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Optimized Graphene Nanoribbon UV Phototransistor Based on ZnO Sensitive Gate for Optical Wireless Communications

F. Djeffal and H. Ferhati

Abstract— **In this paper, we demonstrate the role of the strategic combination between Graphene Nanoribbon (*GNR*) channel and Particle Swarm Optimization (*PSO*) technique in designing high UV photoresponse sensors for optical wireless communication systems (*OWCSs*) Accurate numerical models are developed based on non-equilibrium Green's function (*NEGF*) formalism, which are used to solve the Schrödinger/Poisson equations self-consistently. The device *UV*-photoresponse mechanism is investigated and thoroughly discussed. Basically, the channel electrostatic behavior is modulated by the photo-induced e/h pairs in the *ZnO* thin-film gate, generating the photogating effect. In addition, *PSO* technique is implemented with the aim of busting up the device performance. It is found that the proposed design showcases the ability for reaching higher responsivity as compared to the traditional *Si*-based devices, exhibiting a high responsivity of 2×10^5 *A/W*. Therefore, the use of *GNR* channel combined with *ZnO* sensitive-gate allows designing an ultra-high ultraviolet photoresponse, making the proposed structure a potential alternative for next-generation chip-level optical communications.**

Index Terms— **ZnO; Graphene Nanoribbon; PSO; Phototransistor; Responsivity; Optical communication**

I. Introduction

Nowadays, traditional optimization techniques face extensive challenges to solve challenges related to global optimization in various domains involving economics, material science, military and engineering [1]. The major reason behind their failure resides on the fact that they can be entrapped in local optima solutions [2]. Alternatively, major research interests have been turned out towards emerging some innovative artificial intelligence tools [1-3]. For instance, metaheuristic methods like Particle Swarm Optimization (*PSO*) and Genetic Algorithm (*GA*) proved promising effectiveness in treating problems in the field of engineering. These complex problems could involve multiple-conflict goals. For this purpose, these evolutionary approaches have triggered a great deal of attention, offering the possibility to deal with global optimization challenges [2-4]. These advantages have allowed the expansion of efficient OWCS [4].

Recently, worldwide research groups are interested in developing high-performance optical interconnection systems (*OISs*), demonstrating large-bandwidth and reduced resistive losses [5]. Accordingly, the performance of the realized long distance *OISs* has previously reached a high level of competitiveness with the traditional ones based on electrical wires [5-6]. However, photodetector or photodiode devices are regarded as the main photoreceiver designs commonly involved in *OISs*. The latter imposes the use of further read-out circuits to ensure the communication voltage level [7-10]. To overcome this challenge, *Ge*-gate, quantum-dots and nanostructuring-based phototransistors were investigated, showing the ability for providing favorable responsivities [11-13]. Despite this characteristic, the use of *Si*-channel not only limits the device ultraviolet photoresponse and optical commutation speed, but also can exhibit a high visible photoresponse. Furthermore, the developed phototransistors utilize rare and high-cost materials such as *Ge* and *GaAs* involving complex manufacturing process. *ZnO UV* Photodetectors have received a great deal of attention during the last few years [12-13]. However, the low carrier mobility associated with *ZnO* material and difficulties for fabricating p-type *ZnO* constitute the main challenges preventing the fabrication of high-performance *ZnO* phototransistors. Therefore, it is important to propose new designs to break the responsivity limits using cost-effective phototransistors compatible with advanced *Si*-photonics.

After decades of continuous downscaling of transistors according Moore’s law, the rise of graphene *2D* material has paved the way for achieving integrated nanoelectronic and *Si*-photonic platforms [14-15]. To this extent, possessing fascinating structural and optoelectronic characteristics including ultra-high carrier mobility, flexibility, *CMOS* compatibility, high-transparency, graphene *2D* material has allowed designing diversity of optoelectronic devices like phototransistors, transparent electrodes, and photodetectors [16-18]. Nevertheless, its short light-matter interaction length causes the weak photoresponse, which limits its application for light-harvesting devices [16]. On the other hand, graphene

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shows extensive recombination losses due to the ultra-short carrier lifetime [17]. Intuitively, capping the *GNR*-based transistor with low-cost earth abundant *ZnO* thin-film acting as *UV*-light sensitive gate can optically modulate the channel conductivity and reach a high photoresponse. In this perspective, this work aims to propose a novel high-responsivity *UV*-phototransistor based on *GNR* channel combined with *ZnO* photo-gate. The sensor photoresponse is studied and thoroughly elucidated by carrying out. It is revealed that the optimized design outperforms the *Si*-based structure regarding the *UV*-photoresponse, making it potential alternative for the future progress of nanoelectronic-photonic integrated systems.

