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Cite as: Appl. Phys. Lett. 118, 053103 (2021); https://doi.org/10.1063/5.0039431
Submitted: 03 December 2020 . Accepted: 24 January 2021 . Published Online: 03 February 2021

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Submitted: 3 December 2020 · Accepted: 24 January 2021 ·
Published Online: 3 February 2021

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ABSTRACT

We theoretically study the efficiency limits and performance characteristics of few-layer graphene–semiconductor solar cells (FGSCs) based on a Schottky contact device structure. We model and compare the power conversion efficiency (PCE) of various configurations by explicitly considering the non-Richardson thermionic emission across few-layer graphene/semiconductor Schottky heterostructures. The calculations reveal that ABA-stacked trilayer graphene–silicon solar cell exhibits a maximal conversion efficiency exceeding 26% due to a lower reversed saturation current when compared to that of the ABC-stacking configuration. The thermal coefficients of PCE for ABA and ABC stacking FGSCs are –0.061%/K and –0.048%/K, respectively. Our work offers insights into optimal designs of graphene-based solar cells, thus paving a route toward the design of high-performance FGSC for future nanoscale energy converters.

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ABSTRACT

We theoretically study the efficiency limits and performance characteristics of few-layer graphene–semiconductor solar cells (FGSCs) based on a Schottky contact device structure. We model and compare the power conversion efficiency (PCE) of various configurations by explicitly considering the non-Richardson thermionic emission across few-layer graphene/semiconductor Schottky heterostructures. The calculations reveal that ABA-stacked trilayer graphene–silicon solar cell exhibits a maximal conversion efficiency exceeding 26% due to a lower reversed saturation current when compared to that of the ABC-stacking configuration. The thermal coefficients of PCE for ABA and ABC stacking FGSCs are –0.061%/K and –0.048%/K, respectively. Our work offers insights into optimal designs of graphene-based solar cells, thus paving a route toward the design of high-performance FGSC for future nanoscale energy converters.

Two-dimensional-material-based heterostructures have been actively explored1–3 in recent years due to their widespread applications in nanoelectronics, nanophotonics, and optoelectronics, such as energy harvesting,4–6 transistors,7,8 photo detection,9 sensors,10 and data storage devices.11 Due to their unusual optical and electronic properties, 2D materials have immense potential for next-generation solar cells.12–14 With the scaling trends in photovoltaics moving toward thin, atomically thin 2D materials with high mechanical strength and flexibility have become the key candidate materials for the development of the next-generation photovoltaic technology. In terms of solar energy harvesting, 2D-metal/3D-semiconductor solar cells, especially graphene–silicon contact, have been extensively studied,15–18 with a particularly strong emphasis on improving the power generation efficiency of the device.19–22 The record power conversion efficiency (PCE) of such devices has been rising steadily in recent years, achieving an exceptional values of 15.6% and 18.5%, respectively, for graphene/silicon23 and graphene/GaAs24 solar cells.

Despite extensive research focusing on monolayer graphene (MLG) solar cells, few-layer-graphene/semiconductor solar cells (FGSCs) with a new transport mechanism remain relatively less explored. Correspondingly, the fundamental efficiency limit and performance characterization of FGSCs remain poorly understood. Importantly, few-layer graphene (FLG) is known to possess completely different electrical and optical properties when compared to monolayer graphene.25–27 The incorporation of FLG with 3D semiconductors has, thus, led to myriads of interfacial transport and charge injection phenomena that are distinctive from the monolayer counterpart.28–32 In relevance to solar cell applications, employing FLG as a top-layer material offers the following advantages. First, FLG possesses high transparency (see Table I) in the visible range of the solar spectrum, thus ensuring sunlight transmission into the semiconductor medium with small optical loss. Second, FLG exhibits a lower reverse saturation current in contrast to conventional metal and monolayer graphene. As the layer number increases, the series resistance and ideality factor in FLG-based Schottky devices are vanishingly small. Third, since the depletion region forms on the right side of the semiconductor surface, FGSCs are characterized by high photocurrent generation and considerable short-wavelength photoreponse. Benefitted by these factors, FGSCs hold strong potential as a candidate materials for low-cost and high-efficiency solar-to-electricity energy conversion.

