Work function, deformation potential, and collapse of Landau levels in strained graphene and silicene

D. Grassano, 1 M. D’Alessandro, 2 O. Pulci, 1 S.G. Sharapov, 3 V.P. Gusynin, 3 and A.A. Varlamov 4

1Dept. of Physics, and INFN, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy
2Istituto di Struttura della Materia-CNR (ISM-CNR), Via del Fosso del Cavaliere 100, 00133 Rome, Italy
3Bogolyubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrolohichna Street, Kyiv 03143, Ukraine
4CNR-SPIN, c/o DICII-University of Rome “Tor Vergata”, Via del Politecnico, 1, 00133 Rome, Italy

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We perform a systematic ab initio study of the work function and its uniform strain dependence for graphene and silicene for both tensile and compressive strains. The Poisson ratios associated to armchair and zigzag strains are also computed. Basing on these results, we obtain the deformation potential, crucial for straintronics, as a function of the applied strain. Further, we propose a particular experimental setup with a special strain configuration that generates only electric field, while the pseudomagnetic field is absent. Then, applying a real magnetic field, one should be able to realize experimentally the spectacular phenomenon of the Landau levels collapse in graphene or related 2D materials.

I. INTRODUCTION

The possibility to tune the work function (WF) of graphene and related new materials is important for engineering new efficient devices. These latter require a cathode and an anode electrodes with a low and high values of the WF respectively. The WF of the system \( W = E_{\text{vac}} - E_F \) is defined as the difference between the values of vacuum level \( E_{\text{vac}} \) and the Fermi energy \( E_F \). The experimental value of the WF extrapolated for pristine undoped graphene is \( W \sim 4.5 \) eV, which turns out to be in between the desired cathode and anode values. It is shown that the p-type doping by Au particles allows to increase the WF (up to 0.5 eV) by controlling the immersion time. Furthermore, it is observed experimentally and confirmed by ab initio calculations that the WF of graphene can be increased up to the value \( \sim 5.5 \) eV (increase by 0.94 eV) by applying a self-assembled monolayer on its surface. A dramatic lowering of the WF is predicted when functionalizing graphene with hydrogen: in the limit of 100% hydrogen coverage, graphene is called graphane, and possess a WF of about 3 eV.

The WF of single and double graphene layers can also be varied by electrostatic gating that changes the doping level. A combination of Cs/O surface coating along with gating allowed to reach the ultra-low value \( W \sim 1 \) eV. It has to be stressed that the tunability of the WF by electrostatic gating in 2D materials is a rather nontrivial property. Indeed, it is well known that in most of the three-dimensional semiconductors the phenomenon of surface state pinning of the Fermi level occurs. Here any change in \( E_F \) is accompanied by an almost equal shift in the band structure and thus in the value of \( E_{\text{vac}} \) at the surface. On the contrary, as it was demonstrated in Ref. 2, in monolayer graphene the WF varies in one-to-one correspondence with the position of the Fermi level with respect to the Dirac point \( E_D \). This relation was verified down to the nanometer scale where, due to inhomogeneities of the sample, the local Dirac point also changes its position.

Finally, it is demonstrated that the WF of chemically vapor deposited graphene can be adjusted by applying strain, viz. under a 7% uniaxial strain it increases by 0.16 eV. The latter result should be considered in a broader context of a new branch of studies called straintronics, that explores the possibilities to use strain for controlling physical properties of graphene and related materials. The effect of deformation on the electronic properties of graphene-like materials is mainly twofold. Firstly, the hopping integrals that describe motion of conducting electrons between the atoms change under the strain. For the uniform strain this results in a linear change of the slope of the density of states (DOS) function in the vicinity of the Dirac point. Secondy, the onsite energies of the electrons change causing a shift of the Dirac point energy \( E_D \) itself, where \( \varepsilon \) is the strain.

The vast majority of the existing literature on the strained graphene focuses on the former effect while neglecting the second one. This probably explains why there is still no agreement on the value of the deformation potential that characterizes the strain dependence of the Dirac point energy. In particular, this effect is not mentioned in the most recent review, while theoretical values of the deformation potential \( \alpha \) recited in the review are rather inconsistent between different sources and vary in a fairly wide range from 0 eV to 20 eV.

