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ABSTRACT

The lack of bandgap in graphene is the main factor that prevents that this outstanding material be implemented in optoelectronics. In this work, we show that by nanostructuring graphene aperiodically it is possible to have an efficient transmission bandgap engineering. In particular, we are considering aperiodic graphene superlattices in which electrostatic barriers are arranged following the basic construction rules of the Thue-Morse sequence. We find that the transmission bandgap can be modulated readily by changing the angle of incidence as well as by appropriately choosing the generation of the Thue-Morse superlattice. Even, this angle-dependent bandgap engineering is more effective than the corresponding one for periodic graphene superlattices.

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I. INTRODUCTION

Graphene^{1,2} is a material with surprising and unique properties that no other material offers, to such degree, that it is regarded as a miracle material. The countless possible uses and technologies that can come from it have been grouped in the so-called graphene roadmaps.^{3,4} In particular, the exceptional electrical conductivity makes that we can think in a possible graphene electronics. However, the lack of bandgap hampers this possibility. In fact, the special band structure of graphene which is closely related to its exotic, unique and unprecedented properties is at the same time the biggest hurdle for electronics. To circumvent this problem there are several proposals. Here, we will summarize the most important ones.

A bandgap engineering is possible by patterning graphene in finite pieces, known as nanoribbons.^{5,6} The lateral confinement of the charge carriers induces a bandgap. The size of the energy bandgap scales inversely with the nanoribbon width. The bandgap is also sensitive to the ribbon edges.⁵ Despite the advances in the control of ribbon edges,⁷ the size

of the bandgap (~ 100 meV) as well as the mass production of reliable nanoribbons are the main obstacles of this proposal. Another possibility is to induce a bandgap via the interaction of graphene with substrates like SiC or hBN, in the range of 50 to 260 meV.^{8,9} However, the substrate degrades considerably the mobility of the charge carriers. In particular, the greater the bandgap the lower the carriers mobility. An alternative for bandgap opening is the hydrogenation of graphene.^{10,11} In fact, it is experimentally reported¹² that patterned hydrogen absorption induces a considerable bandgap, 450 meV. The absorption is mediated by the graphene/Ir(111) Moiré superlattice. Furthermore, the bandgap owes its existence to the confinement effect that takes place between the covered and uncovered hydrogen regions. Under this context, options in which the bandgap can be tuned readily by applying external electric fields are always welcomed. This can be achieved with electrically gated bilayer graphene.^{13,14} This technique allows the continuous modulation of the bandgap, from 0 up to 250 meV. In this case, the bandgap owes its origin to the symmetry breaking between the graphene layers due to the applied electric field. By gating it is also possible to take

advantage of the highly anisotropic propagation of the charge carriers in the so-called gated graphene superlattices (GSLs).^{15,16} So, we can think in an angle-dependent bandgap engineering in gated graphene superlattices.¹⁷ In this case, the bandgap can be tuned by modulating the angle of the incident electrons. The bandgap has a parabolic dependence for moderate angles, and an exponential variation for large ones. Furthermore, the bandgap can be tuned from meV to eV. In principle, the manipulation of the propagation of the charge carriers at angular level is challenging, however nowadays there are important advances in the angular control of the charge transport.^{18,19} Here, it is important to mention that the base for this angular-dependent bandgap engineering are periodic superlattices. However, an extra dimension can be incorporated through the aperiodic order that superlattices based on sequences like Fibonacci, Thue-Morse, Cantor, etc. offer. In fact, aperiodicity induces special characteristics on the band structure and transport properties of Fibonacci and Thue-Morse superlattices.²⁰⁻²² So, the highly anisotropic propagation of charge carriers in graphene and aperiodicity open the possibility for an angle dependent aperiodic bandgap engineering.

