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REGULAR ARTICLE

OFET Biosensor: Simulation and Analysis for Various Biomolecules

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A *p*-type (DiketoPyrroloPyrrole as organic semiconductor) Dual Gate OFET based biosensor is proposed for the detection of biomolecules in the nanocavity provided at the source end underlapping the region of the structure both at the top and at the bottom. Various biomolecules have been investigated for their effect on Drain current, ID which is a measure of sensitivity of the device. This device is then compared with different organic p-type semiconductor materials such as pentacene and tetracene based OFET biosensor. Drain current and sensitivity of these devices have also been calculated which shows that DPP (DiketoPyrroloPyrrole) based OFET biosensor has higher sensitivity of 3.0×10^3 as compared to pentacene and tetracene based OFET biosensors. Simulation of these devices has been done in SILVACO ATLAS TCAD tool. The simulation results also show that the proposed device even shows higher sensitivity for high-k dielectrics such as HfO_2, Ta_2O_5, TiO_2.

Keywords: DPP, OFET, High-K dielectric, Sensitivity, Pentacene, Tetracene.

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1. INTRODUCTION

Field effect transistors (FETs) are extensively used for biosensing applications. They show high sensitivity due to their inherent property of amplification. FET based biosensors are used in various fields such as healthcare, military, environmental and agriculture protection and food analysis. These biosensors are based on inorganic materials which show high drain current, high mobility, label free detection and are easy to use. Still these materials degrade with time, have less selectivity and operate at high temperatures which limits their applications hence organic materials-based biosensors comes into picture [1]. These materials are biodegradable, low cost, flexible, have large area applications [2] and have plenty of availability of organic semiconductors [3-4] but mobility and stability are still a challenge in organic FETs [5].

The most investigated organic semiconductor is pentacene with its potential applications due to its high hole mobility [6]. However, DiketoPyrroloPyrrole (abbreviated as DPP) and its derivatives have been widely studied in the past few years due to its good thermal and photo stability [7]. Various OFET based sensors using pentacene [8-9] and DPP [10-11] have been fabricated and studied in the past.

In this paper a DPP based Dual Gate OFET biosensor is designed by introducing biomolecules such as DNA ($k = 8.7$), Cellulose ($k = 6.1$), APTES ($k = 3.57$), Biotin ($k = 2.63$) and Streptavidin ($k = 2.1$) in the cavity region and the change in the Drain current, electric field, potential, band diagram and hence the sensitivity of the device is measured [12]. This Dielectric Modulated (DM) [13] OFET is designed in SILVACO TCAD ATLAS tool, and the simulation results are obtained. These results are then compared with pentacene [14] and tetracene [15] based OFET biosensors. Comparison results show that DPP based Dual Gate (DG) OFET biosensor are more sensitive to biomolecules as compared to its counterparts. These results are calibrated with the results in literature where sensitivity of DPP based sensor [16] is higher than Pentacene based sensor [17]. DPP based OFET biosensor is also simulated for high-k dielectrics such as HfO_2 ($k = 25$), Ta_2O_5 ($k = 22$) and TiO_2 ($k = 95$) and the results show highest sensitivity for TiO_2 whose dielectric constant is highest as comparison to the others.

The manuscript is catalogued as follows, the introduction is covered in section I, the proposed device schematic and parameters specifications used for designing is discussed in section II. The results obtained and analyzed with the discussion carried out in section III. A fair conclusion is drawn in section IV with all the enhancements considered.

2. DEVICE DESIGN AND PARAMETERS SPECIFICATIONS

A Dual Gate OFET with DPP (DiketoPyrroloPyrrole)

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as p-type organic semiconductor, Al_2O_3 as gate dielectric, gold as the source and drain regions is designed [18]. DPP based materials are more stable to heat and show high mobility. A nanocavity is provided at the source end underlapping the region of the structure both at the top and at the bottom. Two-dimensional modulated device structure of the proposed DPP based DG-OFET configuration with underlap [19] nanocavity is shown below in Fig. 1.

