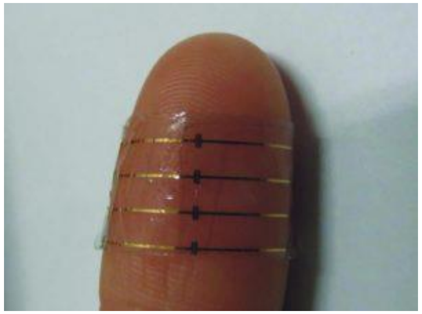
- ✓ **Ion Sensors**: react on change of ions consentration and composition
- ✓ **Enzimatic Sensors**: react on change of local pH, on oxidation of species or transfer of electrons to the gate of the device (e.g. penicillin, glucose, ascorbic acid)
- ✓ **Immunosensors/Nucleotide Sensors**: detect presence of cells and biomolecules

- Campana,A.;Cramer,T.;[illegible]on,D.T.;Berggren,M.; Biscarin i, F. Adv. Mater. (Deerfield Beach, Fla.) 2014, 26, 3874.
- Strakosas, X., Bongo, M. and Ow[illegible] R. M. (2015), The organic electrochemical transistor for biological applications. J. Appl. Polym. Sci., 132, 41735.

Biosensors based on Organic Electrochemical Transistor (OECT)

OECT-Conductive polymer based transistor consists of three electrodes (source, drain and gate) and two conducting layers: electrolyte and conducting polymer





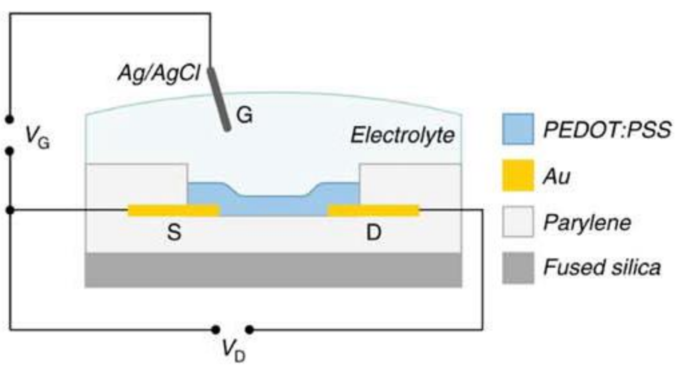
- Wide variety of fabrication methods (also by low-cost printing techniques)
- High curent modulation
- High sensitivity
- High stability in aquarious solutions
- Biocompatability

- Campana,A.;Cramer,T.;Sim[illegible]T.;Berggren,M.; Biscarin i, F. Adv. Mater. (Deerfield Beach, Fla.) 2014, 26, 3874.

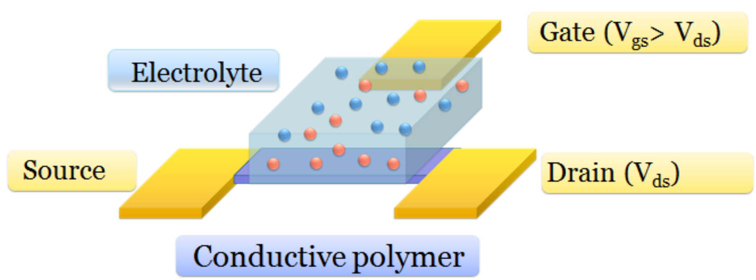
Typical OECT Structure

Structure: OECT consists of three electrodes (source, drain and gate), conductive doped polymer layer and electrolyte.

Operation mode: Normally-on transistor. Voltage applied between source and gate modulate the current on the drain