In this work, we propose a bandgap engineering based on the angular dependence of the propagation of Dirac electrons in aperiodic Thue-Morse graphene superlattices (TM-GSLs). We find that the transmission bandgap can be modulated by changing the angle of incidence as well as by appropriately choosing the generation of the Thue-Morse superlattice. Even, this angle-dependent bandgap engineering is more effective than the corresponding one for periodic graphene superlattices (Periodic-GSLs).¹⁷

II. MODEL AND METHOD

Our object of study is an aperiodic graphene superlattice that obeys the construction rules of the Thue-Morse sequence. Namely, $g(A) = AB$ and $g(B) = BA$. For us A and B represent a quantum well and barrier, respectively. Then, by applying these rules we can obtain a series of barriers and wells that will represent the generations of our system. For instance, with A as generation zero, generations one, two and three become AB, ABBA and ABBABAAB. At experimental level, in principle, this structure can be obtained by placing a graphene sheet on substrates like SiO₂ or hBN and by depositing top gate electrodes in Thue-Morse fashion.^{23,24}

In Fig. 1a we show the schematic representation of the possible device for the fourth generation ($N = 4$) of the Thue-Morse graphene superlattice. By applying voltages to the top gates we can generate-modulate the height (V_0) and width (d_B) of the potential barriers. The regions between potential barriers correspond to quantum wells of width d_W . As the main effect of the voltages on the top gates is to shift the Dirac cones, the band edge profile of the conduction band can be modeled as an aperiodic arrangement of potential barriers and wells, abrupt potential model, which in turn results in minibands and gaps that strongly depend on the electron angle of incidence, see Fig. 1b.

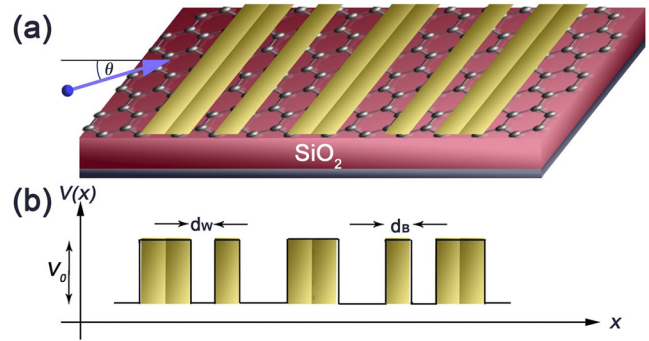


FIG. 1. (a) Schematic representation of the possible device for Thue-Morse graphene superlattices. The graphene sheet is placed on a non-interacting substrate like SiO₂ and top gates are deposited in Thue-Morse fashion. (b) As the main effect of gating is to shift the Dirac cones, the band-edge profile of the conduction band can be modeled as a series of abrupt potential barriers and wells. The device structure and the band-edge profile correspond to the fourth generation ($N = 4$) of the Thue-Morse superlattice. d_W , d_B and V_0 represent the width of wells and barriers and the height of barriers, respectively.

The transmission properties of this system can be computed directly using the transfer matrix approach.^{25,26} The basic information needed to apply this methodology is the dispersion relation, wave vectors and wave functions in the barrier and well regions as well as in the left and right semi-infinite regions. In the well and semi-infinite regions, the dispersion relation is $E = \pm \hbar v_F k$ and the wave functions come as:

$$\psi_k^\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ u_\pm \end{pmatrix} e^{\pm i k_x x + i k_y y}, \quad (1)$$

where v_F is the Fermi velocity, k is the magnitude of the wave vector in these regions, k_x and k_y are the longitudinal and transversal components of k , and $u_\pm = \text{sgn}(E) e^{\pm i \theta}$ the coefficients of the wave functions that depend on the angle of the impinging electrons, $\theta = \arctan(k_y/k_x)$.

The eigenenergy associated with the barrier region q takes the form $E - V_0 = \pm \hbar v_F q$ and the eigenfunctions as,

$$\psi_q^\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ v_\pm \end{pmatrix} e^{\pm i q_x x + i q_y y}, \quad (2)$$

where V_0 is the strength of the electrostatic potential, q is the magnitude of the wave vector in the barrier regions, q_x and q_y are the components of q , and v_\pm the coefficients of the wave functions.