In this Letter, we investigate the various performance metrics and efficiency limits of FGSCs (see Fig. 1) by harnessing the thermionic...
emission process in FLG–semiconductor Schottky junctions. Here, we consider two forms of FLG: ABA and ABC stacking order configurations, which exhibits layer- and stacking-dependent electronic band structures. To gain physical insights into the main limiting factors and further improve the device performance, we perform a computational study to understand how the device performance is influenced by the effect of stacking order, semiconductor bandgap, series resistance, layer number of FLG, and temperature. Our results offer practical insights into the optimum design of high-performance FGSCs, thus offering an important theoretical basis for the exploration of 2D-material-based solar energy harvesting technology.

We model an ideal FGSC and determine its theoretical efficiency limit based on the following assumptions: (i) Each incident photon with energy higher than the semiconductor bandgap \([E_g \text{ in Fig. 1(b)}]\) can produce an electron–hole pair that contributes to the photocurrent, i.e., negligible recombination of excess carriers. (ii) The device ideality factor is \(n = 1\), and Ohmic loss due to the series resistance is expected to be small. Such ideal conditions may be approached practically via FLG because both the series resistance and ideality factor are shown to decrease with the number of graphene layers.\(^3\) The \(J-V\) characteristic of the 2D-material/semiconductor Schottky contact at room temperature exhibits a rectifying behavior, as governed by the Shockley diode equation,

\[
J(V, T) = J_{SC} - J_{SAT} \left\{ \exp \left[ \frac{q(V - IR_S)}{k_B T} \right] - 1 \right\},
\]

where \(J_{SC}\) represents the short-circuit photocurrent density, and \(J_{SAT}\) denotes the reversed saturation current density (RSCD) due to thermionic emission over the Schottky barrier \([\Phi_B, \text{ see Fig. 1(b)}]\) under a bias voltage \(V\). Here, \(q\) is the electron charge, \(k_B\) is the Boltzmann constant, and \(T\) is the operating temperature of the cell. \(R_S\) is the series resistance, which compactly contains the resistance contributed from the semiconductor bulk, FLG, and the contacts. The inevitable existence of \(R_S\) lowers the effective voltage applied to the junction.

The short-circuit current or photocurrent density generated by sunlight absorption in FGSCs is

### Table I. Absorption coefficient, light transmittance, and short-circuit current density (FLG-Si) for a different number of graphene layers.\(^3\)

| Layer number | Absorption coefficient \((\text{cm}^{-1})\) | Light transmittance (%) | Short-circuit current density \((\text{mA/cm}^2)\) |
|--------------|------------------------------------------|--------------------------|-----------------------------------------------|
| 2            | \(4.3 \times 10^6\)                      | 95.4                     | 45.2                                          |
| 3            | \(6.4 \times 10^6\)                      | 93.1                     | 43.8                                          |
| 4            | \(8.5 \times 10^6\)                      | 90.8                     | 42.1                                          |
| 5            | \(1.06 \times 10^7\)                     | 88.5                     | 39.9                                          |
| 6            | \(1.28 \times 10^6\)                     | 85.3                     | 37.5                                          |

![FIG. 1.](image-url) (a) Schematic of the vertical few-layer graphene–semiconductor solar cell for sunlight-to-electricity energy conversion. (b) Band diagram showing the thermionic transport over a Schottky barrier \(\Phi_B\). (c) ABA- and (d) ABC-stacking-order trilayer graphene with low-energy dispersion (left) and crystal structure (right).
\[
J_{SC} = q \int_{E_g}^{\infty} \mathcal{F} I_{AM1.5D}(h\omega) \, d\omega,
\]

where \(I_{AM1.5D}\) is the incident photon flux of AM1.5D terrestrial solar spectrum with a wavelength range of 280–4000 nm. Here, \(\mathcal{F}\) represents the optical transmittance of FLG, which can be obtained from experimental data.\(^{26,27}\) \(E_g\) is the bandgap of the semiconductor, and \(h\omega\) represents the photon energy with frequency \(\omega\). The open-circuit voltage can then be obtained as

\[
V_{OC} = \frac{k_B T \ln \left( \frac{J_{SC}}{J_{SAT}} + 1 \right)}{q}.
\]