II. DEVICE STRUCTURE AND MODELING FRAMEWORKS

Fig.1 depicts the cross-section of the investigated *GNR*-based phototransistor structure. It consists of capping the *GNR* transistor with a *ZnO* photo-gate generating photo-gating effect under illumination. In this figure, *L* denotes the channel length, d_{ZnO} represents the *ZnO* sensitive layer thickness and t_{ox} is the HfO_2 dielectric gate thickness. To investigate the optical performances of the device, the phototransistor is exposed to *UV*-light with an optical power P_i at normal-incidence with λ=*365 nm*. Principally, offering a high derived current capability, an armchair-edge *GNR* with *12* atoms of carbon, band-gap value of *0.60 eV* and *1.35 nm* of width is suggested as a channel in our device [18]. Besides, HfO_2 is inserted in the device as dielectric gate with t_{ox} of thickness.

In our *GNR*-based phototransistor device, the channel length (*L*) with tens of nanometers is assumed, underlining the presence of quantum effects. In this framework, the device is modeled using the quantum transport simulation achievable by *NEGF* technique. The *GNR* charge density is calculated by taking into account the ballistic transport. In this sense, the Schrödinger equation is solved by means of *NEGF* formalism in mode space [17]. The Schrödinger/Poisson equations are solved self-consistently, as it is described in the flowchart shown in Fig.2. Thus, based on the Hamiltonian matrix (*H*) of the *GNR* [19], the retarded Green's function is estimated from [20]

$$G(E) = [EI - H - \Sigma_S - \Sigma_D]^{-1} \tag{1}$$

where E is the energy, Σ_S and Σ_D are the self-energy matrices of source and drain extremities and I is the identity matrix.

Sharp levels at the sub-band minimum energies are considered for density of states of the device channel. Besides, the S/D electrodes are assumed with continuous distribution of states. So, the level broadening quantities Γ_S, Γ_D are estimated by means of the following formula [11-18]

$$\Gamma_S = i\left(\Sigma_S - \Sigma^{+}{}_S\right) \tag{2-a}$$

$$\Gamma_D = i\left(\Sigma_D - \Sigma^{+}{}_D\right) \tag{2-b}$$

The local density of states resulted from S/D injection is determined by subsequent equations

$$D_S(E) = G\,\Gamma_S\,G^{+} \tag{3-a}$$

$$D_D(E) = G\,\Gamma_D\,G^{+} \tag{3-b}$$

The charge density related to channel position can be computed by the model presented in previous work [17].

Besides, *2D* Poisson equation can be solved by Finite Difference Method (*FDM*)

$$\nabla^2 U = \frac{-q}{\varepsilon}\rho \tag{4}$$

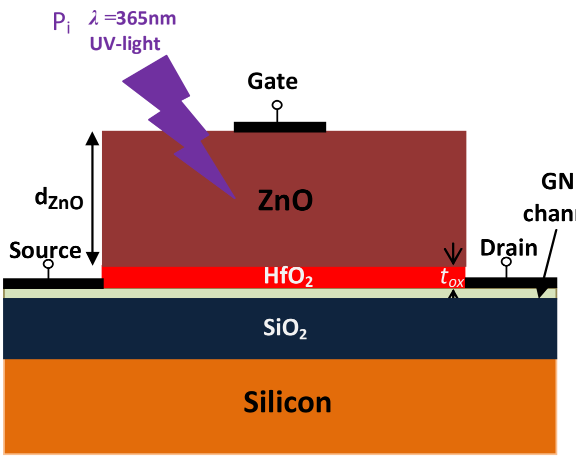

Fig. 1 The investigated GNR-phototransistor structure based on ZnO capping layer.