By imposing the continuity of the wave function at the different boundaries between barriers and wells as well as the conservation of the transverse momentum $q_y = k_y$, we can obtain the transfer matrix of the structure.^{25,26} For instance, for generation 4 the transfer matrix is given as

$$M = M_W M_B^2 M_W M_B M_W^2 M_B^2 M_W^2 M_B M_W M_B^2 M_W, \quad (3)$$

with M_W and M_B the transfer matrices of the wells and barriers, respectively. In fact, these matrices come in terms of the so-called dynamic and propagations matrices D_i 's and P_i 's,^{27,28}

$$M_W = D_W^{-1} P_W D_W, \quad (4)$$

$$M_B = D_B^{-1} P_B D_B. \tag{5}$$

The transmittance of the Dirac electrons through the Thue-Morse superlattice can be computed with the (1,1) element of the transfer matrix,

$$T_N(E, \theta) = \frac{1}{|M_{11}|^2}. \tag{6}$$

Here, N denotes the generation of the TM-GSL.

III. RESULTS

In order to unveil the fundamental differences between the angle-dependent bandgap engineering of aperiodic and periodic graphene superlattices we will calculate the transmission properties of TM-GSLs for specific generations and the corresponding ones for Periodic-GSLs, taking care that number of barriers in both systems be the same.

In Fig. 2 we present the transmittance for the fifth ($N = 5$) and seventh ($N = 7$) generation of TM-GSLs. As the number of barriers N_B scales as 2^{N-1} , the mentioned generations have 16 and 64 barriers. Periodic-GSLs have been chosen such that the periods (barriers) correspond to precisely these numbers. Likewise, the superlattice parameters, for all cases in Fig. 2, are the same: $V_0 = 1.0$ eV, $d_B = d_W = 10a$, and $\theta = 30^\circ$. Here, a represents the carbon-carbon distance in graphene, with a value of $a = 0.142$ nm. As we can see the aperiodic order changes notably the transmission characteristics. Two main modifications are introduced with the Thue-Morse aperiodicity. First, the width and number of resonances in the minibands are greatly reduced. For instance, the well-defined minibands of Periodic-GSLs at about 1 and 2 eV collapse to a bunch of resonances when the aperiodicity is incorporated, compare the red and blue curves in Fig. 2a. By increasing

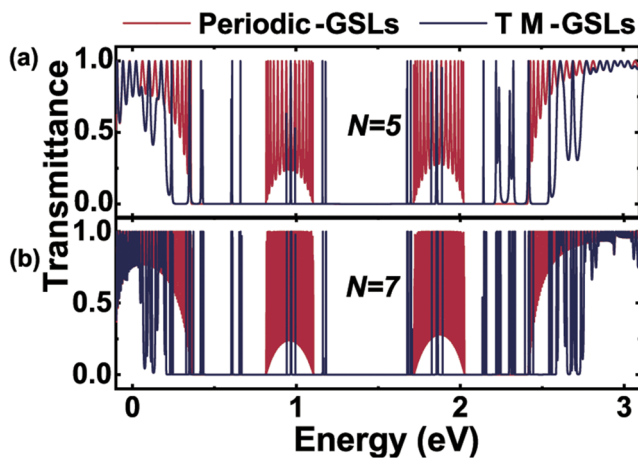


FIG. 2. Transmittance vs Energy for TM-GSLs with (a) $N = 5$ and (b) $N = 7$. As reference, the transmittance of Periodic-GSLs has been included, gray curves. The angle of incidence considered is $\theta = 30^\circ$. The superlattice parameters are: $V_0 = 1.0$ eV and $d_B = d_W = 10a$. With the carbon-carbon distance in graphene, $a = 0.142$ nm. The number of barriers in the aperiodic and periodic superlattices is the same.