For an ideal Schottky contact, the transport of charge carriers is governed by the thermionic emission over the Schottky barrier at the contact interface, and the corresponding RSCD is given by a generalized thermionic emission model,

\[
J_{SAT} = \alpha T^\beta \exp \left( - \frac{\Phi_B}{k_B T} \right),
\]

where the prefactor \(\alpha\) and the scaling exponent \(\beta\) are the material- and interface-dependent parameters, respectively. The scaling exponent takes the form of \(\beta = 2\) and \(\alpha = 120 \text{ A/cm}^2\text{K}^2\) for a classic Schottky contact composed of 3D bulk metals with parabolic energy dispersion. For FLG-based vertical Schottky contact, the electronic properties of the FLG\(^{28–32}\) deviate significantly from the parabolic energy dispersion. Furthermore, the electronic properties of FLG exhibit nontrivial dependences on the number of layers and the layer stacking order. For instance, the bernal (i.e., the ABA stacking order) and the rhombohedral (i.e., the ABC stacking order) FLG—the most thermodynamically stable stacking orders\(^{24}\) [see Figs. 1(c) and 1(d)]—display highly nonparabolic energy dispersions. Such band structure nonparabolicity gives rise to an unconventional and non-Richardson RSCD whose temperature scaling behavior is drastically different from that of the classic Richardson thermionic emission model. In this case, the vertical FLG–semiconductor Schottky heterostructures obey a current–temperature scaling exponent of \(\beta = 1\), with the following layer number \(N\) and stacking order–dependent prefactor:\(^{20}\)

\[
\alpha = \begin{cases} \frac{2 N q}{\pi \tau_{inj} \left( \hbar \nu_F \right)^2} & \text{(ABA, } N \geq 1 \text{)} \\ \frac{2 q}{\pi N \tau_{inj} \left( \hbar \nu_F \right)^2 r_L^{2N-2}} & \text{(ABC, } N \geq 3 \text{),} \end{cases}
\]

where \(N\) represents the FLG layer number, \(\tau_{inj}\) is a charge injection characteristic time constant whose value is influenced by the quality of the contact, \(r_L \approx 0.39 \text{ eV}\) is the interlayer hopping parameter,\(^{20}\) \(\hbar\) is the reduced Planck’s constant, and \(v_F = 10^6 \text{ m/s}\). Here, the RSCD shows an \(N\)-fold enhancement in ABA FLG due to the presence of \(N\) conduction subbands. This is in stark contrast to ABC FLG where the RSCD has a nonlinear \(N\)-dependent prefactor.

The PCE of the FGSC is defined as the ratio of the maximum electric power to the total incoming solar photon energy flux \(P_{sun}\), i.e.,

\[
\eta = \frac{(JV)_{\text{max}}}{P_{\text{sun}}} = \frac{J_{SC} \cdot V_{OC} \cdot FF}{I_{AM1.5D}(h\omega) \, d\omega},
\]

where \(FF\) is the fill factor. The maximum power point \((JV)_{\text{max}}\) can be determined by solving \(d(JV)/dV = 0\).

In an ideal metal/semiconductor junction, the Schottky barrier height is dependent on the work function and the electron affinity of the semiconductor, as dictated by the Schottky–Mott rule.\(^{33}\) However, due to the inevitable presence of the metal–semiconductor interaction, the formation of mid-gap states, interface dipole, and defects, the Schottky barrier height (S BH) can deviate substantially from the ideal Schottky–Mott rule.\(^{34}\) For graphene–silicon Schottky contact, the SBH has been experimentally found to vary across a sizable range from 0.32 eV to 0.89 eV.\(^{35}\) Here, we set the SBH to the ultimate magnitude of \(\Phi_{B_{\text{max}}} = E_F\) in order to examine the upper limits of the PCE for the FGSC.\(^{36}\) We choose a relatively larger injection time of \(\tau_{inj} = 40 \text{ ps}\) to represent the inevitable presence of defects at the Schottky contact interface and a low series resistance of \(R_S = 0.1 \text{ \Omega cm}^2\). Figure 2(a) shows the PCE of the FGSC as a function of the semiconductor bandgap at room temperature. The small oscillations originate from the atmospheric absorption in the incident AM1.5D solar spectrum. The efficiency bounds of the FGSC reveal a broad range from 0.6 to 1.7 eV with PCE exceeding 20%. For narrow-bandgap semiconductors, although a high photocurrent density is warranted, the output voltage remains low due to the limited Schottky barrier height (or bandgap), as expected from Eq. (3). On the other hand, for wide-bandgap semiconductors, the photon absorption is significantly impeded by the larger bandgap, which leads to a low photocurrent density [see Fig. 2(b) and Eq. (2)]. The interplay between these two counteracting behaviors leads to an optimal semiconductor bandgap for achieving maximum PCE. The open-circuit voltage is associated with \(\alpha\) and is, thus, sensitively influenced by the stacking order. Importantly, the
The open-circuit voltage of the ABA-trilayer FGSC is higher than that of the ABC FGSC. The stacking order dependence becomes particularly more pronounced at the wide-bandgap regime and causes an enhancement of the fill factor.