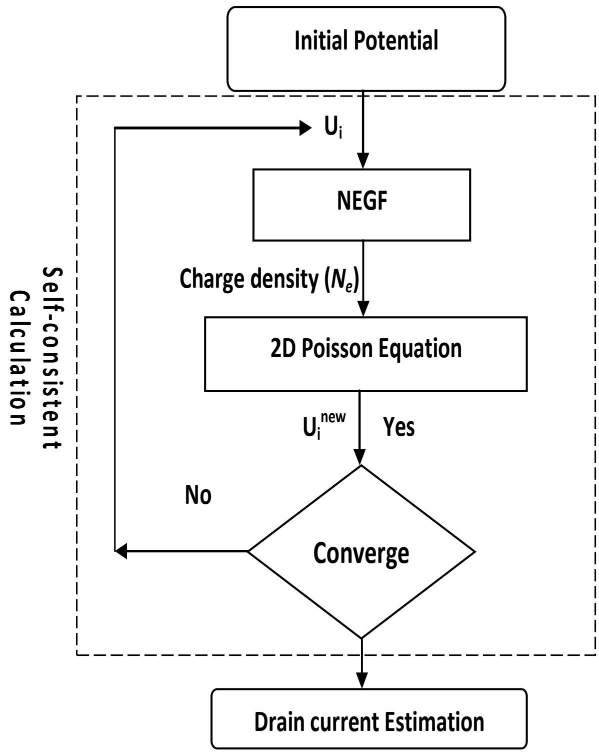

Fig. 2. Flowchart representing the adopted numerical modeling approach.

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where U is the electrostatic potential, ε refers to HfO_2 dielectric constant, q denotes the electron charge and ρ is the net charge density distribution.

The UV illumination of the analyzed UV-phototransistor leads to generate electron-hole pairs within the *ZnO* thin-film. This effect can alter electrostatic behavior of the channel. Besides, the applied gate voltage is modified due to the generation of the photogating effect, leading to induce an effective gate voltage, which can be given by

$$V_{gs}^{*} = V_{gs} + V_{ph}(P_i) \quad (5)$$

where V_{ph} represents the optically induced voltage, V_{gs} refers to the gate voltage [21] and P_i is the incident light power

$$V_{ph} = V_t \ln\left(\frac{I_{ph}}{I_s}\right) \quad (6)$$

where V_t is the thermal voltage, I_{ph} denotes the photocurrent density generated in the *ZnO* gate and the saturation current is I_s.

Therefore, the channel current is determined by the Landauer-Büttiker model [16]

$$I = \frac{2q}{h}\int dE\, T(E)\left[f(E-E_{FS}) - f(E-E_{FD})\right] \quad (7)$$

where *T(E)* is the transmission coefficient given by

$$T(E) = T_r\left(\Gamma_S G\ \Gamma_D\ G^{+}\right) \quad (8)$$

III. Results and Discussions

To elucidate the operating mechanism of the *GNR UV*-phototransistor capped with *ZnO* thin-film as photosensitive gate, the extracted I_{ds}-P_i characteristic of the proposed device using the developed numerical model presented in the last sub-section is compared to the conventional *Si*-channel based phototransistor and illustrated in Fig.3 with $V_{gs}=0.1V$, $V_{ds}=0.3V$, $d_{ZnO}=75nm$ and $\lambda=365nm$. Obviously, *GNR*-based phototransistor shows photocurrent generation then that provided by *Si*-channel counterpart. . in this context, a high photocurrent of $20\mu A$ is achieved. *GNR* material possesses ultra-high carrier mobility, leading to enhance the device drain current. In addition, the investigated phototransistor based on *GNR* channel and *ZnO* capping layer demonstrates a high-photoresponse at lower optical power densities as compared to the conventional one, resulting in decreasing the overall energy consumption of the IOSs system. The optical power increase leads to increasing the optical voltage through photogating effect, which can in turn allow the modulation of the *GNR* channel electrostatic properties. Therefore, introducing a *ZnO* capping layer acting as photo-gate combined with *GNR* channel, we were able to attain enhanced control of the channel under UV light illumination. This benefit offers wider possibilities to reach enhanced ultraviolet photosensing properties with respect to the traditional sensors based on Si building blocks.

These interesting results of *GNR*-based phototransistor inspire the study of the device responsivity behavior with respect to the channel length. In this framework, Fig. 4 shows the obtained device responsivity values against *GNR* channel lengths. This figure showcases that short channel phototransistors are in fact worse choice for *GNR UV* sensors. In other words, the downscaled devices show a low photoresponse. This is due to the reduced photosensitive area when the sensor is scaled down. Moreover, the dark current will be increased leading to increase dark-noise effects. On the other hand, long channel devices demonstrate an ultra-high responsivity exceeding 2.5×10^{5} A/W. Therefore, we believe that the performed study can be useful for elucidating the role of using *ZnO* capping *GNR* channel for achieving high-responsive phototransistors. The next step is devoted to the performance optimization of the device using new emerging artificial intelligence techniques in order to boost the device *FoM* for *OWCS*. For this reason, *PSO* approach is implemented in the next sub-section.