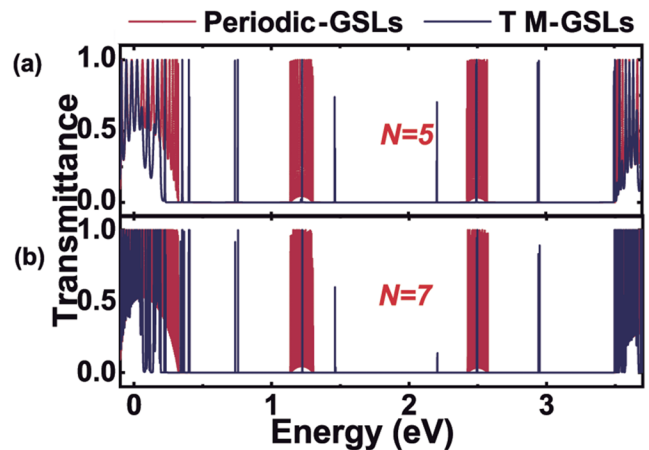


FIG. 3. The same as in Fig. 2, but here the angle of incidence is 45° .

the generation of TM-GSLs the mentioned bunch becomes a sharp resonance at the center of the minibands, see Fig. 2b. Second, several resonances are induced in the transmission gaps of the Periodic-GSLs. This characteristic is associated to the predominant random character of Thue-Morse superlattices.²⁹ With N these gap resonances cluster in narrow minibands that modifies totally the transmission landscape. These gap resonances also impede that we can define the main transmission bandgaps as simple as in the case of Periodic-GSLs.¹⁷ However, by increasing the angle of incidence we can swept (eliminate) most of the gap resonances giving rise to a huge transmission bandgap. In particular, with a moderate increase of 15° , we obtain a transmission bandgap four times greater than the corresponding one for Periodic-GSLs, see Fig. 3. We can also notice remaining

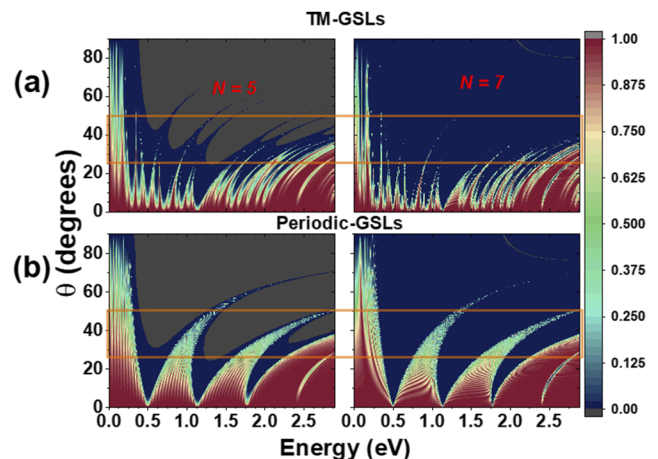


FIG. 4. Transmittance as function of the energy and the angle of incidence for (a) TM-GSLs and (b) Periodic-GSLs. The left and right panels correspond to $N = 5$ and $N = 7$. The height of the barriers and the widths of barriers and wells are the same as in Fig. 2 and 3.