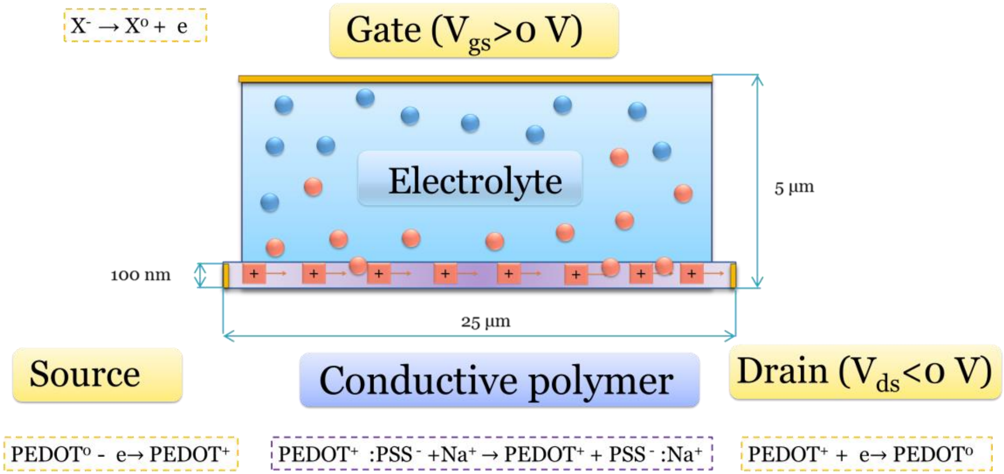


Immerced electrode structure

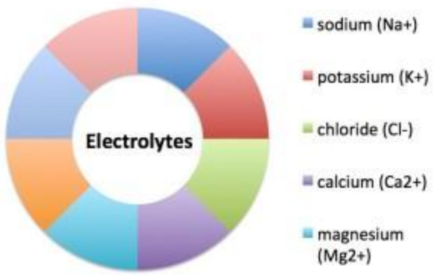


Planar structure

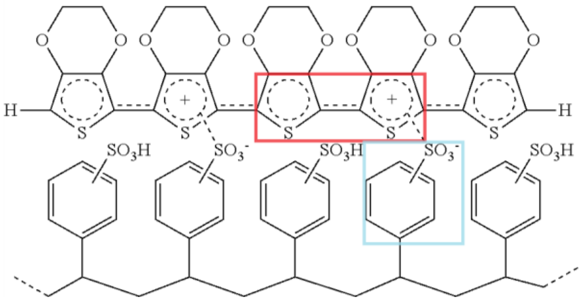
Typical OECT Structure



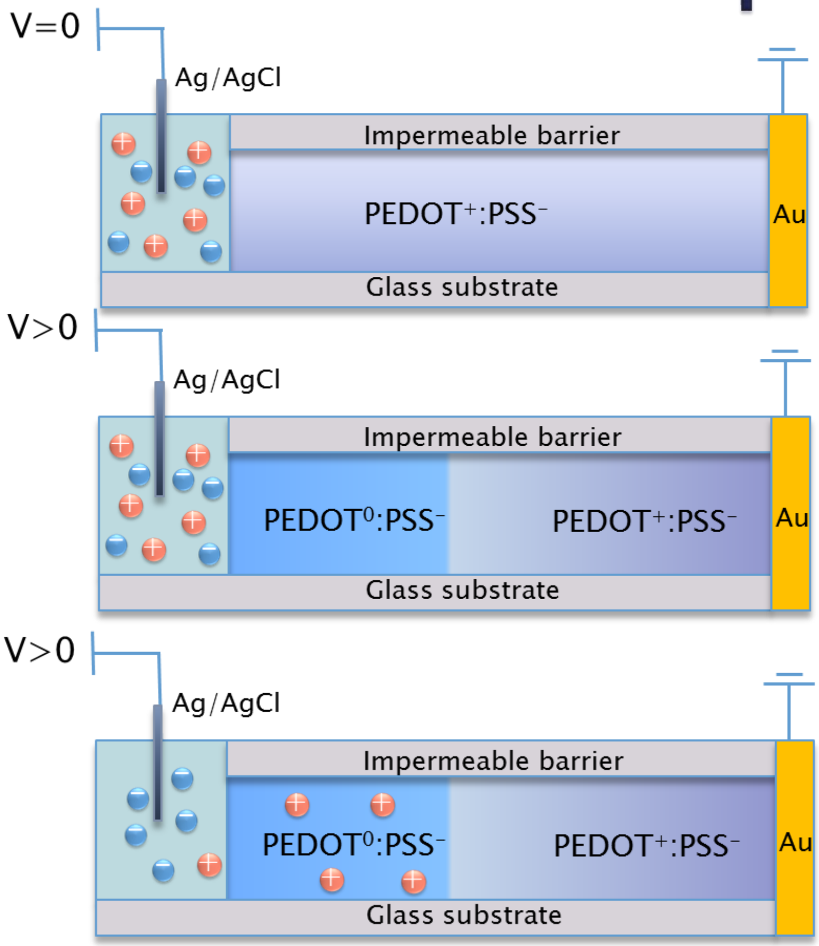
Ionic conductor: Electrolyte



Conductive polymer:
PEDOT :PSS p-type semiconductor



Dedoping Process. Moving front experiment



Before voltage application

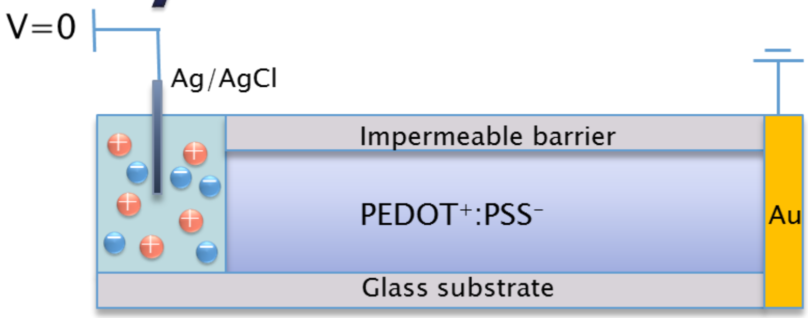
Voltage applied between gate and source electrodes reduces amount of holes by polymer reduction.

Then positive electrolyte ions penetrate inside conductive layer to maintain electro neutrality.

Result in OECT: current is decreasing with gate voltage increasing.

Stavrinidou, E., Leleux, P., Rajao[illegible], Khodagholy, D., Rivnay, J., Lindau, M., Sanaur, S. and Malliaras, G. G. (2013), Direct Measurement of Ion Mobility in a Conducting Polymer[illegible] Mater., 25: 4488–4493.

