Numerical modelling of ionically gated small molecule OPV structure

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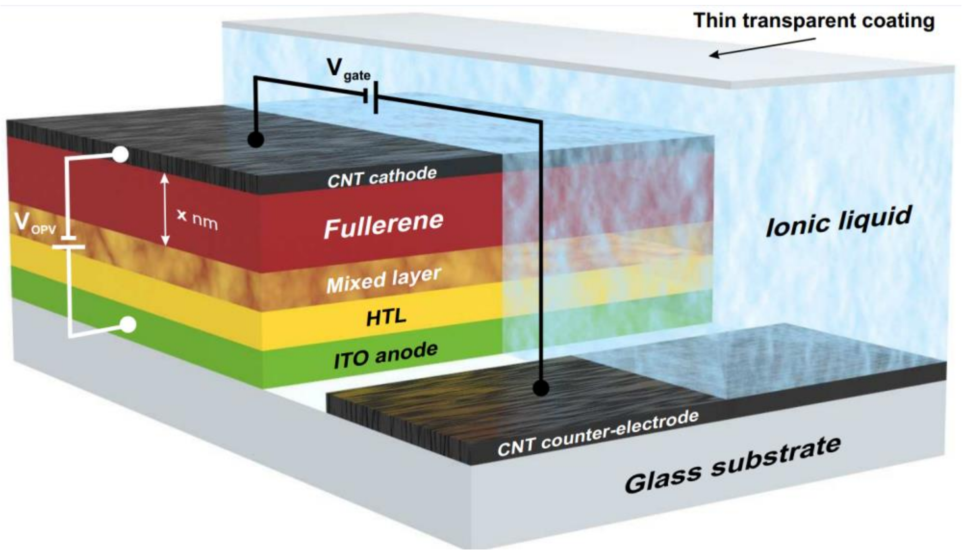

Fig.1- OPV Schematic

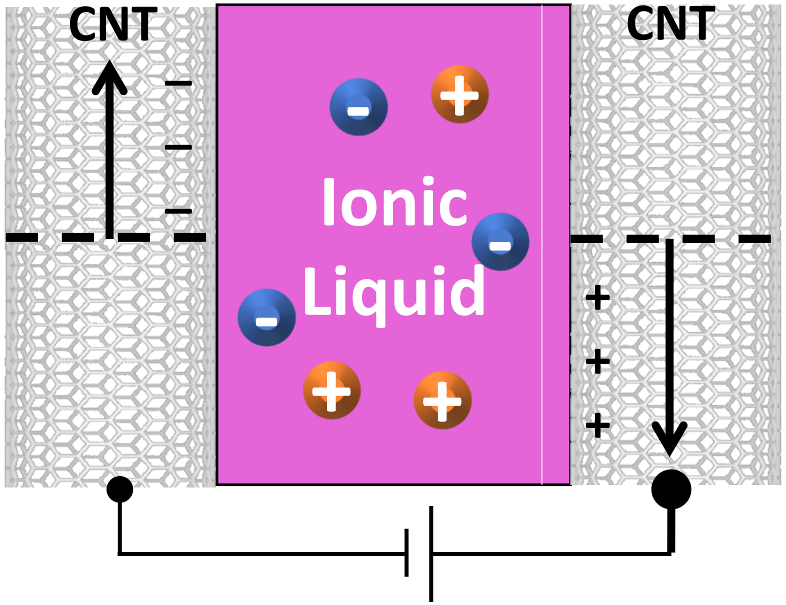

Fig.2- Ionic Liquid Penetration inside layers

Ionic Liquid penetrates inside MWCNT and C60 and improve the IV curve through the reduction of cathode work function and doping of C60

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Optical part → Transfer Matrix Method

$$Q(x,\nu) = \frac{1}{2} c\epsilon_0 \alpha n \mid E(x) \mid^2$$

$$G(x,\nu) = Q(x,\nu)/(h\nu)$$

$$G(x) = \int G(x,\nu) d\nu$$

[1] Koster, L. J.; Smits, E.; Mihailetchi, V.; Blom, P. Device model for the operation of polymer/fullerene bulk heterojunction solar cells. Physical Review B2005, 72, 085205.