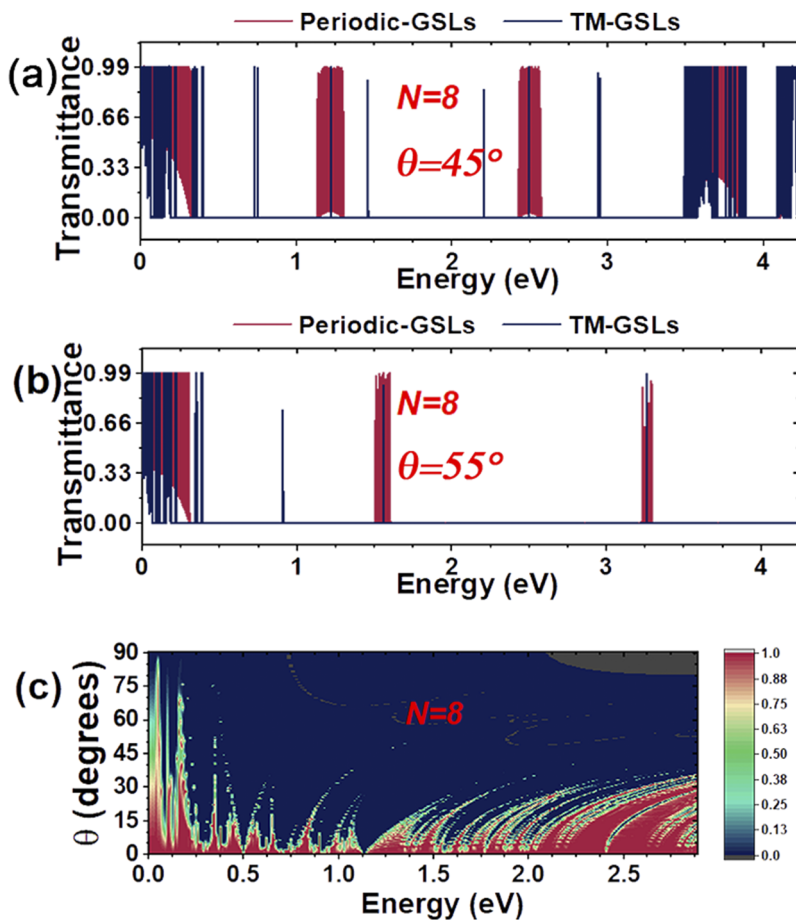


FIG. 5. The same as Fig. 3 ((a) $\theta = 45^\circ$ and (b) $\theta = 55^\circ$) and Fig. 4a (c), but here $N = 8$.

resonances at the center of the minibands and bandgaps of the Periodic-GSL. The former persist regardless of the generation (Fig. 5a) and the latter can be diminished by increasing the angle of incidence (Fig. 5b). Actually, these well-localized resonances are quite interesting for sensor applications.

In Fig. 4 we show the transmittance as a function of the energy and the angle of incidence for (a) TM-GSLs and (b) Periodic-GSLs. This figure allows us to have a broader picture of the transmission properties. From this figure, it is clear that the well defined minibands of Periodic-GSLs, semi-circular black regions, are greatly affected when the Thue-Morse aperiodicity is incorporated. In fact, the low-energy minibands are distorted and eventually destroyed as the angle of incidence increases. This gives rise to transmission gaps of 1-4 eV in the angular range of 25° - 50° . As reference see the orange rectangle in Fig. 4. For angles greater than 50° there is practically no difference between aperiodic and periodic GSLs. The corresponding results for $N = 8$ are shown in Fig. 5b. As we can see the fragmentation and diminishing of the transmittance is covering most of the energy range shown. So, the aperiodic order can be used as an additional parameter to tune the angle-dependent bandgap engineering in gated graphene

superlattices. In particular, aperiodicity gives access to transmission bandgaps that are not achievable with Periodic-GSLs and provides well-localized resonances that can be exploited in optoelectronic sensors.

IV. CONCLUSIONS

In summary, we have studied the angle-dependent bandgap engineering in TM-GSLs. This bandgap engineering is based on the angular dependence of the propagation of Dirac electrons in graphene superlattices. Specifically, transmission minibands and gaps can be formed at different energy ranges depending on the angle of the incident electrons. We find that the formation and size of the different gaps at different angles of incidence is notably more efficient in TM-GSLs than in periodic GSLs for the same number of barriers. In particular, this bandgap engineering is more effective in the angular range of 25° to 50° , while for other angles there is practically no qualitative difference between periodic and aperiodic GSLs. Another notable property of TM-GSLs is the existence of well localized states in the transmission gaps. These states may be of great interest for the development of optoelectronic sensors.

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