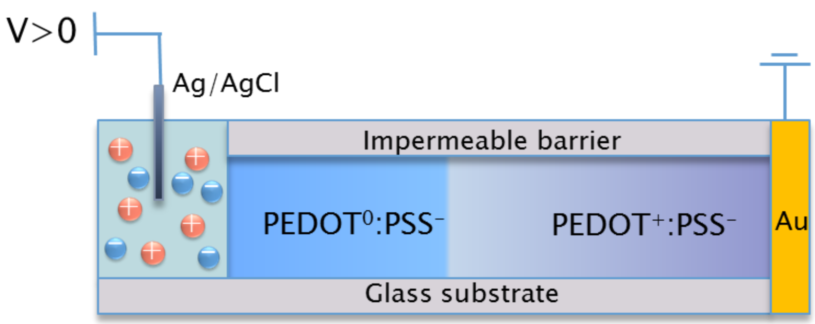
Physics and Chemistry of process



Ions of electrolyte, electrons and holes distribution

Nernst-Planck equation $J_i(x) = -D_i \frac{\partial C_i(x)}{\partial x} - \frac{z_i F}{RT} D_i C_i \frac{\partial \varphi(x)}{\partial x} + C_i V(x)$

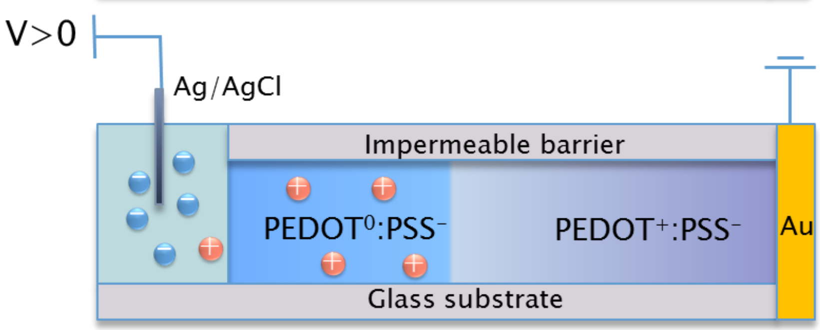
Poisson-Boltzmann equation $\frac{\partial E}{\partial x} = \frac{e}{\varepsilon \varepsilon_0}(h - e + C - A)$



PEDOT+ reduction, positive ions injection

$$PEDOT^+ + e \rightarrow PEDOT^o$$

Nernst equation $c_{pedot+} = \frac{c_{initial\_pedot+}}{1 + \exp(\frac{zF}{RT}(V_0 - V))}$



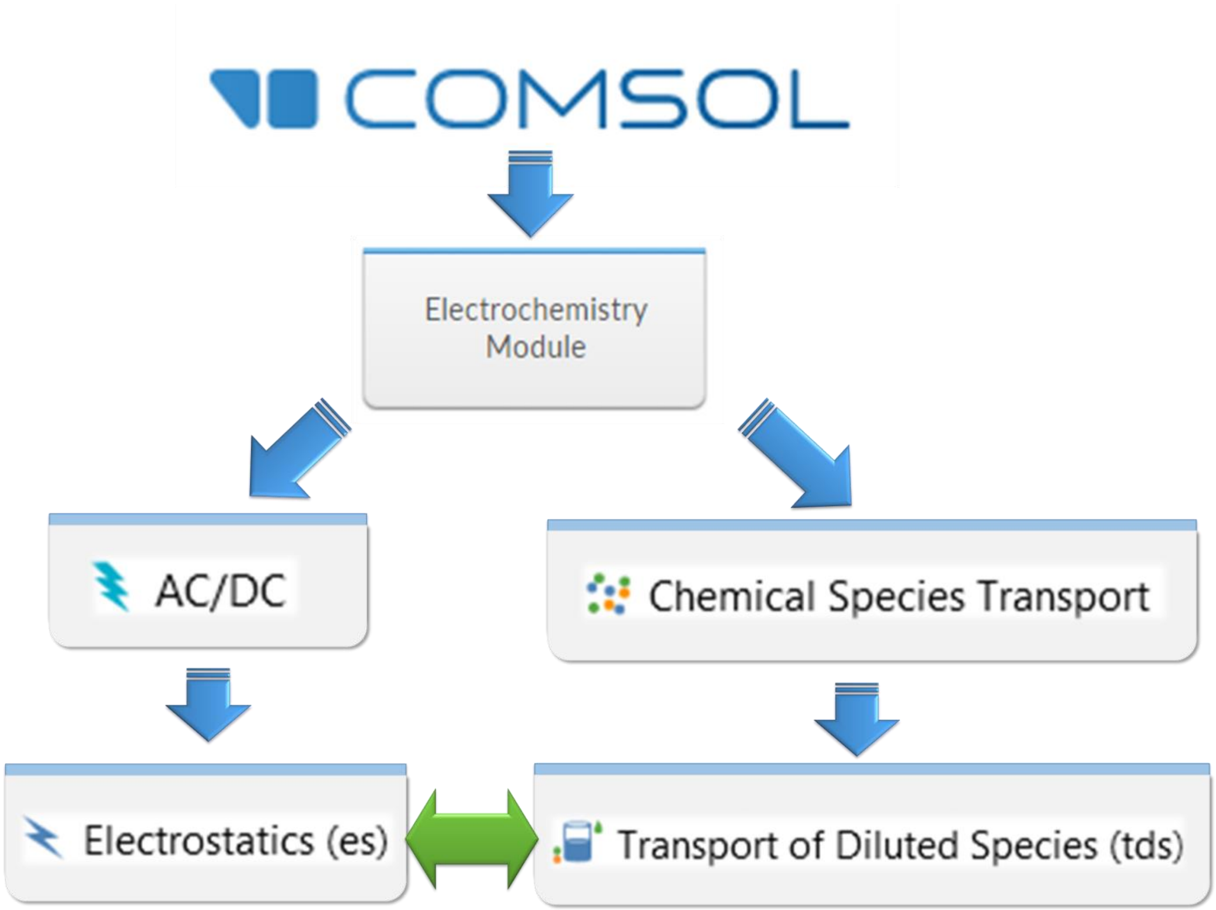
Negative ions reaction at the electrode

$$X^- \rightarrow X^o + e$$

Butler-Volmer equation $i = nFk^0[C_o e^{-(\frac{\alpha nF}{RT})(E-E^0)} - C_r e^{(\frac{(1-\alpha)nF}{RT})(E-E^0)}]$