[2] Grove, A. S. Physics and Technology of Semiconductor Devices; John Wiley & Sons, Inc., 1967.

Electrical Part → Drift Diffusion Model

Main system of equation

$$\nabla^2 V = \rho/\epsilon,$$

$$\nabla \cdot J_i = \pm qU \qquad i = n, p,$$

$$J_n = qn\mu_n \nabla V_{\mathrm{LUMO}} + \mu_n k_B T \nabla n$$

$$J_p = qn\mu_p \nabla V_{\mathrm{HOMO}} + \mu_p k_B T \nabla p$$

Boundary Conditions

$$n_{\mathrm{th}} = N_{\mathrm{LUMO}} \cdot exp\left(\frac{-q\phi_n}{k_B T}\right)$$

$$p_{\mathrm{th}} = N_{\mathrm{HOMO}} \cdot exp\left(\frac{-q(\phi_n - E_{\mathrm{gap}})}{k_B T}\right),$$

$$n_{\mathrm{th}} = N_{\mathrm{LUMO}} \cdot exp\left(\frac{-q(\phi_p - E_{\mathrm{gap}})}{k_B T}\right)$$

$$p_{\mathrm{th}} = N_{\mathrm{HOMO}} \cdot exp\left(\frac{-q\phi_p}{k_B T}\right),$$

$$V_{\mathrm{anode}} - V_{\mathrm{cathode}} = V_a - V_{\mathrm{bi}}$$

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Excitons Generation → Onsager-Braun theory

$$k_{\text{diss}} = \frac{3\gamma}{4\pi a^3} exp\left(\frac{E_b}{k_B T}\right)\left(1 + b + \frac{b^2}{3} + \frac{b^3}{18} + \frac{b^4}{180} + \ldots\right).$$

$$b = q^3 \nabla V / (8\pi \epsilon_0 \epsilon_r k_B^2 T),$$

$$p = \frac{k_{\text{diss}}}{k_{\text{diss}} + k_F}.$$

$$P = \int_0^\infty p \frac{4}{\sqrt{\pi} a^3} r^2 exp\left(\frac{-r^2}{a^2}\right) dr.$$

for considering local disorder in organic material the dissociation rate is integrated over a Gaussian distribution of binding distances

$$U = -q(PG - (1 - P)R),$$

[3] Mingebach, M.; Walter, S.; Dyakonov, V.; Deibel, C. Direct and charge transfer state mediated photogeneration in polymer-fullerene bulk heterojunction solar cells.Appl. Phys. Lett2012, 100

[4] Barker, A.; Ramsdale, C. M. Modeling the current-voltage characteristics of bilayer polymer photovoltaic devices.Phys. Rev. B2003, 67

Recombination → Langevin recombination

$$R_L = \zeta \gamma (np - n_i^2).$$

$$n_i = \sqrt{N_{\text{HOMO}} N_{\text{LUMO}}} exp\left(-\frac{E_{\text{gap}}}{2k_B T}\right)$$

$$\gamma = q(\mu_n + \mu_p)/(\epsilon_r \epsilon_0).$$

[5] Langevin, P. Recombinaison et mobilites des ions dans les gaz. Ann. Chim. Phys.1903,
28, 433–530.

