Graphene is nowadays one of the most attractive materials in several research fields because of its unusual, and in many respects, excellent physical properties, as a consequence of its two-dimensional honeycomb lattice. In particular, it is expected to be a good channel material in high-frequency electronic devices, flexible devices, spintronic devices, and to provide outstanding properties for photonics and optoelectronics, sensors, energy storage and conversion and so on [1]. However, with a view to digital applications in electronics, the lack of bandgap in graphene is known to make it difficult to turn off the current of transistors leading to low $I_{ON}/I_{OFF}$ ratio and poor current saturation [2, 3], which is a strong limitation for practical applications. So far, many efforts in engineering bandgap in graphene have been made to solve this issue. For instance, techniques such as cutting 2D graphene sheets into narrow nanoribbons [4], depositing graphene on hexagonal boron nitride substrate [5], nitrogen-doped graphene [6], applying an electric field perpendicularly to Bernal-stacking bilayer graphene [7], graphene nanomeshes [8], using hybrid graphene/hexagonal boron-nitride [9] or vertical graphene channels [10] have been explored. Although they are certainly promising options for opening a bandgap in graphene, some of them have their own drawbacks while the others still need experimental verification and realization. Hence, bandgap engineering is still a timely topic for the development of graphene in nanoelectronics.

In this context, it has been also shown that the lattice orientation is an additional degree of freedom to control the electronic properties of graphene layers. For a given transport direction ($Ox$-axis), we define two classes of rotated graphene lattice distinguished by difference in lattice symmetry and, hence, in Brillouin zone. In particular, these two classes correspond to two different cases where the position of their Dirac cones in the $k_y$-axis is determined differently, i.e. $K_{y}' = K_y = 0$ or $K_{y}' = -K_y = 2\pi/3L_y$ ($L_y$ is the periodic length along the $Oy$ axis). As a consequence, in devices made of two layers of different lattice classes, the misalignment of Dirac cones between the left and right graphene sections opens a finite energy-gap of conductance that can reach a few hundreds of meV. We also show that strain engineering can be used to further enlarge the transport gap and to diminish the sensitivity of the gap on the twist angle and on the commensurateness of the layer stack.

Keywords: energy gap, graphene, tight binding approach

(Some figures may appear in colour only in the online journal)
dispersion in the vicinity of \(K\)-points, saddle points emerge at the crossing of Dirac cones (i.e. at the \(M\)-point in the Brillouin zone), yielding van Hove singularities in the density of states at low energies and remarkable renormalization of the Fermi velocity. Moreover, several properties (e.g. magnetic, optical, phonon transport etc.) are strongly modified when tuning the twist angle [14–17]. The dependence of conductance on the twist angle in misoriented graphene multilayers has been also investigated in a number of works, e.g. in [18–21]. Especially, controlling the orientation of graphene layers has been demonstrated as a good strategy to modulate the resonant tunneling effects and non-linear transport characteristics in graphene/hexagonal boron-nitride/graphene heterostructures [22–24].

It is worth mentioning that recently, many researches in graphene-based electronics are being oriented toward devices made of vertical heterostructures of graphene and other layered materials [10, 22–32]. This new direction lies on the fact that inserting large bandgap layers between graphene sheets is an effective strategy to solve the main drawback of graphene, i.e. its gapless character, which makes it possible to block the current in the OFF state of graphene devices. Indeed, the ON/OFF current ratio in vertical graphene devices is significantly improved, compared to that in the case of pristine graphene [23–25].

...and answering this question is our aim in the current work. Additionally, even if the two layers in the commensurate systems have different orientations, their Dirac cones are still at the same position in the \(k\)-space, which leads to a zero energy gap, if strain is not applied. We will demonstrate here that this issue can be solved in the case of incommensurate layers and, on this basis, we will explore the new possibilities of energy-gap engineering in this type of vertical graphene hetero-channels.