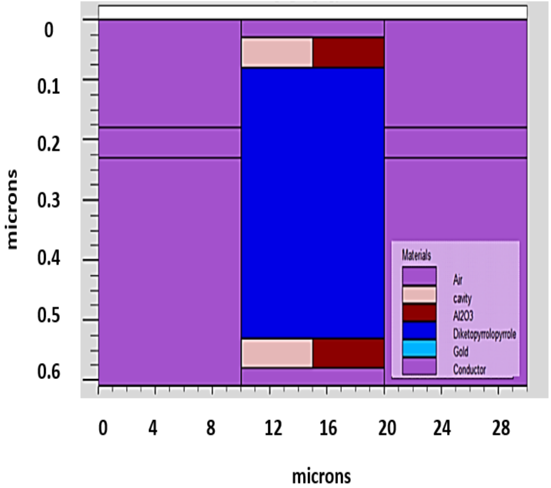

Fig. 1 – Cross sectional (2D) view of proposed DG DPP based OFET with underlap nanocavity

The structure of the device consists of an Aluminium layer as gate electrode of thickness 30 nm. On top of it there is a nanocavity underlap region at the source end of thickness 50 nm and Al_2O_3 as gate dielectric of thickness 50 nm. Above it, a DPP based organic semiconductor is deposited of thickness 400 nm with source and drain regions coated with gold of thickness 50 nm. On top of it again there is a nanocavity and gate dielectric of 50 nm which is finalized by gate electrode of Al of thickness 30 nm.

Device design parameters are mentioned in Table 1.

Table 1 – Device design parameters

Device Dimensional Parameters	**Values**
Thickness of Gate electrode	30 nm
Thickness of cavity region	50 nm
Thickness of organic semiconductor (DPP)	400 nm
Thickness of Source and Drain	50 nm
Work function of gate metal, Al	4.1 eV
Work function of source and drain regions, Au	5 eV

3. RESULT AND DISCUSSION

Modelling and Simulation of the above said device is done on SILVACO TCAD ATLAS tool. The various models used in our simulation are fldmob and langevin. The Poole–Frenkel mobility model (pfmob) and Langevin recombination models report the transport and recombination mechanism. The device shown in Fig. 1 is simulated and transfer characteristics are generated for various biomolecules such as DNA, Cellulose, APTES, Biotin, Streptavidin. The simulated results are shown in Fig. 2.

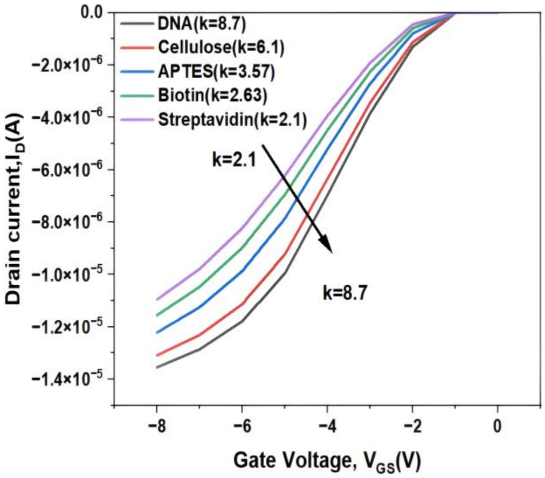

Fig. 2 – Transfer characteristics with $V_{DS} = -3$ V

VGS varies from 0 to – 8 V with VDS kept constant at 3 V. It can be seen from Fig. 2 that as the dielectric of biomolecule increases, drain current also increases. This is due to the fact that gate capacitance increases with an increase in dielectric constant which increases the inversion charge and hence drains current increases. The drain current of DNA ($k = 8.7$) is highest whereas drain current of Streptavidin ($k = 2.1$) is lowest.

Fig. 3 shows Energy band diagram with respect to various biomolecules of the proposed DPP based DG-OFET. A cutline is made at 1 nm below oxide-channel interface and energy levels of HOMO and LUMO are extracted. Variations in the band gap can be seen as the cavity is filled with biomolecules of different dielectrics.