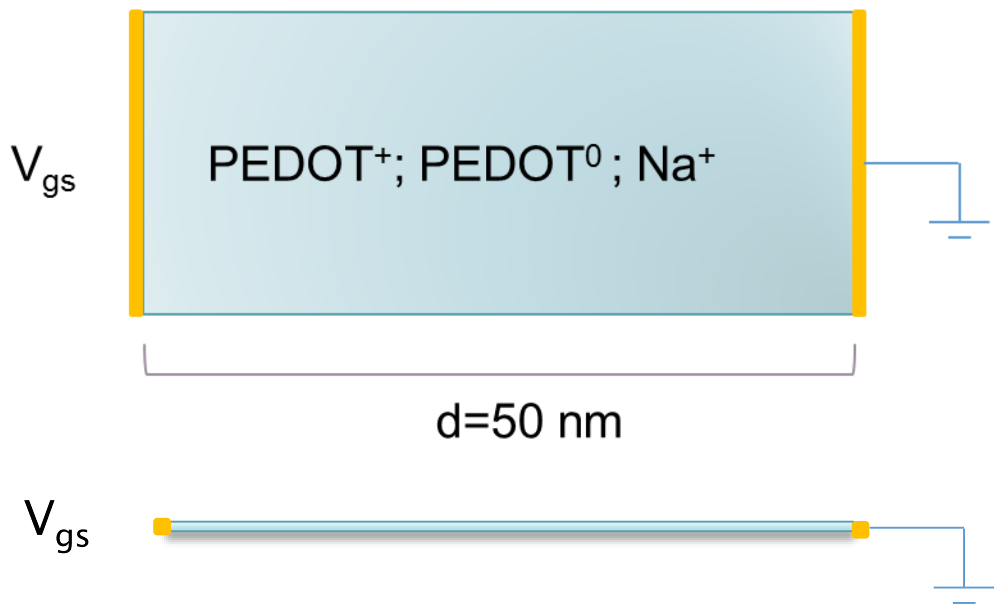
$$PSS^- + Na^+ \rightarrow PSS^- : Na^+$$

Comsol Modelling



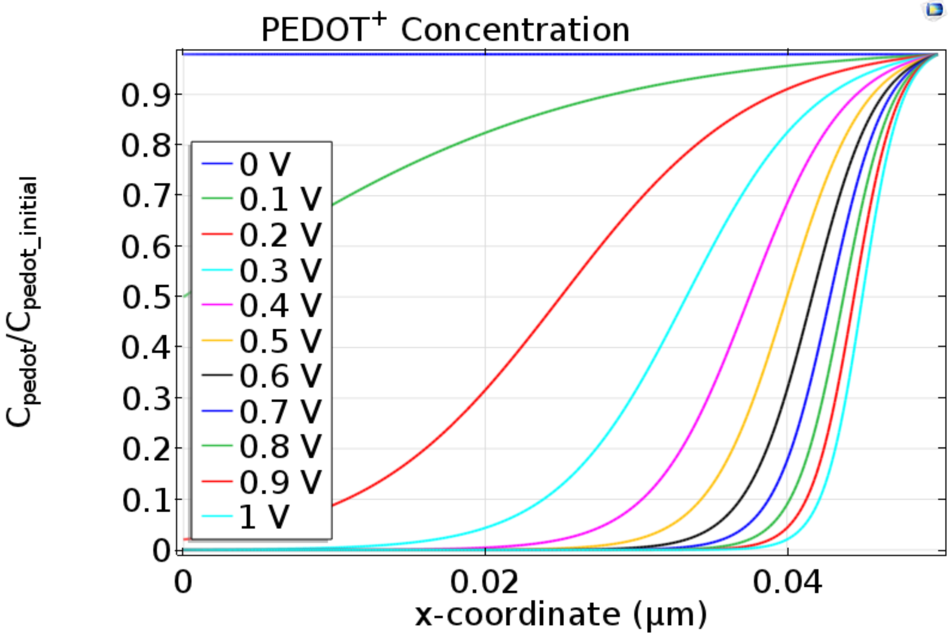
*COMSOL Multiphysics® simulation software was used to obtain following results