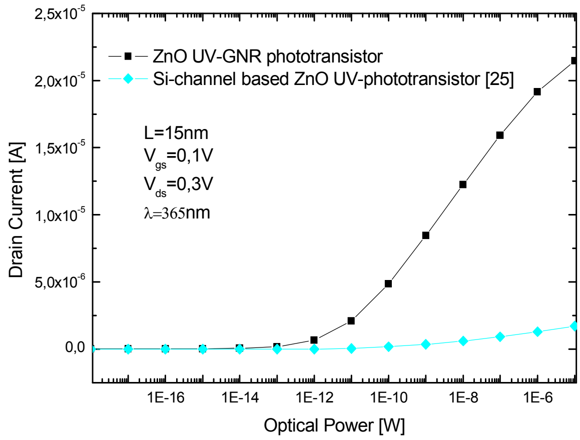

Fig. 3. *I-P_i* curves of the proposed *GNR* phototransistor with *ZnO* capping layer compared to that of the conventional Si-channel based counterpart with $V_{gs}=0.1V$ and $V_{ds}=0.3V$.

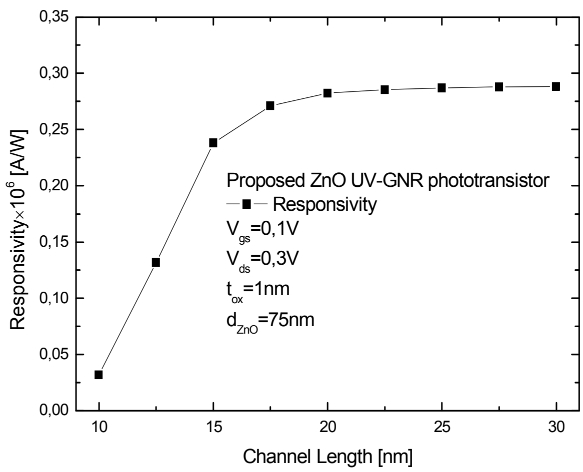

Fig. 4. Responsivity versus *GNR* channel length with $\lambda=365nm$, $d_{ZnO}=75nm$, $V_{gs}=0.1V$ and $V_{ds}=0.3V$.

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A. PSO optimization ZnO GNR FET-based UV sensor

Basically, several design parameters such as the *ZnO* photosensitive layer and oxide thickness can influence the performance of the investigated phototransistor and can induce a complex photoelectrical behavior. In order to boost up the device performance, *PSO* metaheuristic method is implemented to select the best configuration of the analyzed *ZnO GNR FET*-based *UV* sensor. This technique is first proposed by Eberhart and Kennedy [22]. It imitates the social behavior of bird flocking to minimize the fitness function using random methods, thus enabling the identification of the global solution. This metaheuristic technique suggests the use of bird flocking behavioral model to minimize the fitness function. The searching mechanism of the global solution is performed by moving the particles around a multidimensional search space and the particles of the swarm are updated from iteration to another according to the defined fitness function. In this sense, the model adjusts and updates the particles velocity (V_i^{k+1}) and position (X_i^{k+1}) in a swarm by exploiting the following expressions

$$V_i^{k+1} = wV_i^k + c_1 r_1 (p_{ij}^k - X_i^k) + c_2 r_2 (g_{ij}^k - X_i^k) \quad (9)$$

$$X_i^{k+1} = X_i^k + V_i^{k+1} \quad \text{with } i = 1..k \quad (10)$$

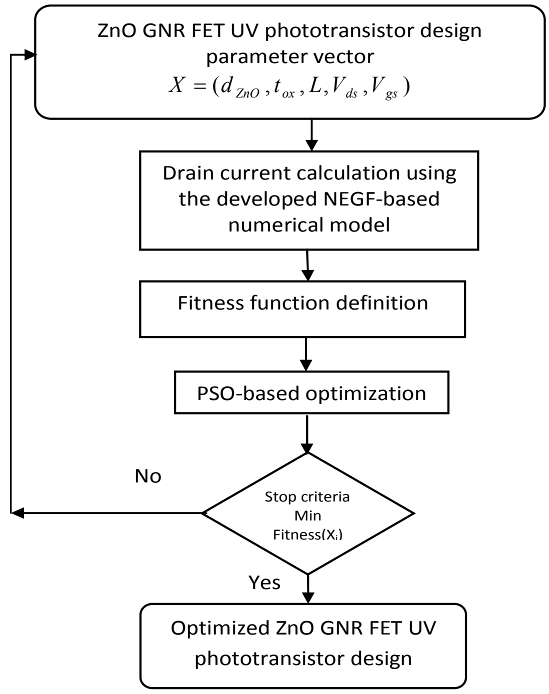
where *k* is the swarm size, p_{ij}^k and g_{ij}^k are best positions of each particle in the swarm and in the particles group, r_1 and r_2 represent random numbers, w represents the inertia weight applied to balance the global exploration. Cognitive and social acceleration factors are given as (c_1 and c_2).