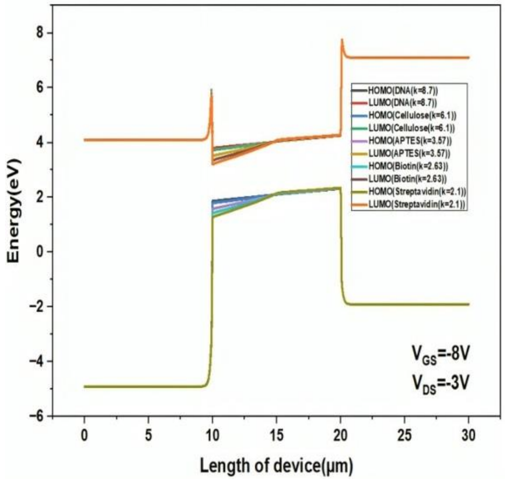

Fig. 3 – Variation of energy band for different biomolecules

Fig. 4 and Fig. 5 represent electric field and potential along the length of the channel of the proposed device. The electric field increases and potential decreases when dielectric of biomolecules increases.

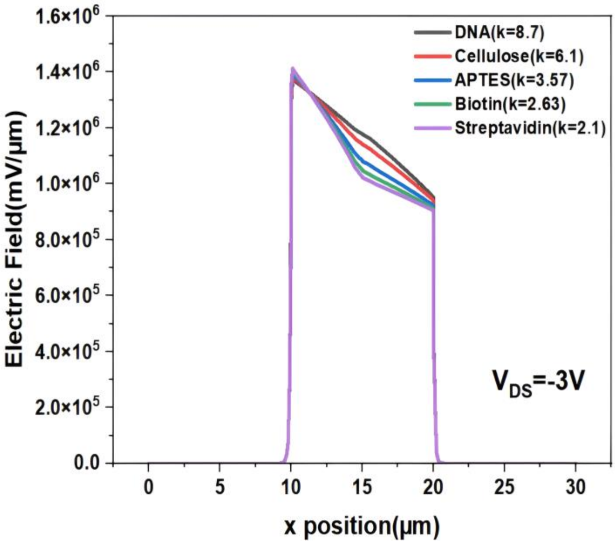

Fig. 4 – Electric field along the length of the device

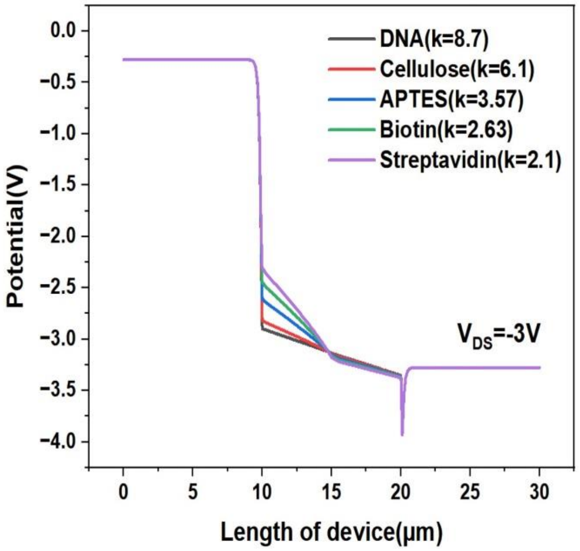

Fig. 5 – Potential along the length of the device

Current sensitivity of the device, SDRAIN [20]is calculated as

$$S_{DRAIN} = I_D(at\ any\ k) - I_D(at\ k = 1)/I_D(at\ k = 1)$$

Sensitivity of various biomolecules have been calculated as function of VGS and it has been observed that maximum sensitivity (3.0×10^3) is achieved for DNA ($k = 8.7$) while taking I_D ($k = 1$) as reference which is the dielectric of air. This is clearly visible in Fig. 6.

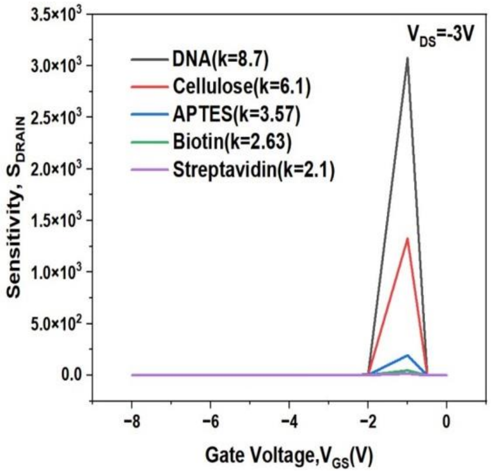

Fig. 6 – Drain current sensitivity at different values of dielectric constant of biomolecules of the proposed device

Sensitivity can also be increased by using high-k dielectrics such as HfO_2, Ta_2O_5 and TiO_2 that can be seen in Fig. 7, 8 and 9 respectively. Maximum sensitivity is achieved (5.13×10^3) when TiO_2 as a dielectric is used ($k = 95$).