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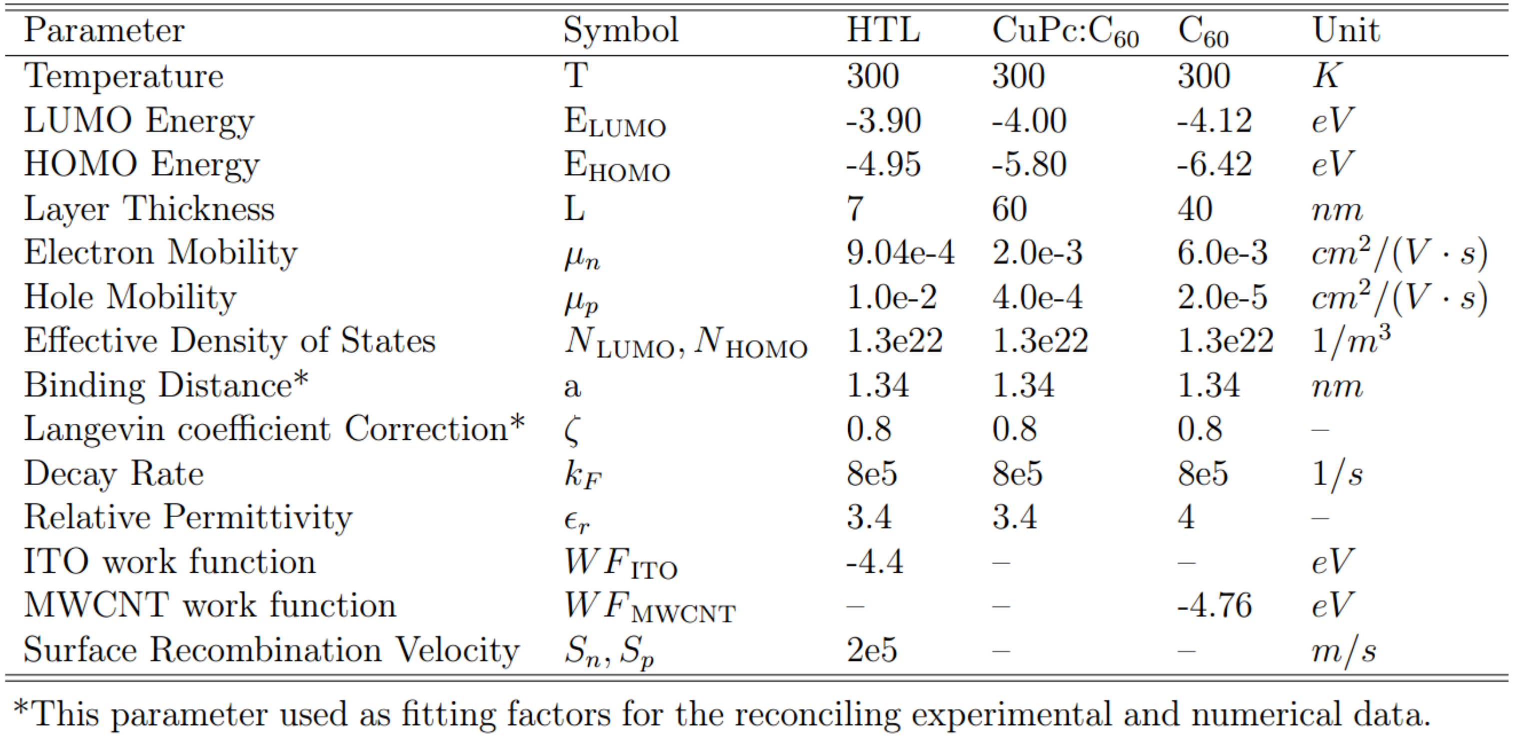
Simulation Parameters

We used finite element method and simulated OPV in one dimension



Parameter	Symbol	HTL	CuPc:C_{60}	C_{60}	Unit
Temperature	T	300	300	300	K
LUMO Energy	E_{LUMO}	-3.90	-4.00	-4.12	eV
HOMO Energy	E_{HOMO}	-4.95	-5.80	-6.42	eV
Layer Thickness	L	7	60	40	nm
Electron Mobility	μ_n	9.04e-4	2.0e-3	6.0e-3	$cm^2/(V \cdot s)$
Hole Mobility	μ_p	1.0e-2	4.0e-4	2.0e-5	$cm^2/(V \cdot s)$
Effective Density of States	N_{LUMO}, N_{HOMO}	1.3e22	1.3e22	1.3e22	$1/m^3$
Binding Distance*	a	1.34	1.34	1.34	nm
Langevin coefficient Correction*	ζ	0.8	0.8	0.8	–
Decay Rate	k_F	8e5	8e5	8e5	$1/s$
Relative Permittivity	ϵ_r	3.4	3.4	4	–
ITO work function	WF_{ITO}	-4.4	–	–	eV
MWCNT work function	WF_{MWCNT}	–	–	-4.76	eV
Surface Recombination Velocity	S_n, S_p	2e5	–	–	m/s

*This parameter used as fitting factors for the reconciling experimental and numerical data.

