Impurity states in doped graphene systems

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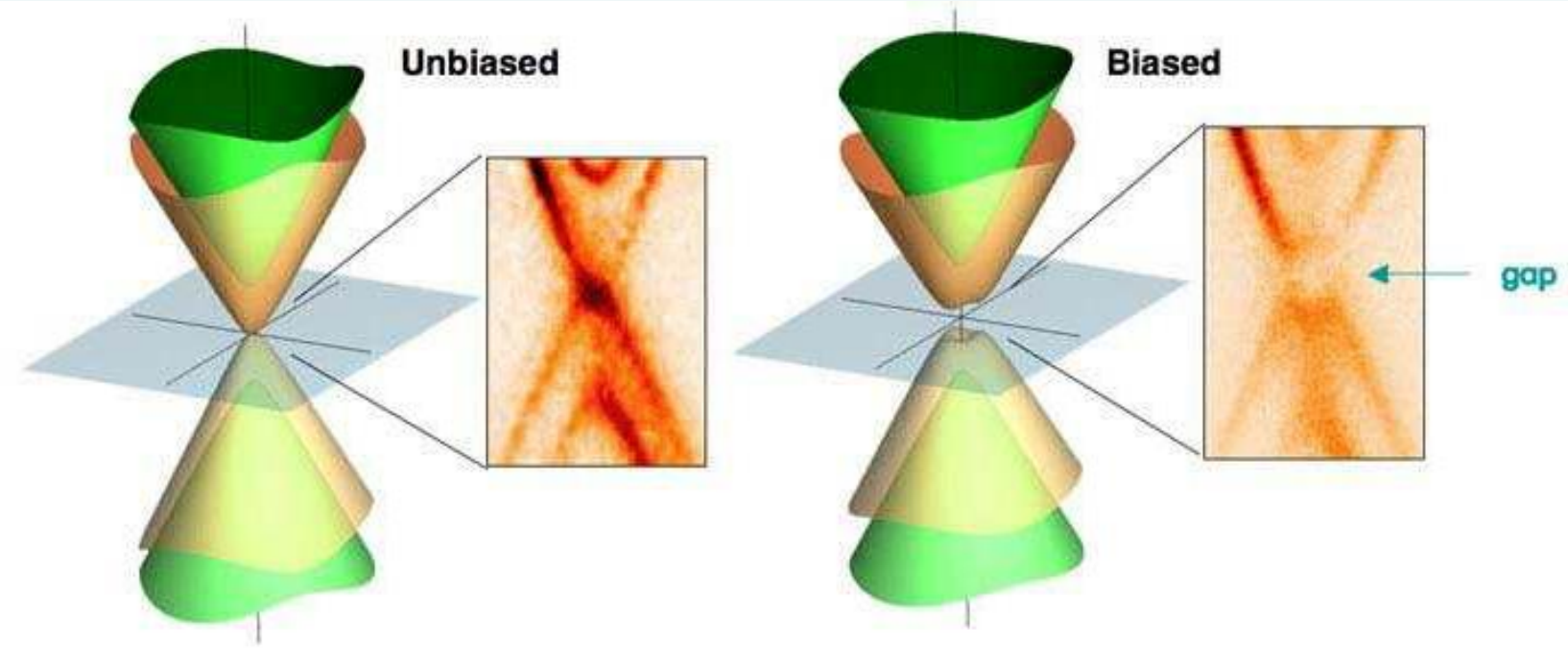
Motivation

Single layer graphene (SLG), a two-dimensional form of carbon, attracted a great theoretical and experimental interest due to Dirac-type spectrum of charge carriers in this gapless semiconductor. It is well known, that the role of the light velocity here plays the parameter , which is smaller by two order than light velocity [1]. The discovery of graphene brought an exciting link between solid-state physics and quantum electrodynamics (QED).

Due to zero band gap, graphene monolayer cannot be applied in on–off devices. To apply graphene in such devices, it is necessary create a band gap between valence and conduction bands in graphene. One of ways to open a gap is placing the graphene monolayer on a polar substrate. By interacting with the substrate, two sublattices of graphene become inequivalent and a finite gap U between the conduction and the valence band may be opened.

The band gap in graphene monolayer is about 106 meV and 260 meV for h-BN [2] and SiC substrate , respectively. Even, the Cu (100) substrate exposed to the air can induce a larger band gap of 350 meV in graphene layer.