The studied structures are schematized in figure 1. They consist in two partially overlapped graphene layers and we assume additionally that the overlap region has two edges perpendicular to the transport (\(Ox\)) direction. The top layer is rotated relatively to the bottom one by an angle \(\phi_{TL}\) but, differently from the study in [33], they are incommensurate layers, i.e. they do not have any common (truly) periodic lattice vector. Here, we consider 2D graphene channels, i.e. the width of graphene layers is very large, or, in other words, assumed to be infinite. Hence, to carry out the calculations, the periodicity of the channel along the transverse (\(Oy\)) direction is a necessary assumption [33–35]. In this regard, we propose to make an approximation as follows. In all incommensurate cases, the two layers have different lengths \(L^1_y\) and \(L^2_y\) of unit cells along the \(Oy\) axis. However, when they are coupled to form a heterochannel, we can always find two periodic vectors \(\vec{L}^1_y = m_1 \hat{L}^1_y\) and \(\vec{L}^2_y = m_2 \hat{L}^2_y\) that satisfy the condition \(\vec{L}^1_y \approx \vec{L}^2_y\).

...and that have only a small difference, i.e. \(<2\%\). Now, we would like to explain the nomenclature of graphene lattices considered in this work. In figure 1, we plot the geometry of two typical devices, i.e. the left (bottom) layer has zigzag and armchair orientation in (a) and (b), respectively, with respect to the \(Ox\) axis. We distinguish two lattice types as follows. For both cases, the lattice is determined by rotating the original (zigzag or armchair) lattice by an angle \(\phi_{TL}\). This angle \(\phi_{TL}\) is computed as \(\cos \phi_{TL} = \frac{L^1_y \cdot L^2_y}{|L^1_y| \cdot |L^2_y|}\), where \(L_y\) is the vector (before the lattice is rotated) defining
Figure 1. Schematic of devices made of vertical stack of misoriented graphene layers. The left layer has a zigzag (a) or armchair orientation (b) along the transport direction.

Figure 2. $(E - k_y)$-maps of transmission probability around the neutrality (Dirac) point in different devices. The devices made of $(\text{AM}7_4 @ \text{AM}4_7)$, $(\text{AM}6_6 @ \text{AM}7_4)$, $(\text{ZZ}4_4 @ \text{ZZ}5_3)$, $(\text{AM}13_7 @ \text{AM}13_8)$ layers are considered in the panels (a),(b),(c) and (d), respectively (see the definition of layers in the text).
the size of unit cells along the $Oy$-axis while $\mathbf{L}_y^0$ is the vector of the original lattice. These vectors are determined as $\mathbf{L}_y = q_1 \mathbf{a}_1 + q_2 \mathbf{a}_2$ and $\mathbf{L}_y^0 = \mathbf{a}_1 + \mathbf{a}_2$. For the type 1 (i.e. ZZ, q2 lattice, see in figure 1(a)) when the original lattice has a zigzag orientation along the Ox axis, $\mathbf{a}_1 = (-\sqrt{3}, 3, a_0/2)$ and $\mathbf{a}_2 = \left(\frac{1}{3}, \frac{1}{3}\right)a_0/2$. For the type 2 (i.e. AM, q2 lattice, see in figure 1(b)) when the original lattice has an armchair orientation, $\mathbf{a}_1 = (3, \sqrt{3})a_0/2$ and $\mathbf{a}_2 = \left(\frac{1}{3}, \frac{1}{3}\right)a_0/2$. Here, $a_0 = 0.142$ nm is the in-plane C-C bond length in graphene.

To compute the electronic transport in the considered systems, we employed atomistic tight-binding calculations and Green’s function techniques as in [33–35, 42–45]. In particular, the hopping parameters are determined similarly as in [42–45], i.e. $t_{ij} = t_0 \exp[-\beta (r_{ij}/r_0 - 1)]$ where $t_0 = \pm 2.7$ eV (resp. 0.48 eV) for ZZ and AM, and $\pm 2q_1 - q_2$ for ZZ and AM, respectively. Note that the two layers ZZ and AM, are commensurate while the other systems are incommensurate. It is clearly shown that in the case of commensurate lattices, even if the two lattices have different orientations, there is no energy-gap of transmission. This can be explained by the fact that the commensurate lattices have the same periodic vectors and hence, because of their same lattice symmetry, they have the same Brillouin zone. Since their commensurate lattices have the same periodic vectors, the transport gap is zero, similarly as reported in [33, 38, 45]. The transport picture, however, can be dramatically changed in the devices made of incommensurate layers, i.e. finite energy-gaps can be achieved as shown in figures 2(b)–(d). The value of energy-gap is quite significant in these cases: $E_g \approx 810.6$ meV in (b), 703.2 meV in (c), and 432.8 meV in (d). This phenomenon is explained as follows. For all cases studied, we can distinguish two classes of rotated graphene lattice as shown in figures 3(a) and (b). In the class 1, the lengths $L_x$ and $L_y$ determining the unit (smallest