The physical meaning of the deformation potential can be immediately understood from the fact that for the undoped graphene the Fermi level coincides with the Dirac point \( E_F = E_D \). Then its WF is \( W_D = E_{\text{vac}} - E_D \) and the
deformation potential $\alpha$ characterizes the slope of its dependence on the strain, viz. $\alpha = -dW_D^H/d\varepsilon$. In its turn the WF and its strain dependence can be found from the ab initio studies as suggested in [14]. In particular, using the result of the ab initio calculations [15], which show that a 12\% uniaxial strain results in an increase of the work function $W_D^H$ by 0.3 eV, one can estimate that $\alpha \approx -2.5$ eV. This is rather large value that implies that the impact of the deformation potential cannot be neglected, since even a moderate 1\% strain causes an observable shift of the Dirac point by 25 meV. Concerning the other related 2D materials, it is found in a recent first-principles density functional theory study [10] that compressive strain of up to 10\% decreases the WF of various metal dichalcogenide monolayers by as much as 1 eV.

The deformation potential is important for various applications. In particular, it is well known that the Landau levels of graphene in a magnetic field would collapse in the presence of an in-plane electric field. This spectacular phenomenon consists in merging of the relativistic Landau levels staircase if the electric field reaches its critical value $E_c$, and the cyclotron frequency turns zero [17, 18]. As previously stated, the WF is calculated as the energy difference between the vacuum level and the Fermi energy. To obtain the vacuum level we have computed the plane-averaged electrostatic potential associated to the ground state density of the system. Then, the vacuum level is given by the limit value of the potential at far distance from the material.

Biaxial and uniaxial strains have been applied by modifying the relative position of the atoms in the lattice. The coordinate system is chosen in such a way that the zigzag direction is parallel to the $y$ axis and the armchair one is parallel to the $x$ axis. A generic uniform deformation is represented by the strain matrix $\hat{\varepsilon}$

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{yx} & \varepsilon_{yy} \end{pmatrix},$$

(2)

In this way the deformation of the lattice is described as

$$\mathbf{x} = \mathbf{x}_0 + \mathbf{u}, \quad \mathbf{u} = \hat{\varepsilon} \cdot \mathbf{x}_0,$$

(3)

where $\mathbf{x}_0$ is the actual position of the atom, $\mathbf{u}$ is the displacement vector. Specifically, the strain matrices describing the deformations for both biaxial strain and uniaxial ones in the armchair and zigzag directions are given by

$$\hat{\varepsilon}_{bi} = \eta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{\varepsilon}_{arm} = \eta \begin{pmatrix} 1 & 0 \\ 0 & -\nu_{arm} \end{pmatrix}, \quad \hat{\varepsilon}_{zig} = \eta \begin{pmatrix} -\nu_{zig} & 0 \\ 0 & 1 \end{pmatrix},$$

(4)

where the strain parameter $\eta$ determines the magnitude of deformation and $\nu_{arm}, \nu_{zig}$ represent the Poisson ratios (PR) associated to armchair and zigzag strain, respectively. These parameters indicate the amount of deformation in the transverse direction, with respect to the applied strain.

In the present analysis the PR have been computed in a full ab initio fashion. To do so we have imposed a fixed strain in a given direction and looked for the value of

II. AB INITIO METHODS

Our ab initio calculations of the effect of strain on the work function of graphene and silicene are based on the Density Functional Theory (DFT) as implemented in the Quantum Espresso package [20, 21]. We have solved the single-particle Schroedinger equation as formulated by Kohn-Sham (KS) [22]
atomic distance in the transverse coordinates that minimizes the total energy of the system. The results of this procedure are reported in Fig. 1 and Fig. 4 for graphene and silicene, respectively. This analysis provides values of the PR that depend both on the deformation direction and the strain value. For silicene, at each applied strain the corresponding buckling has also been determined.