On the other side, a bilayer graphene (BLG) is a semiconductor that exhibits more intriguing properties: the charge carriers here are chiral quasiparticles with a dominantly parabolic dispersion. In pristine BLG the conduction and valence bands touch at the corners of the Brillouin zone. However, by applying a perpendicular electric field a band-gap U can be opened, and continuously tuned from a few meV to nearly 300 meV .

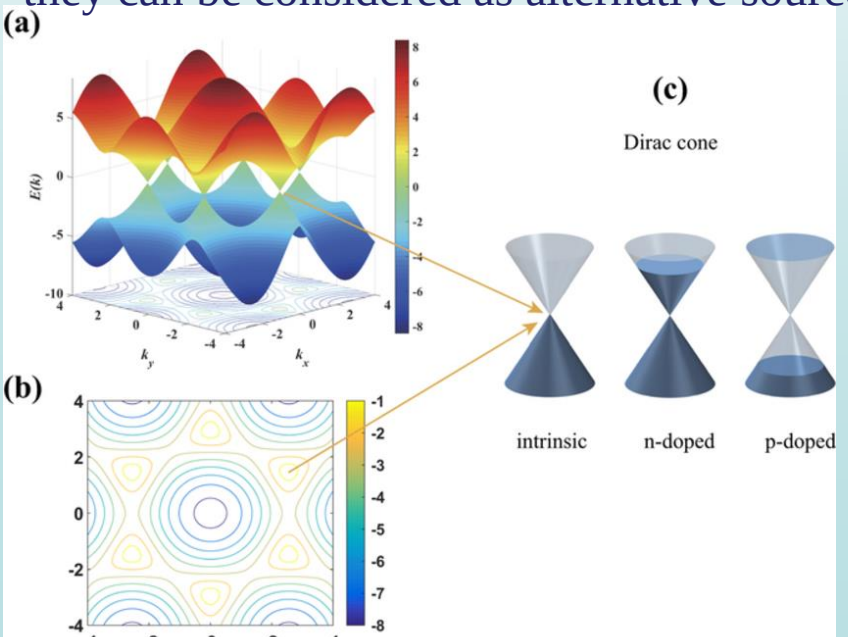


1.K.S.Novoselov et al., Science 306,666 (2004).
2.C.R. Dean, A.F. Young, I. Meric, C. Lee, L. Wang, S. Sorgenfrei, K. Watanabe, T. Taniguchi, P. Kim, K.L. Shepard, J. Hone, Nat. Nanotechnol. 5 (2010) 722.

The problem of the finding of new and effective sources of terahertz radiation is very important since such devices can be largely used in different fields of science and technology, e.g in biology, medicine, astronomy, environmental monitoring and security systems [3].

One of the most promising mechanisms for generation of terahertz radiation in the far-infrared region is based on optical transitions between the energy levels of shallow impurity centers in semiconductors and semiconductor nanotructures . It is interesting to investigate similar phenomena in in graphene systems, where bound states exist for arbitrary weak impurity potential and their binding energies and localization lengths can be changed in a desirable way by a gate voltage [4].

From this point of view it is very interesting to investigate the optical response and the problem of a Coulomb impurity in doped SLG and BLG systems since they can be considered as alternative source of terahertz radiation.



3.A.V.Andrianov, A.O.Zakhar'in,Yu.L. Ivanov, and M.S. Kipa, JETP Letters 91, 96 (2010)

4. A.A. Avetisyan, A. Djotyan, and K. Moulopoulos, Physics of Atomic Nuclei, 80, No. 2, 307 (2017)

ABSTRACT

In this work we focus on the problem of energy levels of isolated Coulomb impurity in gapped graphene systems. It is interesting to investigate the impurity states in doped graphene systems- SLG and BLG with opened energy gap, where the binding energy of impurity and its localization length depends on the doping concentration of charge carriers, tight binding parameters, and can be controlled by external electric and magnetic fields.

For fundamental physics as well as for different applications it is interesting to develop transparent analytical methods for a better understanding the physics of a single impurity in graphene systems and the influence of band structure parameters on the impurity electron binding energy, oscillator strengths etc.

We develop a clear variational approach in the momentum space for calculation of the ground state energy of an impurity electron in doped monolayer and bilayer graphene with opened energy gap.