Energy Diagram of OPV

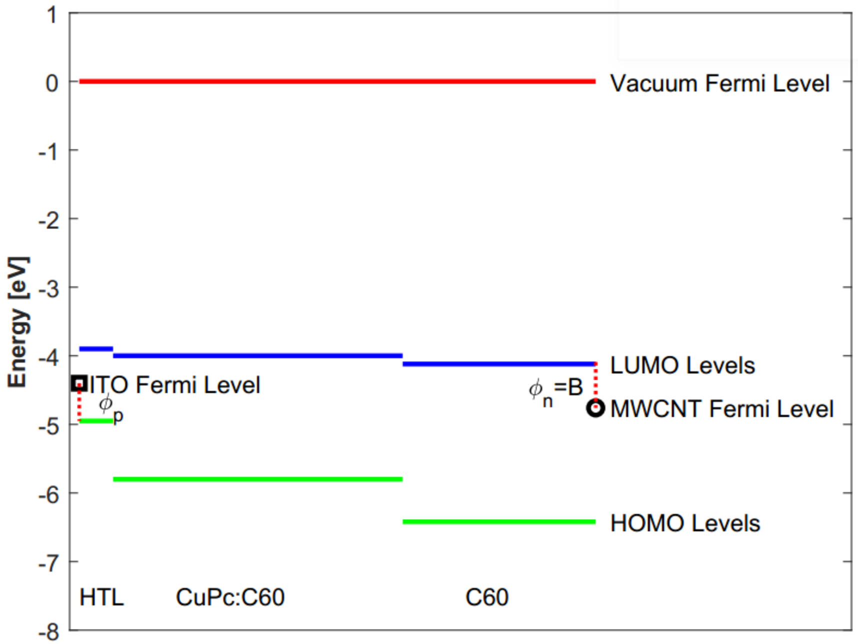


Fig.3- Energy diagram of OPV

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We changed the barrier and defined dopant concentration and profile, and used the generation rate from optical part