FIG. 1. Plot of the total energy of graphene against the values of $\varepsilon_{xx}/\varepsilon_{yy}$. The dark orange (red) curve represents the value of the $\varepsilon_{yy}$ ($\varepsilon_{xx}$) strain that minimize the energy of the system given the constrain $\varepsilon_{xx} (\varepsilon_{yy}) = \text{const.}$

III. AB INITIO RESULTS

A. Strain dependence of the WF and extraction of deformation potential for graphene

The strain dependence of the work function in graphene has been computed using the PBE functional, since, as shown in Fig. 2 for biaxial strain, the value the WF turns out to be quite sensitive to the choice of the XC but its slope is not. This implies that physical quantities like the deformation potential, which is basically related to the first derivative of these curves, can be assessed with less ambiguity.

The WF dependence of graphene on biaxial and uniaxial strains have been computed. For the uniaxial cases, deformation in both zigzag and armchair directions have been investigated and the associated PR have been taken into account. In all the cases, we have considered the values of strain in the range from -16% up to +16%. Results are reported in the top panel of Fig. 3 and show good agreement with the literature [12, 25–30].

Knowing the WF dependence of the strain we have extracted the deformation potential $\alpha$, defined as

$$\alpha_s = -\frac{dW(\eta)}{d\eta},$$

where the index $s$ takes the values (bi, arm, zig). We emphasize that for the uniaxial armchair and zigzag strains

FIG. 2. Dependence of the work function of graphene on the values of strain for the PBE and LDA XC functionals.

FIG. 3. Results for graphene. Top panel: Work function dependence on the biaxial (blue dots), the uniaxial-zigzag (green dots), and the uniaxial-armchair (orange dots) strain from -16% (compressive) to +16% (tensile). Bottom panel: Deformation potential $\alpha$ associated to biaxial and uniaxial strains.
the deformation potential in Eq. (5) was calculated taking into account the PR.

Here, the *ab initio* estimate of equation (5) is evaluated through a polynomial fitting of the WF curves in the top panel of Fig. 3 and by the subsequent computation of the first derivative for each value of strain. This procedure is restricted to a limited range (from -6% to +6%), since the WF curves become less smooth for higher strain values, and the numerical extraction of the derivative becomes less trivial. Corresponding results, reported in the bottom panel of Fig. 3 show that in graphene the zigzag and armchair deformation potentials are practically identical, and much weaker than the biaxial one.

**B. Strain dependence of the WF and extraction of deformation potential for silicene**

The same analysis described for graphene has been performed also for silicene, using the PBE functional both for tensile and compressive deformations. The optimized equilibrium lattice constant was found to be equal 3.867 Å with a buckling of 0.448 Å. Even in this case the PR of the system has been computed *ab initio* by employing the same procedure used for graphene (see Fig. 4).

Results are reported in Fig. 5 and show the strain dependence for both the WF and the deformation potential. In particular, the behavior of the WF is presented for values of strain that range from the +16%, in the tensile region down to -10%, in the compressive part. We restricted our analysis at compressive strain of -10% since we observed that the electronic properties of the material are not preserved below this value. The obtained data show that, analogously to what happens for graphene, the WF increases as long as the material is stretched. The curves present a smooth behavior for values of strain limited from the -4% up to the +4%. In this range the deformation potential has been computed by extracting the numerical derivative of the WF. A comparison with the results for graphene evidences that the values of the deformation potential for silicene are much smaller than those for graphene, in all the considered cases.

**FIG. 4.** Plot of the total energy of silicene against the values of $\varepsilon_{xx}/\varepsilon_{yy}$. The dark orange (red) curve represents the value of the $\varepsilon_{yy}/\varepsilon_{xx}$ strain that minimize the energy of the system given the constrain $\varepsilon_{xx}(\varepsilon_{yy}) = \text{const}$.

**FIG. 5.** Results for silicene. Top panel: Work function dependence on the biaxial (blue dots), the uniaxial-zigzag (green dots), and the uniaxial-armchair (orange dots) strain. Bottom panel: Deformation potential $\alpha$ associated to biaxial and uniaxial strains.

**IV. DEFORMATION POTENTIAL IN THE TIGHT-BINDING STRAINED HAMILTONIAN**

In this section we relate the obtained above results to the parameters of the the tight-binding Hamiltonian. The electrons in the valence and conduction bands of graphene and silicene are described by the following Hamiltonian

$$H = H_{\text{hop}} + H_{\text{pot}}.$$  (6)
Here \( H_{\text{hop}} \) is conventional tight-binding Hamiltonian for \( \pi \) orbitals that describes hopping between nearest-neighbors [11, 12]. We do not write down its explicit form since the corresponding hopping parameters and their strain dependence are not considered in the present work.