Variational approach in the momentum space for monolayer graphene

The Hamiltonian for monolayer graphene in the presence of asymmetry between two sub-lattices that gives rise to a gap U, has the form:

$$H_0 = \begin{pmatrix} -U/2 & v_F(p_x - ip_y) \\ v_F(p_x + ip_y) & U/2 \end{pmatrix}$$

$v_F = \sqrt{3}\gamma_0 a / 2\hbar \approx 10^6 cm/\mathrm{s}$ $\quad \gamma_0 = 3.1\ eV$; a is the lattice constant.

The equation for determination of hydrogenlike impurity energy in SLG:

$$H_0 \begin{pmatrix} \phi \\ \chi \end{pmatrix} = \left(E + \frac{Ze^2}{r} \right) \begin{pmatrix} \phi \\ \chi \end{pmatrix}$$

The equation for the spinor component ϕ (using the system of two equations)

$$\left[\frac{U^2}{4} + (v_F \hat{p})^2 \right] \phi = \left(E + \frac{Ze^2}{r} \right)^2 \phi$$

The charged impurity does not need to be embedded in the graphene plane, and can be simply adsorbed to its surface.

Dopants: K, Na, NH_3 , Z=1

We take into account the term $Z^2 e^4 / r^2$ that becomes crucial for large values of fine structure constant, when impurity level is not shallow, and approaches to the middle of the gap.

The potential energy (the operator of multiplication in the coordinate space)

becomes the integral operator in the momentum space with the kernel ***V(q)*** defined as:

$$V(\mathbf{q}) = \frac{1}{(2\pi)^2}\int d\varphi \int V(\rho)\exp(-iq\rho\cos\varphi)\rho d\rho$$

The Fourier transform of two-dimensional Coulomb potential

$$V\left(\left|\mathbf{k}-\mathbf{k}'\right|\right) = -\frac{2\pi e^2}{\chi q} = -4\pi a_B R^* / \sqrt{k^2 + k'^2 - 2kk'\cos\vartheta}$$

$$R^* = \mu e^4 / 2\chi^2\hbar^2 \quad a_B = \hbar^2\chi / \mu e^2$$

Effective fine structure constant $\alpha = e^2\chi^2 / \hbar^2 v_F^2$ $\alpha = 2.2/\chi$

In SLG the ground state of two-dimensional hydrogen like impurity exists only for $\alpha < 0.5$
The value of dielectric constant plays the crucial role for the formation of bound impurity states.

The large range of values for dielectric constant χ , namely from 2 to 15 is found for graphene by different experiments.

The Fourier transform (2D) of the potential $1/\rho^2$

$$V_1(\mathbf{q}) = \frac{1}{(2\pi)^2}\int d\varphi \int V_1(\rho)\exp(-iq\rho\cos\varphi)\rho d\rho = \frac{1}{8\pi}\left[H_0(qb) - N_0(qb)\right]$$

b is the cutoff parameter, b ~ 0.1 a_B

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In dimensionless units $\tilde{E} = E / R^*$ $\tilde{U} = U / R^*$ $R^* = \mu e^4 / 2\chi^2 \hbar^2$

the equation for energy of an impurity electron can be presented in the form:

$$\tilde{E}^2 - \tilde{U}^2 + \frac{2\tilde{E}}{\pi} \int \phi(k)\ k dk \int \int \frac{k' dk' \phi(k') d\varphi}{\sqrt{k^2 + k'^2 - 2kk' \cos\vartheta}} + \int d\varphi \int \phi(k')\ V_1(|\mathbf{k} - \mathbf{k}'|) k' dk'$$
$$- \frac{4}{\alpha^2} \int d\varphi \int k^3\, \phi^2(k) dk = 0\,.$$

The masse is defined by the relation: $m v_F^2 = U / 2$

We choose a trial wave function in the form:

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$$\phi(k) = N / (k^2 + \lambda^2)^2$$

Screening in graphene systems

One of the most important fundamental quantities for understanding physical properties of graphene is the dynamical polarization function Π(ω, k) which describes the screening of the Coulomb potential due to many body effects and determines the collective excitations [5,6]. It is interesting to investigate the impurity states in doped graphene systems- *SLG* and *BLG* with opened energy gap, where the binding energy of impurity and its localization length depend on the doping concentration of charge carriers, tight binding parameters, and can be controlled by external electric and magnetic fields.