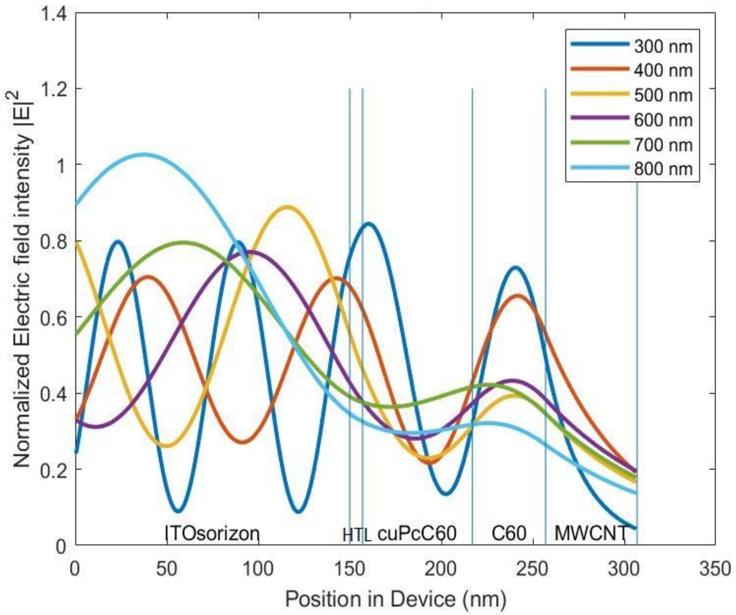

Fig.4- Electric field distribution in OPV

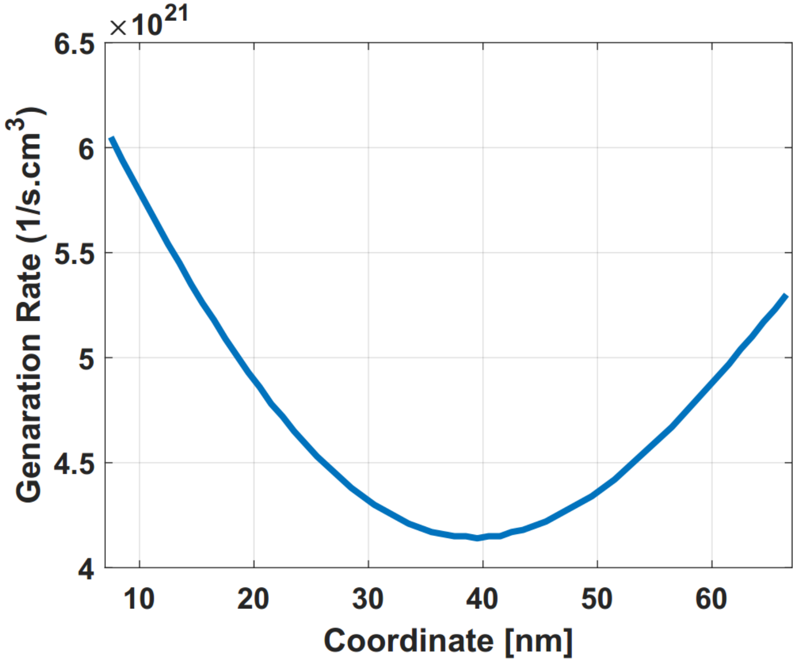

Fig.5- Generation Rate

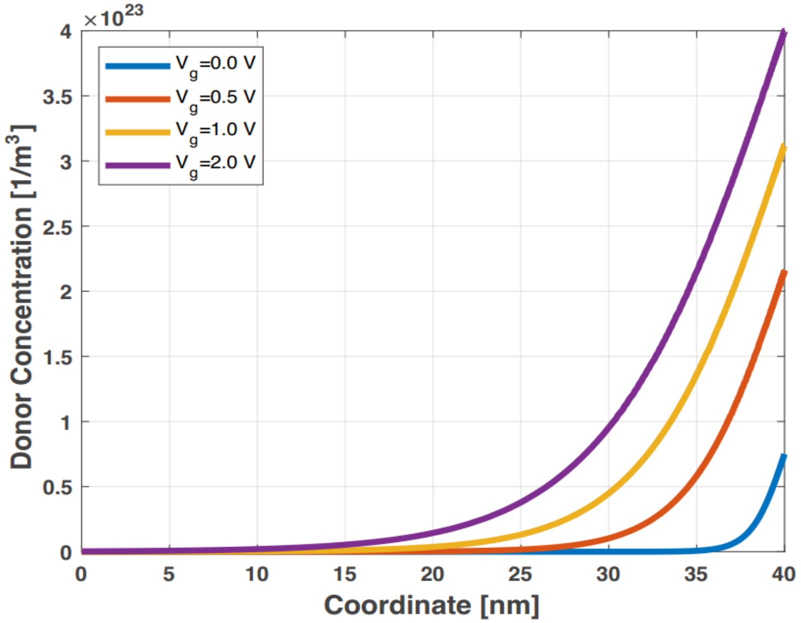

Fig.6- Dopant Concentration in C60 layer

[6] Torben Menke, Debdutta Ray, Hans Kleemann, Karl Leo and Moritz Riede, Determining doping efficiency and mobility from conductivity and Seebeck data of n-doped C60 layers, Basic Solid State Physics, 252(8), 1877–1883

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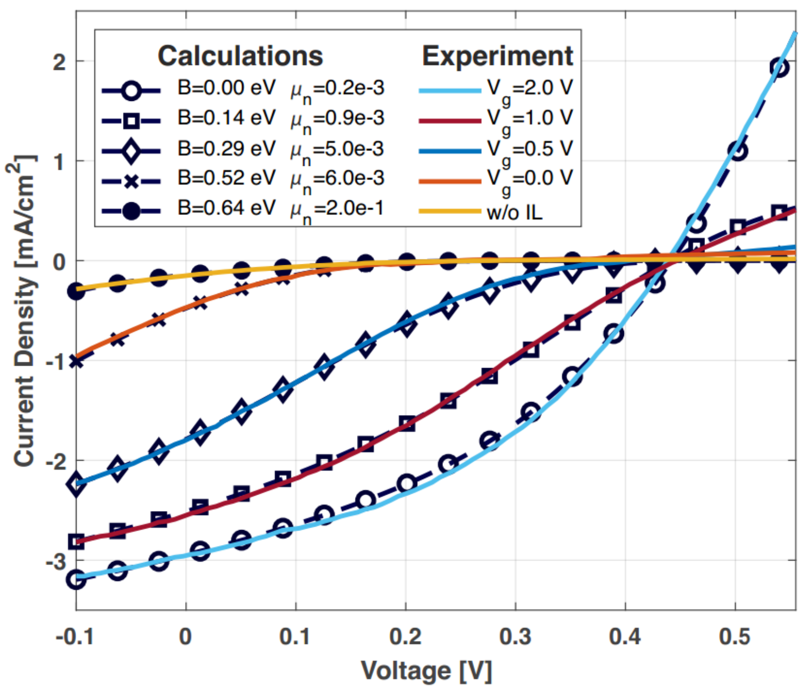