Table 1. Description of some concrete devices investigated in this work and their transport gap $E_g$. 

| Layer 1  | Layer 2  | $\phi_{TL}$ | $L_y (a_0)$ | $\eta$ (%) | $E_g$ (meV) |
|----------|----------|-------------|-------------|------------|-------------|
| ZZ4, 4   | ZZ5, 3   | 8.21°       | 12.062      | 1.031      | 703.2       |
| ZZ5, 5   | ZZ6, 1   | 24.18°      | 14.899      | 1.351      | 569.3       |
| ZZ13, 1  | ZZ14, 1  | 11.25°      | 23.366      | 0.549      | 363.0       |
| ZZ8, 8   | ZZ12, 2  | 22.94°      | 24.216      | 1.790      | 350.2       |
| ZZ15, 1  | ZZ13, 4  | 9.80°       | 26.776      | 0.836      | 316.7       |
| ZZ19, 1  | ZZ17, 4  | 7.78°       | 33.629      | 1.061      | 252.2       |
| AM6, 6   | AM7, 4   | 25.28°      | 10.464      | 1.369      | 810.6       |
| AM8, 9   | AM10, 7  | 16.99°      | 15.491      | 1.250      | 547.5       |
| AM13, 7  | AM13, 8  | 5.04°       | 19.595      | 0.781      | 432.8       |
| AM14, 9  | AM13, 11 | 12.41°      | 21.141      | 1.342      | 401.2       |
| AM14, 14 | AM16, 11 | 17.78°      | 24.402      | 1.259      | 347.6       |
| AM17, 9  | AM17, 10 | 3.87°       | 25.573      | 0.458      | 331.6       |
| ZZ41, 14 | AM14, 13 | 18.59°      | 23.366      | 0.549      | 362.9       |
| ZZ13, 2  | AM16, 11 | 24.83°      | 24.494      | 0.500      | 346.2       |
| ZZ15, 1  | AM17, 13 | 16.20°      | 26.776      | 0.836      | 316.7       |
| ZZ15, 4  | AM19, 14 | 26.22°      | 29.798      | 1.689      | 284.6       |

Note: Here, $\phi_{TL}$ is the twist angle, $L_y$ is the average periodic length along the $Oy$ axis, and $\eta$ indicates the mismatch between $L_y^0$ and $L_y'$ of the two layers.
per-\(c\)tic) cell satisfy \(L_x = \sqrt{3} L_y\) while \(L_y = L_x/\sqrt{3}\) for the class 2. Accordingly, the Brillouin zone and Dirac cones (at the \(K\)-points) of these two lattice classes have different properties: \(K_y^1 = K_y = 0\) for the class 1 while \(K_y^2 = 2\pi/3L_y\) for the class 2, as schematized in figure 3. Similarly to the case of commensurate lattices, if the channel is made of two layers of the same class, the Dirac cones of both layers are located at the same \(k\)-points and the transport gap is zero (not shown). However, if the channel is made of layers of different classes, the misalignment of their Dirac cones in the \(k\)-space generates a finite transport gap, which explains the results obtained.