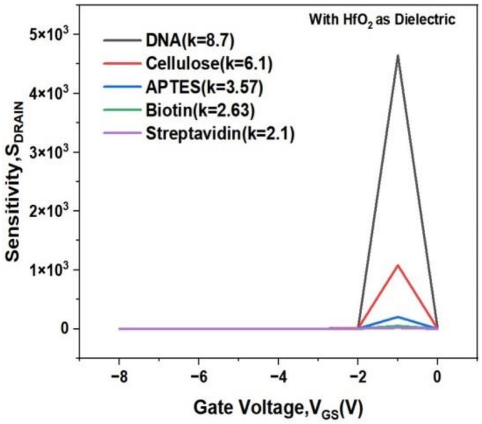

Fig. 7 – Drain current sensitivity with HfO2 as dielectric at different values of dielectric constant of biomolecules

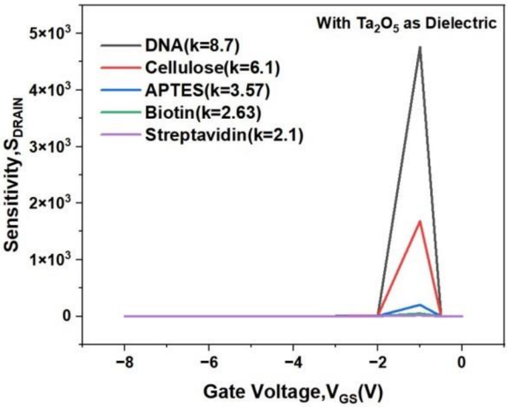

Fig. 8 – Drain current sensitivity with Ta_2O_5 as dielectric at different values of dielectric constant of biomolecules

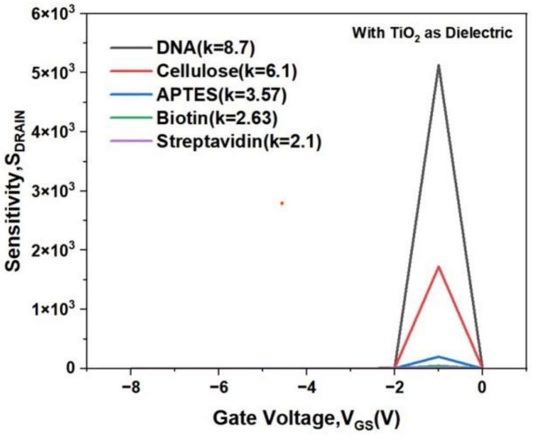

Fig. 9 – Drain current sensitivity with TiO_2 as dielectric at different values of dielectric constant of biomolecules

This proposed device is also compared with pentacene and tetracene based DG-OFET biosensor. Drain current and sensitivity of pentacene based DG-OFET has been shown in Fig. 10 and 11 whereas that of tetracene based DG-OFET is shown in Fig. 12 and 13. It has been clear from these figures that Drain current and sensitivity of our proposed DPP based DG-OFET is found maximum.