Fig.7- Fitted IV curves for different barrier, different mobility and different dopant concentration

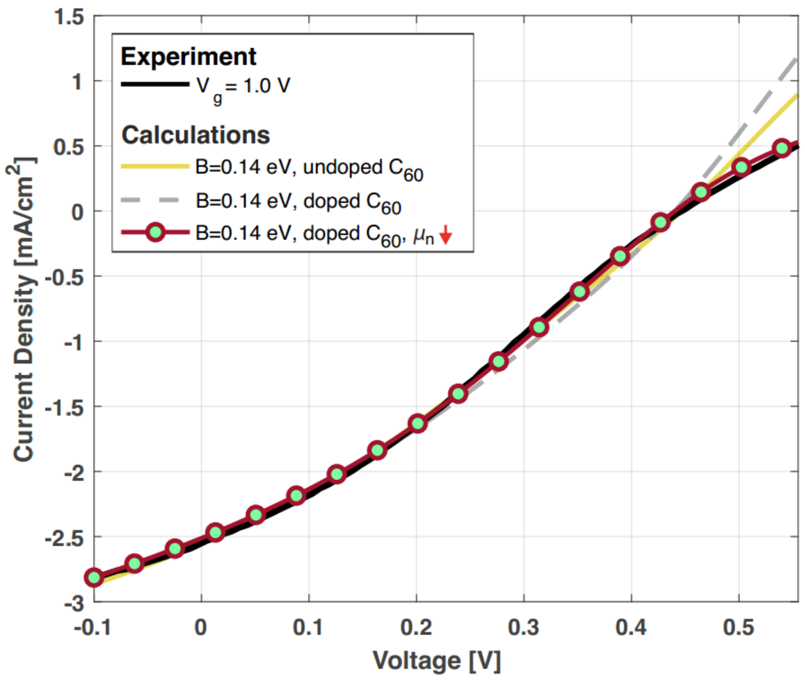

Fig.8- Fitted IV curve for 0.14 V barrier and considering different phenomena

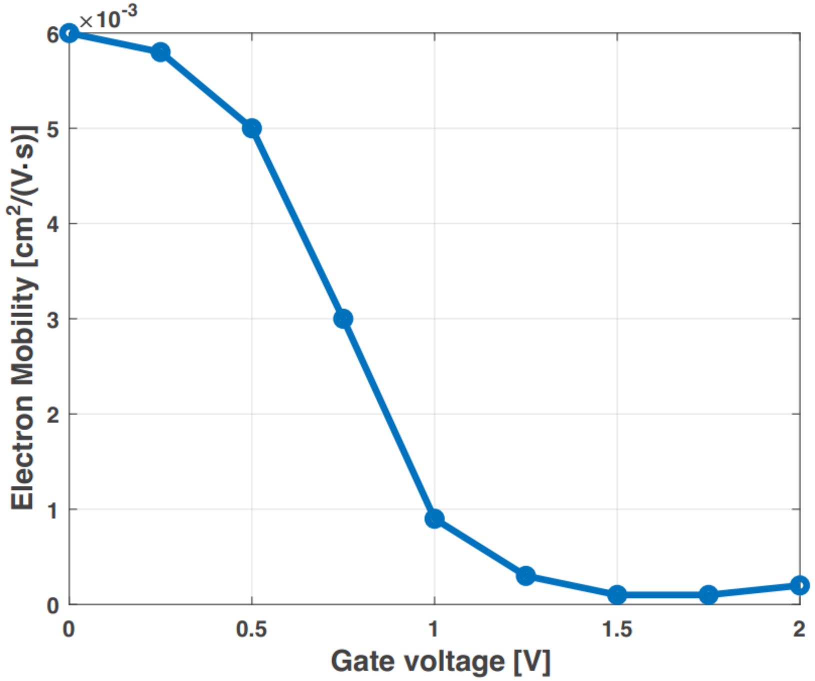

Fig.9- Mobility changing for different dopant concentration correspond to different gate voltage