In the table 1, we show the detailed description of some concrete devices investigated in this work and their transport gap. \(\hat{L}_y\) is the average periodic length of two layers along the \(O_y\) axis and \(\eta\) denotes the mismatch between \(\hat{L}_y\) and \(L_y\), i.e. \(\eta = |\hat{L}_y - L_y|/L_y\). As mentioned above, our calculations were performed with \(\eta < 2\%\) in all cases. First, we find that there are various possibilities of finite energy-gap using this design strategy and \(E_g\) can reach a few hundreds meV. Important, the dependence of \(E_g\) on the twist angle is quite complicated but \(E_g\) is simply inversely proportional to \(\hat{L}_y\). This is essentially explained as follows. The value of \(E_g\) is basically proportional to the distance \(\Delta K_y\) between the Dirac cones of the two layers along the \(k_y\)-axis [3, 5, 8]. In the considered channels, \(\Delta K_y\) is actually equal to \(2\pi/3L_y\), which fully explains the property above. On this basis, we can also analytically compute the value of \(E_g\). Note that in the low energy regime (i.e. \(|E| \ll 1\) eV around the Dirac point), the energy dispersion of graphene is well described by the simple formula \(E(\hat{k}) = \pm \hbar v_F |\hat{k}|\) with \(v_F = 3a_0\delta_0/2\hbar\) and \(\hat{k} = \mathbf{k} - \mathbf{K}\) (i.e. \(\delta_0 = 2.7\) eV and \(a_0 = 0.142\) nm). The band edge is thus defined as a function of \(\hat{k}_y\) as \(E_{\text{edge}}(\hat{k}_y) = \pm 3a_0\delta_0|\hat{k}_y|/2\). In the considered channel, the Dirac cones of the two layers are located at different \(k_y\)-points, i.e. at \(K_y^1 = 0\) and \(K_y^2 = 2\pi/3L_y\), respectively, and the energy-gap is thus determined as the value of \(E_{\text{edge}}(\hat{k}_y)\) at the middle point [33, 35, 38], i.e. \(\hat{k}_y = \pi/3\hat{L}_y\) (see also in figures 2(b)–(d)). Hence, we have

\[
E_g \approx \pi \frac{a_0}{\hat{L}_y} \delta_0
\]

In figure 4, we summarize the results obtained in all studied devices. They indeed confirm an excellent agreement with the analytical formula above.

Now, new questions arise. Since the dependence of \(E_g\) on the twist angle is quite complicated, it shall not be easy to control well this energy-gap in practice. Additionally, the control of the commensurateness of the two layers is also an open question. To partly solve these issues, we propose to use strain engineering as an additional ingredient. As suggested in [33], the strain effects are very efficient to open a finite transport-gap in devices made of commensurate lattices. Similarly, this idea can be used here to open an energy-gap in the channels where two incommensurate layers are of the same lattice class, i.e. when \(E_g = 0\) without strain. Additionally, in the cases of device with a small gap (i.e. if the two layers are from different lattice classes and \(\hat{L}_y\) is large), strain can be used to further enlarge \(E_g\). These points are clearly shown in figure 5 for three typical cases: commensurate (\(\text{AM}_{7, 4} @ \text{AM}_{4, 7}\)), incommensurate (\(\text{AM}_{14, 16} @ \text{AM}_{9, 16}\)) with zero gap and incommensurate (\(\text{AM}_{11, 20} @ \text{AM}_{13, 20}\)) with a small gap if no strain is applied. The gap is significantly broadened, i.e. by a few hundreds meV, when a small strain of only 4% is applied.

In conclusion, we have investigated the transport properties of vertical devices made of two incommensurately mis-oriented graphene layers. For given \(O_{xy}\) coordinates with
transport direction parallel to the Ox axis, there are two different classes of graphene lattice depending on their lattice symmetry and on the properties of their Brillouin zone. In particular, depending on the graphene lattices, the two Dirac cones are either located at the same \( k_y \)-point (\( K_0 = K_0 = 0 \)) or at different \( k_y \)-points (\( K_0 = -K_0 = 2\pi/3L_y \)). As a consequence, in devices made of two layers of different lattice classes, the misalignment of Dirac cones of the two layers leads to a significant energy-gap (i.e. a few hundreds of meV) of conductance. The gap is shown to be inversely proportional to the length \( L_y \). We have also shown the possibility of using strain to enlarge the energy-gap and to diminish the sensitivity of the gap on the twist angle and commensurateness of the layer stack. Thus, our study suggests an alternative strategy to open an energy gap in graphene channels without altering the graphene lattices, by controlling the misorientation of two partially overlapped graphene layers, which should be helpful for broadening the practical applications of graphene.

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Figure 5. Strain effects on the transport gap in different devices. The strain of angle \( \theta \) with respect to the transport direction (Ox) is applied [33].
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