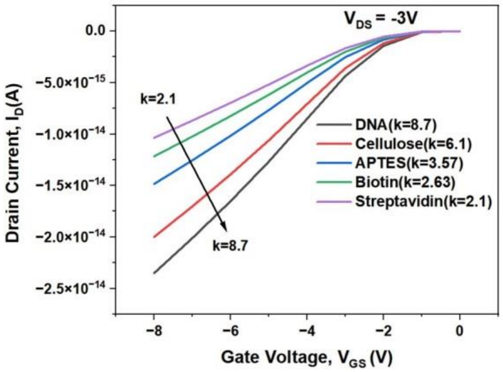

Fig. 10 – Transfer characteristics of pentacene based DG-OFET at $V_{DS} = -3$ V

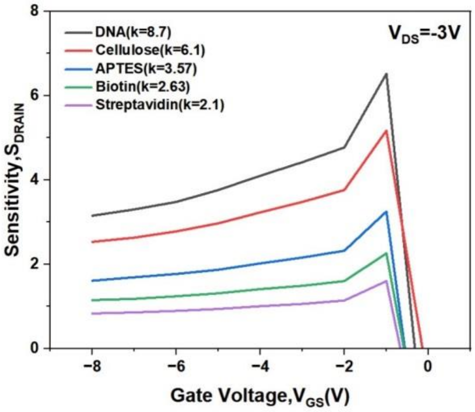

Fig. 11 – Drain current sensitivity of pentacene based DG-OFET at different values of dielectric constant of biomolecules

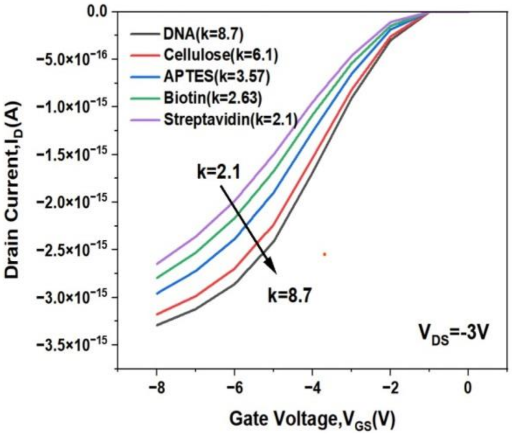

Fig. 12 – Transfer characteristics of tetracene based DG-OFET at $V_{DS} = -3$ V

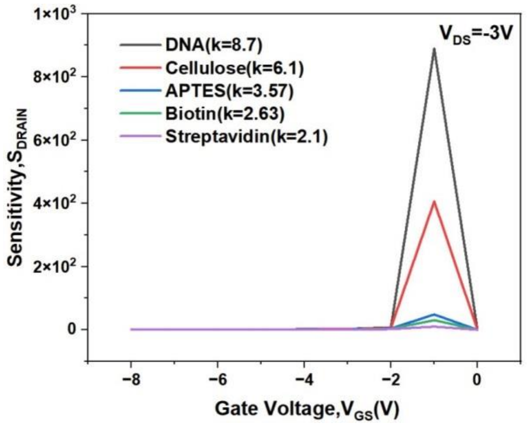

Fig. 13 – Drain current sensitivity of tetracene based DG- OFET at different values of dielectric constant of biomolecules

4. CONCLUSION

OFET based biosensors have been studied to increase the diagnosis of biomolecules in various applications such as health monitoring, environmental research, food analysis etc. Here, in this paper, a p-type (DPP as organic semiconductor) DG-OFET is proposed with higher sensitivity (3.0×10^3) as comparison to its counterparts, pentacene and tetracene. Further sensitivity is also increased when high-k dielectrics are used. Maximum sensitivity (5.13×10^3) is achieved when TiO_2 as gate dielectric is used.

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Біосенсор OFET: моделювання та аналіз різних біомолекул

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Біосенсор на основі OFET із подвійним затвором *p*-типу (DiketoPyrroloPyrrole як органічний напівпровідник) пропонується для виявлення біомолекул у нанопорожнині, що забезпечується на кінці джерела, що перекриває область структури як у верхній, так і в нижній частині. Було досліджено вплив різних біомолекул на струм витоку, ID, який є мірою чутливості пристрою. Потім цей пристрій порівнюється з різними органічними напівпровідниковими матеріалами *p*-типу, такими як OFET біосенсор на основі пентацену та тетрацену. Також було розраховано струм стоку та чутливість цих пристроїв, які показують, що біосенсор OFET на основі DPP (DiketoPyrroloPyrrole) має вищу чутливість $3{,}0 \times 10^3$ порівняно з біосенсорами OFET на основі пентацену та тетрацену. Моделювання цих пристроїв виконано в інструменті SILVACO ATLAS TCAD. Результати моделювання також показують, що запропонований пристрій навіть демонструє більш високу чутливість для діелектриків з високим показником *k*, таких як HfO_2, Ta_2O_5, TiO_2.

Ключові слова: DPP, OFET, High-K, Діелектрик, Чутливість, Пентацен, Тетрацен.