As shown in Fig. 2(a), the theoretical upper limit of the PCE for the FGSC with ABA trilayer graphene is predicted to be 26.1% at $E_g = 1.13$ eV—a value that is very close to the bandgap of silicon. To explain why ABA stacking order reflects better performance than ABC, we choose the trilayer graphene/Si solar cell as an illustrative example and further access its $J$–$V$ characteristics under different operating conditions [see Fig. 2(c)]. We show that the open-circuit voltage of ABA FGSCs (0.66 V) is higher than that of ABC FGSCs (0.58 eV), although both of them exhibit the same short-circuit current density of 43.8 mA/cm$^2$. These facts demonstrate the key advantage of the ABA stacking order in achieving high-performance Schottky-contact-based solar energy converters. It is worth mentioning that the classic Richardson thermionic emission model, which does not accurately capture the reduced dimensionality and the nonparabolic nature of the energy dispersion in FLG, can yield a discrepancy in the thermionic current density of about 2 orders of magnitude.

In relevance to the modeling of FGSC, using the classic Richardson model of $\alpha_d = 120$ A/cm$^2$K$^2$ and $\beta = 2$ can lead to a relatively small open-circuit voltage, as well as PCE ($V_{OC} = 0.62$ V and PCE = 25.3%). This finding highlights the importance of utilizing the appropriate thermionic emission that better captures the material properties of FLG during the modeling of Schottky-contact-based energy converters.

Figures 3(a)–3(d) show the PCE, fill factor, short-circuit current density, and open-circuit voltage of the ABA and ABC FGSC as a function of the layer number of graphene. We consider $N \leq 6$ because the work function of FLG with more than six layers tends to saturate at that of graphite. We identify an optimal layer number of $N = 3$ that yields the maximum PCE for ABA stacking. When the layer number is increased, the fill factor increases substantially. However, as the layer number is further increased, the FF becomes saturated [Fig. 3(b)]. In contrast, the short-circuit current density and the open-circuit voltage exhibit a decreasing trend with the layer number in Figs. 3(c) and 3(d). Table I shows the experimentally measured absorption coefficient and the transmittance of FLG with varying graphene layers. As the layer number increases, the light transmittance reduces gradually from 95.4% to 85.3%. Correspondingly, the short-circuit current density drops from 45.2 to 37.5 mA/cm$^2$. The trade-off between the fill factor, the short-circuit current density, and the open-circuit voltage leads to an optimal layer number maximizing the PCE. To compare the RSCD of FLG with ABA and ABC stacking, we define the ratio of $J_{SAT}^{(ABC)}/J_{SAT}^{(ABA)}$ and plot the layer dependence of this ratio in Fig. 3(c). The $J_{SAT}^{(ABA)}$ is about an order of magnitude larger than $J_{SAT}^{(ABC)}$, which reveals the fundamental origin of the better ABA FGSC performance in providing a larger open-circuit voltage and a higher PCE when compared to that of the ABC FGSC. As a comparison, the MLG–silicon solar cell exhibits PCE = 25.5%, $FF = 0.84$, $J_{SC} = 43.64$ mA/cm$^2$, and $V_{OC} = 0.69$ V. Importantly, our results suggest that the ABA FGSC with 2–4 graphene layers exhibits a better performance than MLG–silicon solar cells due to the higher FF. Note that the short-circuit current density in Ref. 6 is lower than the 45.2 mA/cm$^2$ ($N = 2$) predicted here as the former calculation is based on an AM 1.5 global tilted irradiance.

We further study the $\tau_{inj}$-dependence of the PCE, fill factor, and the open-circuit voltage in Figs. 4(a)–4(c). The $\tau_{inj}$ is related to the contact quality between the FLG and the semiconductor. Here, we consider a representative range from 0.1 ps to 100 ps, which is consistent with the values reported experimentally. A larger $\tau_{inj}$ corresponds to the situation in which the contact resistance across the Schottky contact is large. In general, the key performance parameters of the FGSC are influenced by the values of $\tau_{inj}$. Particularly, when $\tau_{inj}$ is small, increasing $\tau_{inj}$ leads to a significant improvement of the PCE, fill factor, and open-circuit voltage.
fill factor, and the open-circuit voltage [see Figs. 4(a)–4(c)]. Such improvement eventually saturates as $T_{\text{op}}$ is further increased. This analysis, thus, suggests that electrical contact engineering may offer a route to improve the system performance of FGSCs.