In our case, the objective function is introduced to maximize the derived current capability (*I*) under *UV* illumination, which can be given by

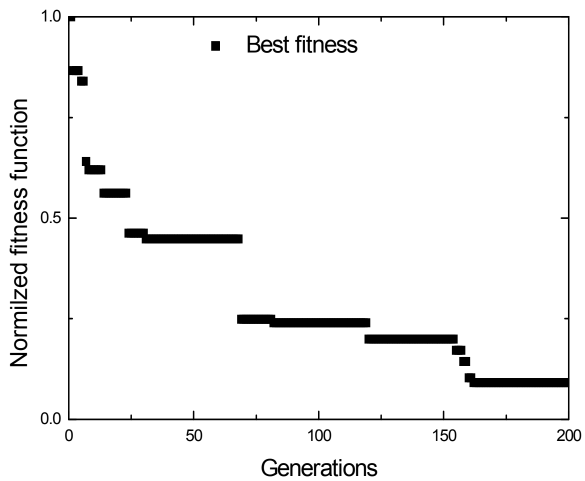
$$Fitness\,(X) = \frac{1}{I(X)} \quad (11)$$

where the design parameters vector is given by $X = (d_{ZnO}, t_{ox}, L, V_{ds}, V_{gs})$.

The stall generation and the size of the swarm are respectively *200* and *10*. The flowchart illustrated in Fig.5 (a) describes the proposed approach based on combining *PSO* method and non- *NEGF* formalism. *PSO* generates a random design parameter vector, which will be applied to the *NEGF*-based numerical model described in Fig.2. Afterwards, the obtained photocurrent is evaluated by the objective function and the iteration process continues until reaching the convergence criteria. In this context, Fig.5 (b) depicts the objective function versus *PSO* generation number. This figure shows that the fitness stabilizes after *150* generations. Moreover, the fitness function is effectively diminished and improvements concerning the device performance are achieved. The optimized design parameter vector of the *ZnO GNR FET UV* sensor is given as $X = (125nm, 4.5nm, 28nm, 0.5V, 0.25V)$. The obtained *FoM* parameters of the optimized *ZnO GNR FET*-based *UV* sensor are summarized and compared with that of the conventional phototransistors in Table.1. It can be concluded that the optimized device gives rise to enhanced FoM parameters as compared to the conventional one, where it yields 2×10^5 *A/W* of responsivity and over than *76 dB of* I_{ON}/I_{OFF} ratio. This makes the optimized *ZnO GNR FET*-based *UV* sensor appropriate for optical wireless communication systems.



(a)



(b)

Fig. 5. (a) Flowchart describing the adopted optimization approach based on *PSO* method. (b) Normalized fitness function versus the generation

TABLE I

PERFORMANCE COMPARISON BETWEEN THE OPTIMIZED GNR ZNO UV PHOTOTRANSISTOR AND THE CONVENTIONAL SI-BASED DEVICE

Phototransistor designs	**I_{ON}/I_{OFF} ratio (dB)**	**Responsivity (A/W)**	**Detectivity (Jones)**	**Ref.**
Si-based ZnO OC-FET	74	0.24	3.5×10^{13}	[21]
InGaZnO Photo-TFT	46	0.08	1.3×10^{10}	[23]
InGaZnO/ $MoSe_2$ heterostructure	60	1.7	-	[24]
ZnO GNR FET UV phototransistor	76.2	2×10^5	1.2×10^{14}	This work

IV. CONCLUSION

This work investigated the role of *GNR* channel and *ZnO* capping thin-film in promoting ultra-high responsivity *UV*-phototransistors. We presented Numerical models based on self-consistent solving of the Schrödinger/Poisson equations using *NEGF* formalism. The results showed that the proposed *UV*-phototransistor paves the way to break the responsivity intrinsic limit associated with the traditional *Si*-channel based counterparts. In addition, we found that long channel devices are highly appropriate for *UV* sensing applications. Importantly, *PSO*-based approach is implemented to optimize the device performances. The optimized design demonstrated 2×10^5 *A/W* of responsivity at very low incident power density of *5pW*. Therefore, the strategic combination between *ZnO* capping layer and *GNR* technology can be effective for realizing ultra-high responsivity *UV*-phototransistors, which are appropriate for newly emerging OWCS.

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