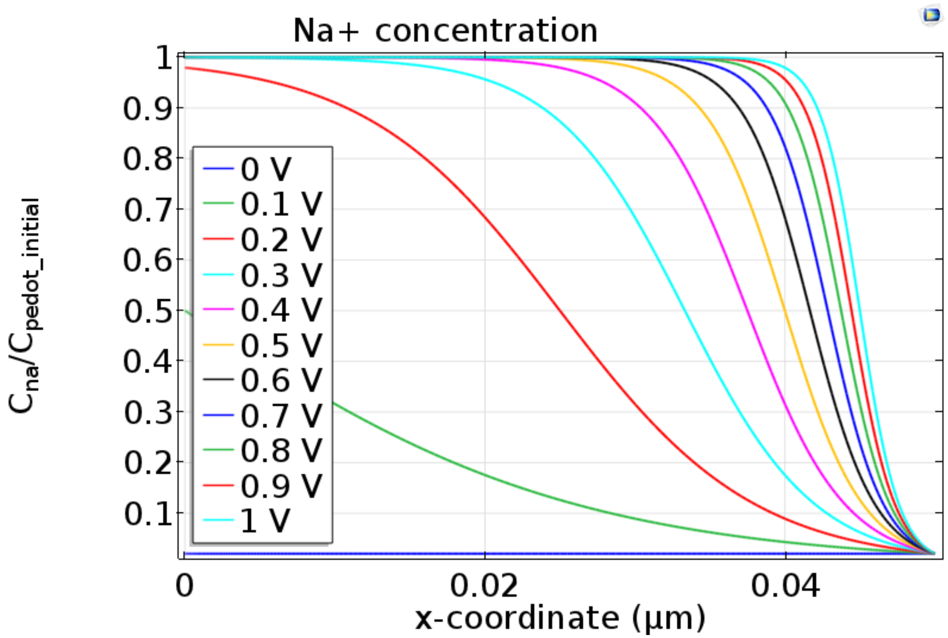
1D Model of Conductive Polymer dedoping and Ions distribution



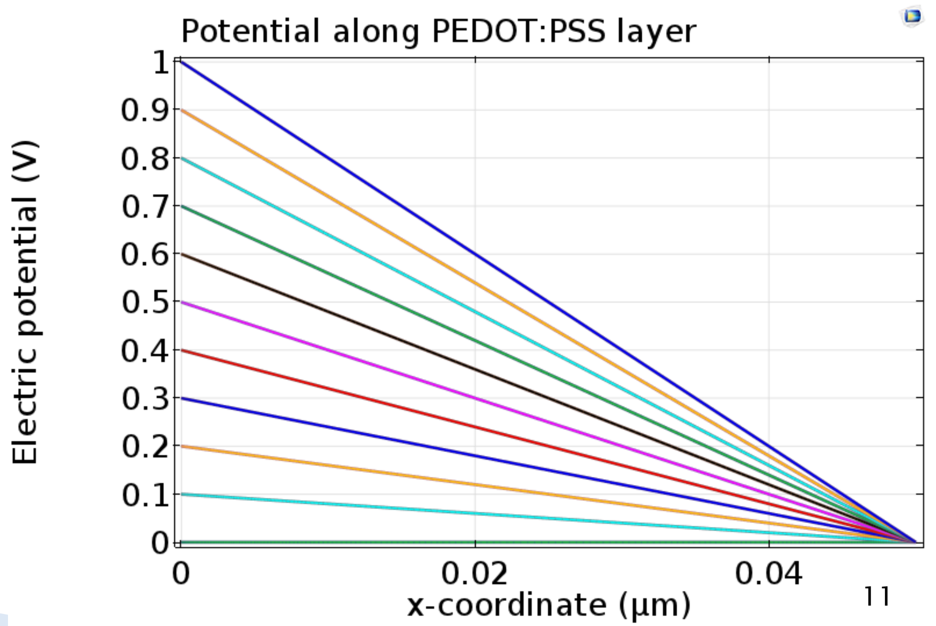
Modelled 1D structure consists of two point electrodes at both sides of line-layer of partially dedoped PEDOT:PSS with Na ions