The main interest for us represents the potential term

\[
H_{\text{pot}} = \sum_{i,\delta} U_{\delta i} c_{\delta i}^\dagger c_{\delta i},
\]

(7)

where \( i \) run over \( N/2 \) lattice cells, indices \( \delta = A, B \) enumerate the sublattices, operator \( c_{\delta i}^\dagger \) (\( c_{\delta i} \)) creates (annihilates) an electron at the corresponding lattice site, the spin index is omitted for brevity, and \( U_{\delta i} \) is the on-site deformation-dependent potential. \( U_{\delta i} \) consists of the strain-independent part \( E_D \), which determines the energy of the Dirac point in unstrained graphene, and the strain-dependent part.

For uniform strain, the potential energy does not depend on the lattice site. Assuming also the linear dependence of the on-site energy on strain, one can rewrite the Hamiltonian (7) as follows

\[
H_{\text{pot}} = \sum_{i,\delta}(\alpha_{xx} \varepsilon_{xx} + \alpha_{yy} \varepsilon_{yy} + E_D) c_{\delta i}^\dagger c_{\delta i}.
\]

(8)

Here we introduced two deformation potential constants \( \alpha_{xx,yy} \). The values of these constants are determined from the strain dependence of the WF:

\[
\alpha_{xx} = -\left( \frac{\partial W}{\partial \varepsilon_{xx}} \right)_{\varepsilon_{yy}=0}, \quad \alpha_{yy} = -\left( \frac{\partial W}{\partial \varepsilon_{yy}} \right)_{\varepsilon_{xx}=0},
\]

(9)

where \( xx \) and \( yy \) correspond to the armchair and zigzag directions, respectively.

In Sec. [11, 12] we have found the values \( \alpha_s \) which describe the deformation of the samples in the presence of Poisson's transverse contraction characterized by \( \nu_s \), with \( s = \text{arm}, \text{zig} \). These parameters can be related to each other by taking into account that

\[
\frac{dW_{\alpha_s}}{d\eta} = \frac{\partial W}{\partial \varepsilon_{xx}} - \nu_{\alpha_s} \frac{\partial W}{\partial \varepsilon_{yy}},
\]

\[
\frac{dW_{\alpha_{zig}}}{d\eta} = -\nu_{\alpha_{zig}} \frac{\partial W}{\partial \varepsilon_{xx}} + \frac{\partial W}{\partial \varepsilon_{yy}}.
\]

(10)

Now we assume that the corresponding derivatives are constants for small values of the strain. Solving the system (10) one obtains

\[
\alpha_{xx} = \frac{\alpha_{\text{arm}} + \nu_{\text{arm}} \alpha_{\text{zig}}}{1 - \nu_{\text{arm}} \nu_{\text{zig}}},
\]

\[
\alpha_{yy} = \frac{\alpha_{\text{zig}} + \nu_{\text{zig}} \alpha_{\text{arm}}}{1 - \nu_{\text{arm}} \nu_{\text{zig}}}.
\]

(11)

The values of the constants \( \alpha_s, \alpha_{xx,yy} \) and the PR for the tensile strain for graphene and silicene are provided in Table I.

|                  | armchair | zigzag | biaxial |
|------------------|----------|--------|--------|
| \( \alpha_s \) (eV) | -3.5     | -3.5   | -8.6   |
| \( \nu_{\text{arm}, \text{zig}} \) | 0.14     | 0.14   | -     |
| \( \alpha_{xx,yy} \) (eV) for \( \nu = 0 \) | -4.1     | -4.1   | -     |

V. COLLAPSE OF LANDAU LEVELS

The behavior of the Dirac fermions in graphene in crossed external magnetic and electric fields was considered in Refs. [17, 18]. The energy shift of the Landau levels and even their collapse was predicted there for values of the in-plane electric field \( E \) larger than the critical value \( E_c = v_F B \), where \( v_F \) is the Fermi velocity in graphene. Some indications of the latter effect have been obtained experimentally in Refs. [31, 32].