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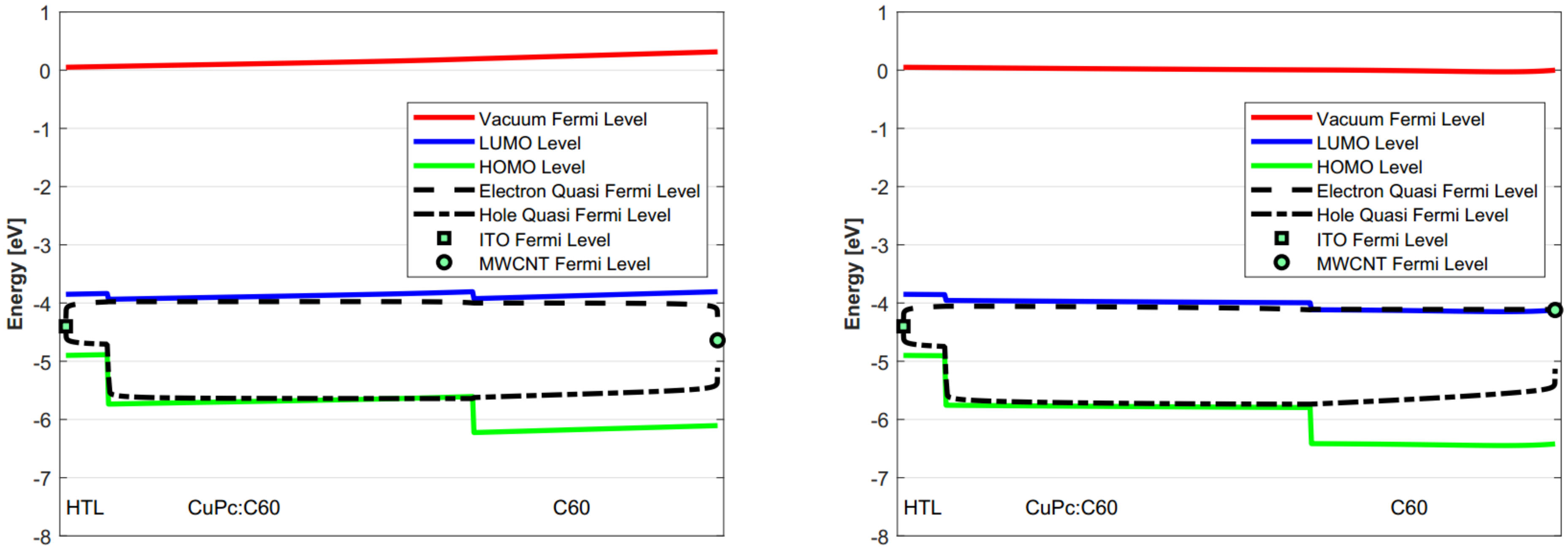

Fig.10- Energy diagram of OPV when the gate voltage is 0 V (left) and 2 V (right) at the point of maximum extracted power

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1. Penetration of dopant from ionic liquid into the cathode raises the Fermi level of the cathode significantly in a way that the potential barrier between LUMO level of the ETL layer and cathode becomes zero.
2. The dopant penetrates further from the cathode side and reaches the ETL layer affecting the macroscopic properties of the ETL layer.
3. The dominant phenomena in improving OPV performance using ionic liquid is raising of the cathode Fermi level and forming an ohmic contact between the ETL layer and cathode.

Danila S. Saranin, Abolfazl Mahmoodpoor, Pavel M. Voroshilov, Constantin R. Simovski, and Anvar A. Zakhidov* ,Ionically Gated Small Molecule OPV: Interfacial doping of Charge collector and Transport layer, arXiv:1805.10954.

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