1D Model results

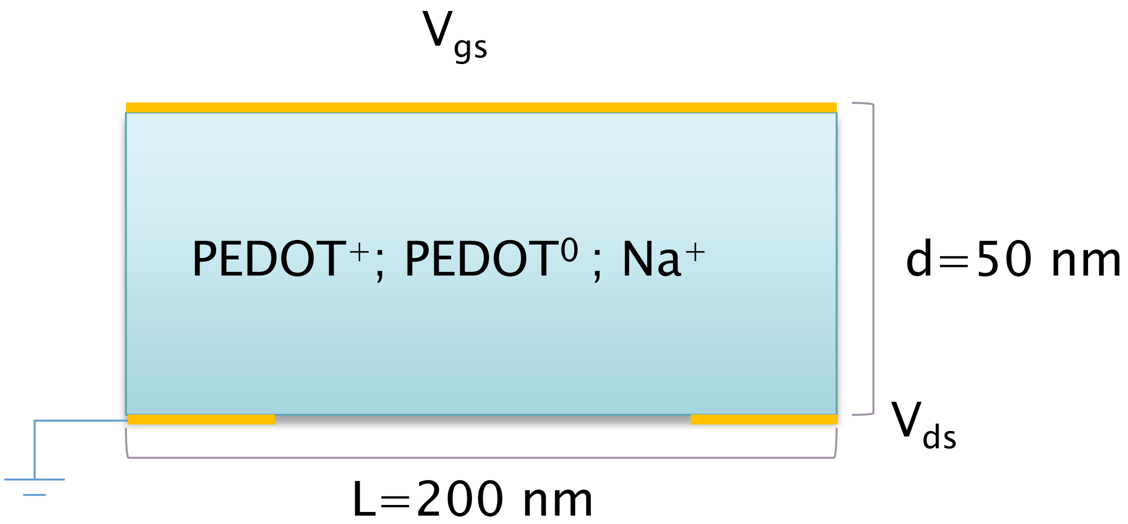




Model of moving front under applied potential



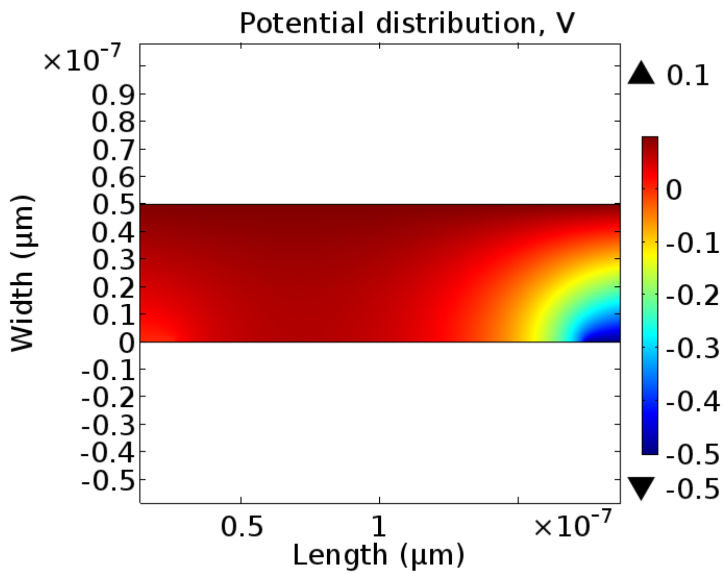
2D Model of Conductive Polymer dedoping and Ions distribution



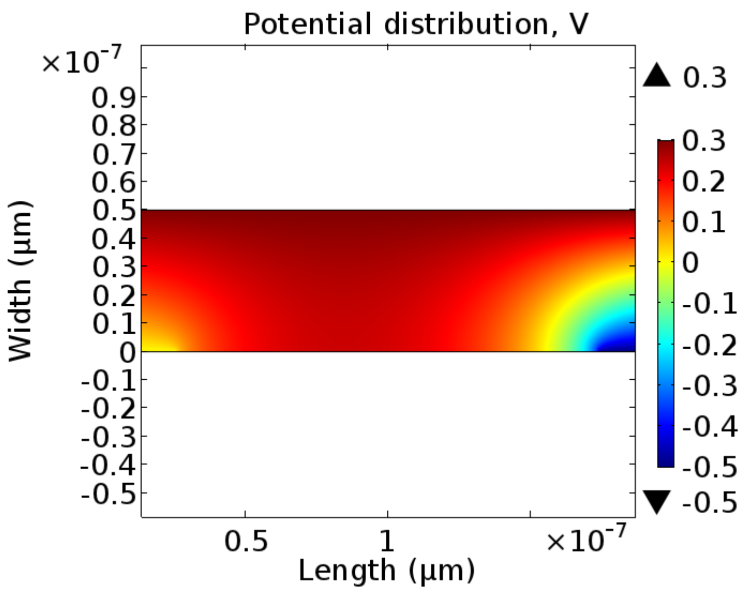
Modelled 2D structure consists of three planar electrodes: Drain and grounded Source at the bottom and Gate at the top of partially dedoped PEDOT:PSS with Na ions.