Interestingly, in Dirac materials the strain can induce the same phenomena. The experimental observation of the Landau levels induced by inhomogeneous strain [33] is probably the most spectacular effect associated with straintronics [33]. The key point is that the strain induced change in the hopping energy between neighboring atoms in the Hamiltonian \( H_{\text{hop}} \) can be described by some kind of vector potential \( A_{\text{pm}} \) (see Refs. [11, 12] for a review). For the \( x \)-axis aligned in the armchair direction it reads

\[
A_{\text{pm}} = \frac{\hbar \beta}{a_0} \left( \frac{2 \varepsilon_{xy}}{\varepsilon_{xx} - \varepsilon_{yy}} \right),
\]

(12)

where \( \beta \) is the dimensionless Grüneisen parameter for the lattice deformation and \( a_0 \) is the lattice constant. The generic position-dependent strain tensor \( \varepsilon_{ij} \) with \( i, j = x, y \) is related to the displacement \( \delta_i \) by the relation

\[
\varepsilon_{ij} = (\partial_i u_j + \partial_j u_i)/2.
\]

The vector potential Eq. (12) generates a pseudomagnetic field \( B_{\text{pm}} = \nabla \times A_{\text{pm}} \). It formally resembles a real magnetic field, with the crucial distinction that it is directed oppositely in \( K \) and \( K' \) valleys. The sign of the pseudomagnetic field depends on the valley, and, for example, in \( K \) valley,

\[
B_{\text{pm}} = \frac{\hbar \beta}{a_0} \left( \frac{1}{2} \partial_y (\varepsilon_{xx} - \varepsilon_{yy}) - \partial_x \varepsilon_{xy} \right),
\]

(13)

whereas it has the opposite sign in \( K' \) valley.

In its turn, the deformation potential part of the Hamiltonian \( H_{\text{pot}} \), Eq. (8), contains the scalar potential \( \alpha A_0 = \alpha (\varepsilon_{xx} + \varepsilon_{yy}) \) which has the same sign in both the \( K \) and \( K' \) valleys. Accordingly, the deformation potential acts as an electric field per unit charge \( E_i = -\alpha \partial_i A_0 \) (it is normally assumed that \( \alpha_{xx} = \alpha_{yy} = \alpha \)).

### Table I. The values of deformation potential constants \( \alpha_s \) with \( s = \text{arm}, \text{zig}, \text{arm}_{xx,yy} \) and the Poisson’s ratios \( \nu_{\text{arm}, \text{zig}} \) (for the tensile strain) for graphene and silicene, calculated in the vicinity of \( \eta = 0 \).

|                  | armchair | zigzag | biaxial |
|------------------|----------|--------|--------|
| \( \alpha_s \) (eV) | -0.8     | -0.7   | -1.3   |
| \( \nu_{\text{arm}, \text{zig}} \) | 0.22     | 0.13   | -     |
| \( \alpha_{xx,yy} \) (eV) for \( \nu = 0 \) | -0.71    | -0.49  | -     |
One can see that uniform strain results in appearance of a constant strain-induced vector potential corresponding to the shift of the $K$ and $K'$ points, so that the pseudomagnetic field is zero. Since $A_0$ is position independent, also an electric field is absent.

On the other hand, creation of the pseudo Landau levels requires a special configuration with inhomogeneous strain. To simplify theoretical modeling, the pseudo Landau levels are very often treated assuming that the deformation is a pure shear, so that $A_0 = \varepsilon_{xx} + \varepsilon_{yy} = 0$, and the corresponding term in the Hamiltonian does not appear. This assumption is rather unphysical and when the deformation potential is included, new effects are expected. For some strain configurations, the deformation potential acts as an in-plane electric field.

A special strain configuration was considered in Ref. [19]. In our notations it can be written as $\varepsilon_{xx} = 2a_0 B x / (\beta \hbar)$, $\varepsilon_{yy} = 0$ and $\varepsilon_{xy} = 0$. It corresponds to the strain induced vector and scalar potentials $A_{pm} = (0, B x)$, $A_0 = 2a_0 B x / (\beta \hbar)$ respectively. Evidently, they generate crossed constant pseudomagnetic and electric fields of the magnitudes $B$ and $E_x = -2a_0 B / (\beta \hbar)$. Then, the condition of the Landau level collapse acquires the form $|\alpha| \gtrsim v_F \beta \hbar / (2a_0)$ [17, 19]. One can see that in this case the condition for the collapse depends on the material constants $\alpha$, $\beta$ and $v_F$, which cannot be tuned easily.