Since the RSCD is exponentially dependent on the temperature, the performance of FGSC exhibits a strong temperature dependence, as shown in Figs. 4(d)–4(f). A high operating temperature decreases the fill factor [Fig. 4(e)] and open-circuit voltage [Fig. 4(f)], which eventually degrade the PCE [Fig. 4(d)]. Reducing the operating temperature is, thus, crucially important to achieve optimal energy conversion efficiency. For the ABA FGSC, the upper limit of the PCE increases (decreases) from 26.1% at room temperature to 32.5% (20.4%) at $T = 200$ (400) K. Similarly, the maximum PCE of the ABC solar cell increases (decreases) from 22.2% at room temperature to 27.7% (18.1%) at $T = 200$ (400) K. For both stacking orders, the efficiency limit of the FGSC acts as a nearly perfect linear function of the operating temperature, thus allowing us to define a thermal coefficient of the PCE as $\gamma_{\text{PCE}} = \Delta PCE/\Delta T$. For ABA trilayer graphene/silicon solar cells, we obtain $\gamma_{\text{PCE}}^{\text{ABA}} = -0.061\%/K$, signifying a drop of 0.061% in the PCE when the temperature is increased by 1 K. In the case of ABC, the thermal coefficient of PCE is found to be $\gamma_{\text{PCE}}^{\text{ABC}} = -0.048\%/K$. When compared to the case of MLG–silicon solar cells ($\gamma = 0.076\%/K$), the performance metrics of MLG-silicon solar cells exhibit a slightly stronger temperature dependence. In addition, we also obtain the thermal coefficient of the fill factor and open-circuit voltage, as depicted in Figs. 4(e) and 4(f).

Finally, we discuss the influence of the series resistance on the performance of FGSCs. Experimentally, the $R_S$ of monolayer- and bilayer graphene-based solar cells are 0.6 $\Omega$ cm$^2$ (Ref. 33) and 0.2 $\Omega$ cm$^2$, respectively. Here, we use three representative values of $R_S$, i.e., 0.1 $\Omega$ cm, 0.5 $\Omega$ cm, and 1 $\Omega$ cm, to illustrate the effects of $R_S$ on the performance metrics of trilayer graphene/Si solar cells. In general, the PEC, FF, and $V_{\text{OC}}$ decrease with an increasing $R_S$ (see Table II for a summary of the results). Lowering $R_S$ is, thus, crucially important in optimizing the performance of the FGSC. We further remark that the active area of graphene/Si heterojunction solar cells is also expected to influence the PCE of the FGSC. In general, a larger active area tends to produce lower PCE in graphene-based solar cells. Nonetheless, a sufficiently large active area is essential to produce a large photocurrent, which is beneficial for energy conversion applications. The interplay between the device active area and the performance should, thus, be systematically scrutinized in future works.

In summary, we have performed a computational modeling on the design of FGSC for solar energy harvesting. The FGSC with ABA trilayer graphene/silicon architectures possess a peak efficiency of 26.1% at room temperature, which is significantly higher than that of ABC-FLG-based devices. The better performance of ABA FLG in FGSC application originates from the lower RSCD. Importantly, an optimal layer number of $N = 3$ is predicted for ABA stacking. Our analysis further reveals an intriguing figure of merit, i.e., the thermal coefficient of the PCE, which allows the temperature dependence of the energy conversion performance to be accessed. Our findings shall provide practical insights useful for the design of high-performance FGSCs, thus paving a potential new avenue toward 2D-material-based solar energy harvesting technology approaching the Shockley–Queser limit.

This project is supported by the National Science Foundation through Grant No. 11811530052. Y.S.A. acknowledges the support of Singapore MOE Tier 2 Grant (No. 2018-T2-1-007).

**DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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**TABLE II.** The PCE, fill factor, and open-circuit voltage in trilayer graphene–silicon solar cells with ABA and ABC stacking for different series resistances.

| $R_S$ ($\Omega$ cm$^2$) | 0.1 | 0.5 | 1 |
|---------------------|-----|-----|---|
| ABA PCE (%)         | 26.1| 25.8| 25.2| 24.4|
| ABA $V_{\text{OC}}$ (V) | 0.66| 0.62| 0.57| 0.5|
| ABA FF              | 0.9 | 0.87| 0.81| 0.78|
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