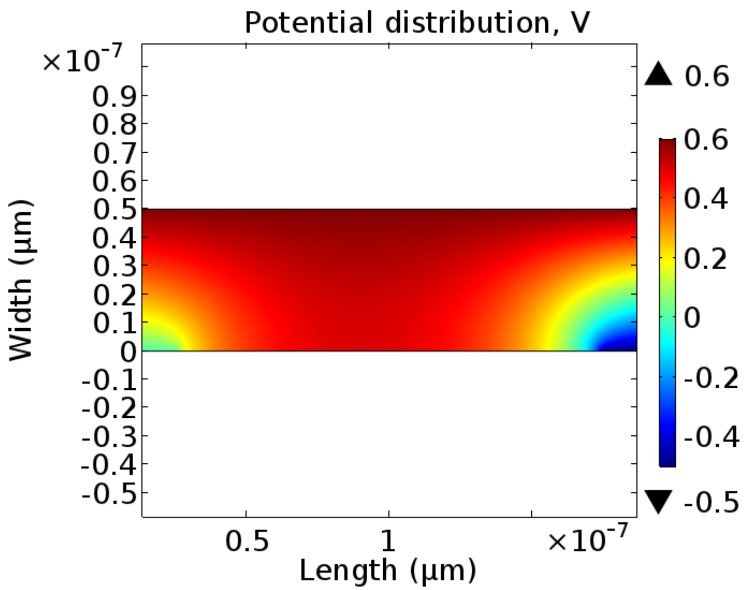
2D Model results

$Vgs = 0.1\ \mathrm{V}$



$Vgs = 0.3\ \mathrm{V}$



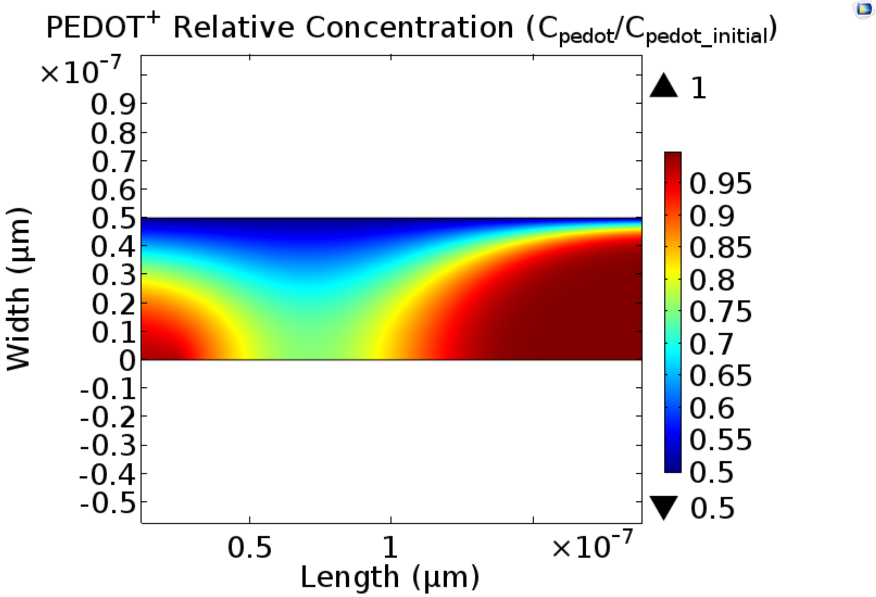


$Vgs = 0.6\ \mathrm{V}$

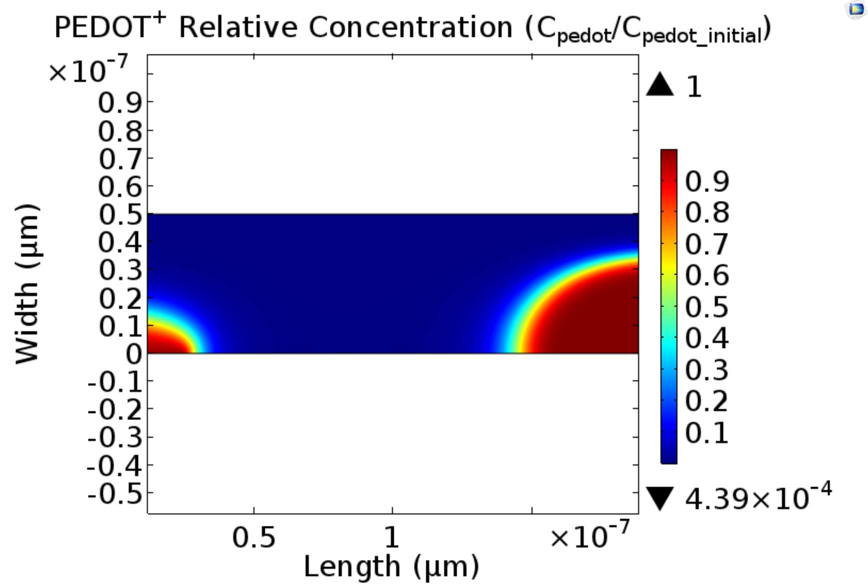
Potential distribution inside PEDOT:PSS layer under applied Gate-Source potential with Drain-Source potential: V_{ds}=-0.5V