Here we propose a different experimental setup with a special strain configuration that generates only electric field, while the pseudomagnetic field is absent. Then, applying a real magnetic field, one should be able to realize the Landau level collapse. In fact, we obtain a pseudomagnetic field $B_{pm} = 0$ when in Eq. (12) the components of the pseudo vector potential are constants, i.e. $A_x = C_1$ and $A_y = C_2$. Then it is easy to see that this is possible when the components of the displacement vector $u_{x,y}(x, y)$ satisfy the two-dimensional Laplace equations

$$\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} = 0,$$

$$\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} = 0. \quad (14)$$

Any harmonic function satisfies Eq. (14), so one can consider the simplest nontrivial example:

$$u_x(x, y) = d(x^2 - y^2) + h_1 x + h_2 y,$n

$$u_y(x, y) = 2d x y + h_3 x + h_4 y. \quad (15)$$

Here $d$ is a constant that has the dimension of an inverse length, while $h_{1,2,3,4}$ are the dimensionless constants that describe the uniform strain. This strain configuration, shown in Fig. 6, generates the potentials

$$A_x = \frac{\beta}{2a_0} (h_2 + h_3), \quad A_y = \frac{\beta}{2a_0} (h_1 - h_4),$$

$$A_0 = 4dx + h_1 + h_4. \quad (16)$$

One can see that this potential corresponds to $B_{pm} = 0$ and a constant electric field $E_x = -4ad / e$, where we explicitly included the electric charge $e$. The constant term $\alpha(h_1 + h_4)$ in $H_{pot}$ corresponds to the uniform strain considered in the previous sections.

When a constant external magnetic field is applied in addition to the strain induced electric field, the condition of the Landau levels collapse $E = v_F B_c$ acquires the following form

$$B_c = \frac{4(|da_0| |\alpha|)}{e a_0 v_F}. \quad (17)$$

Thus, as the magnetic field decreases to this critical value $B_c$, the collapse occurs. Taking into account that $1 \text{T} = \text{V} \cdot \text{s} / \text{m}^2$ and using the value of the Fermi velocity $v_F = 1 \times 10^6 \text{m/s}$, and $a_0 = 2.46 \text{Å}$, one obtains the following estimate

$$B_c = 1.6 \times 10^4 (da_0) \alpha, \quad (18)$$

where $B_c$ is expressed in Tesla, while $\alpha$ is measured in eV.

Assuming a value $da_0 = 10^{-5}$, one finds that the Landau levels collapse for graphene (see Table II) would occur at $B_c = 0.67 \text{T}$. This estimate confirms that corresponding experiment, where the electric field is generated by the non-uniform strain and an external real magnetic field $B$ is tuned to its critical value, can be implemented in practice.

VI. CONCLUSIONS

We have studied \textit{ab initio} how the WF of graphene and silicene depends on uniform compressive and tensile strains. For small deformations the dependence is linear and corresponding values of the deformation potential parameters are provided in the Table II. In accordance to both the experiment [10] and the \textit{ab initio} results the
WFs of graphene and silicene increase under the tensile strain. For small values of strain the armchair and zigzag deformation potentials turn out to be practically identical and approximately correspond to one half of the deformation potential associated to biaxial strain.

It has to be noted that strain tuning of the WF of different materials has been a topic of research for a long time. As an example we refer to the experiment that shows the opposite strain dependence of the WF in Cu and Al, viz. in the elastic range, tensile strain results in the decrease of the WF. The corresponding \textit{ab initio} calculation that agreed with the experiment was presented in \cite{34}. Thus one of the questions for the future is to address how the corresponding strain dependence of the WF is material dependent.

Finally, we proposed the experimental setup with a special strain configuration that generates only electric field, whereas the pseudomagnetic field is absent. In this case, in order to obtain the Landau levels staircase, an external magnetic field should be applied. Such setup allows to explore the phenomenon of the Landau levels collapse more easily, since the strain induced electric field and the magnetic field can be controlled independently.

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