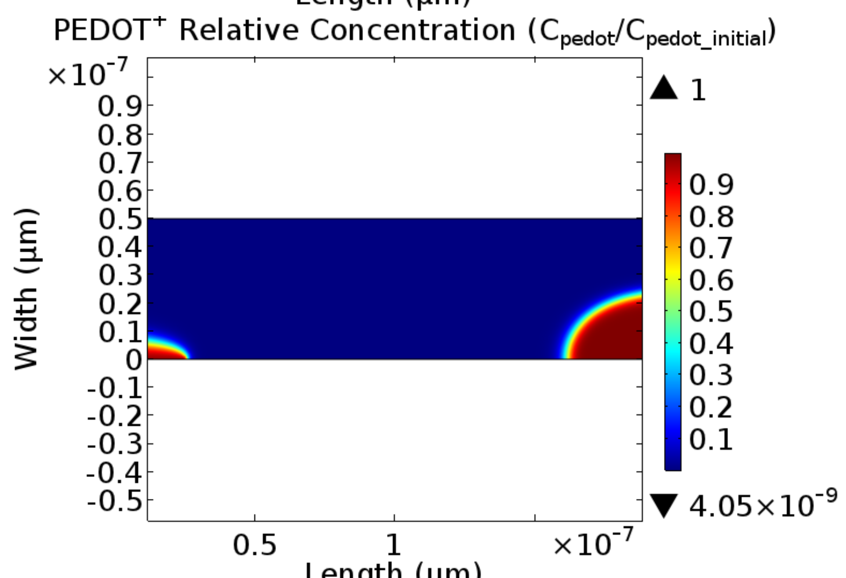
2D Model results

$Vgs = 0.1\ \mathrm{V}$



$Vgs = 0.3\ \mathrm{V}$



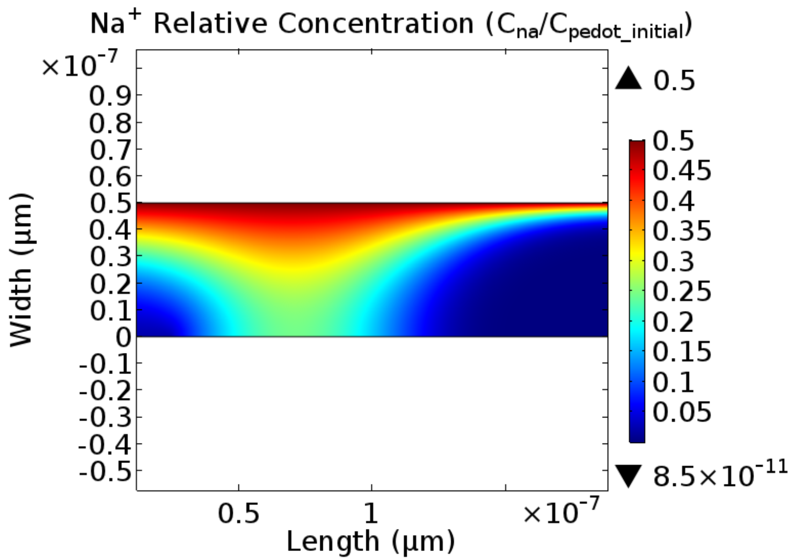


$Vgs = 0.6\ \mathrm{V}$

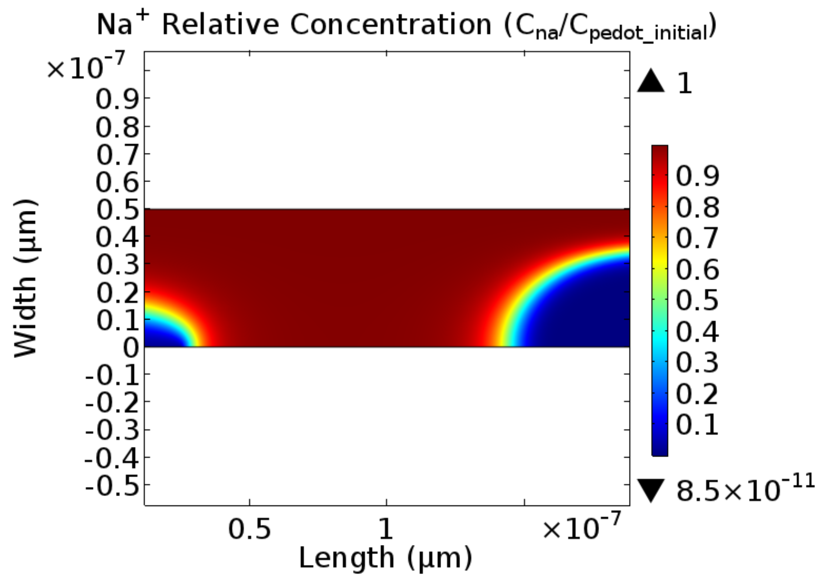
Reduction of $PEDOT^+$ in PEDOT:PSS layer under applied Gate-Source potential with Drain-Source potential: V_{ds}=-0.5V

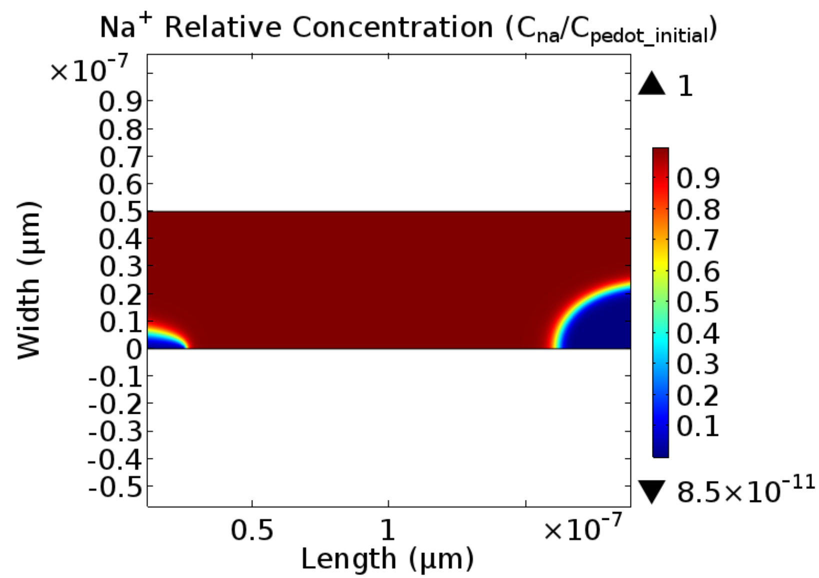
2D Model results

$Vgs = 0.1 \text{ V}$



$Vgs = 0.3 \text{ V}$





$Vgs = 0.6 \text{ V}$

Penetration of Na^+ into PEDOT:PSS layer under applied Gate-Source potential with Drain-Source potential: V_{ds}=-0.5V

Results…

- Moving front experiment was numerically modelled
- Color chandge of PEDOT:PSS layer could be explaned by introduction of Nernst equation of redox reaction

… and following investigation

Further investigations would be dedicated to 3D model of full OECT transistor with different real geometries to build up a full model of this type of biosensor

рахмат
danke
謝謝
ngiyabonga
spas
teşekkür ederim
Баярлалаа
mersi
kia ora
barka
welalin
tack
mahalo
tapadh leat
спасибо
faafetai lava
vinaka
спасибі
blagodaram
dank je
misaotra
matondo
paldies
grazzi
kiitos
dankie
thank you
gracias
хвала
nanni
nandri
dhanyavad
mauruuru
köszönöm
açiü
asante
manana
obrigada
tenki
bedankt
bayarlalaa
gràçie
hvala
akun
dankon
djiere dieuf
tau
mochchakkeram
murakoze
enkosi
dziękuję
дякую
mamnun
chokrane
chnorakaloutioun
gratias ago
gràcies
sulpáy
go raibh maith agat
sobodi
dĕkuji
sagolun
sukriya
kop khun krap
taiku
obrigado
mèsi
didi madloba
najis tuke
ありがとう
tanemirt
grazie
arigatô
takk
dakujem
trugarez
kam sah hamnida
rahmat
terima kasih
rahmet
ευχαριστώ
diolch
dhanyavadagalu
shukriya
mercê
мерси
তোমাকে ধন্যবাদ
감사합니다
xièxie
merci