The screened charged impurity potential: $V(q) = \frac{2\pi e^2}{\chi q \varepsilon(q)}$ $\varepsilon(q) = 1 + \frac{q_s}{q}$

$\varepsilon(q) = 1 + \frac{2\pi e^2}{\chi q}\Pi(q)$ $V(q) = \frac{2\pi e^2}{\chi(q + 4\alpha k_F)}$ $q_s = 4\alpha k_F$ $k_F = \sqrt{\pi n}$

In order to take into account the screening effects we should in the Coulomb term (in the equation for the energy) make the transform:

$$q \to q + q_s$$

5. E. H. Hwang and S. Das Sarma, Phys. Rev. Lett. 101, 2008
6. P K Pyatkovskiy, Journal of Physics: Condensed Matter, 2008

Variational approach in the momentum space for gated bilayer graphene

In the two band approximation:

$$H_0 = \begin{pmatrix} -U/2 & v_3(p_x + ip_y) - (1/2m)(p_x - ip_y)^2 \\ v_3(p_x - ip_y) - (1/2m)(p_x + ip_y)^2 & U/2 \end{pmatrix}$$

U is the gap induced by a static perpendicular electric field

$$v_3 = \sqrt{3}\gamma_3 a / 2\hbar \approx 0.1 v_F \qquad m = \gamma_1 / 2v_F^2$$

tight-binding parameter γ_3 describes the interaction between different *B* atoms in neighboring layers.

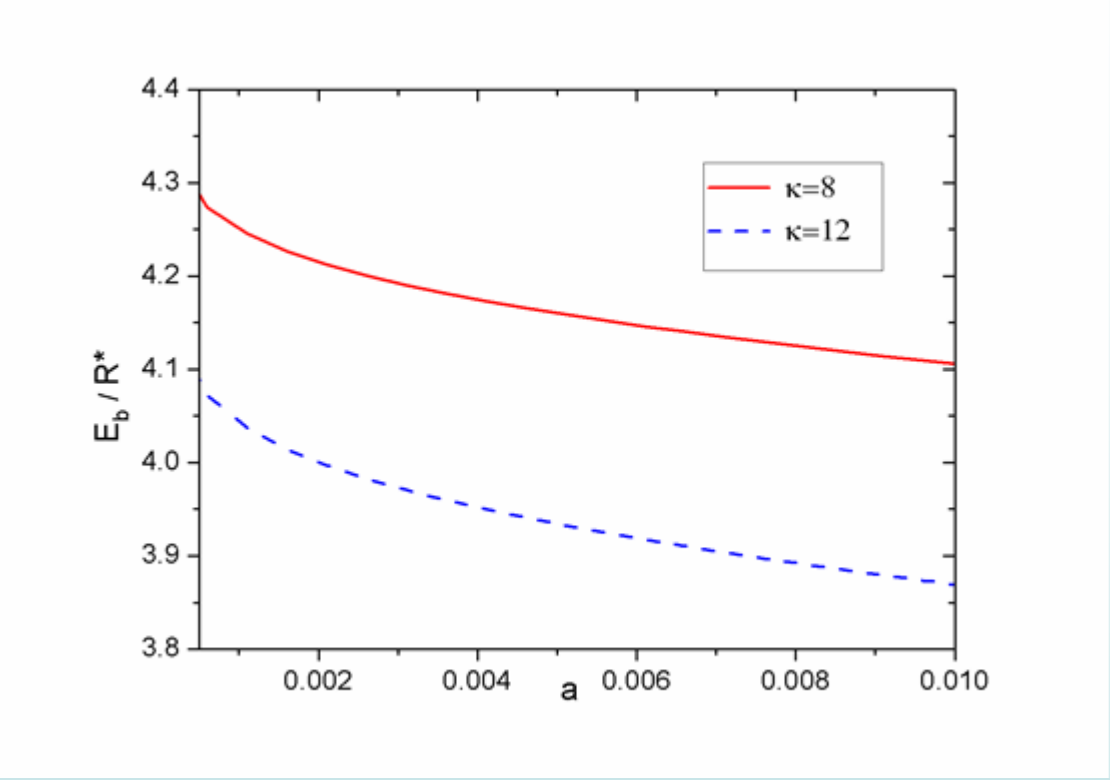
γ_1 describes the interaction between A atoms in different layers, that are on the top of each other.

The equation for the spinor component ϕ for the bilayer

$$\left[\frac{U^2}{4} + (v_3 p)^2 - \frac{v_3 p^3}{m}\cos 3\theta + \left(\frac{p^2}{2m}\right)^2\right]\phi = \left(E + \frac{Ze^2}{r}\right)^2 \phi$$

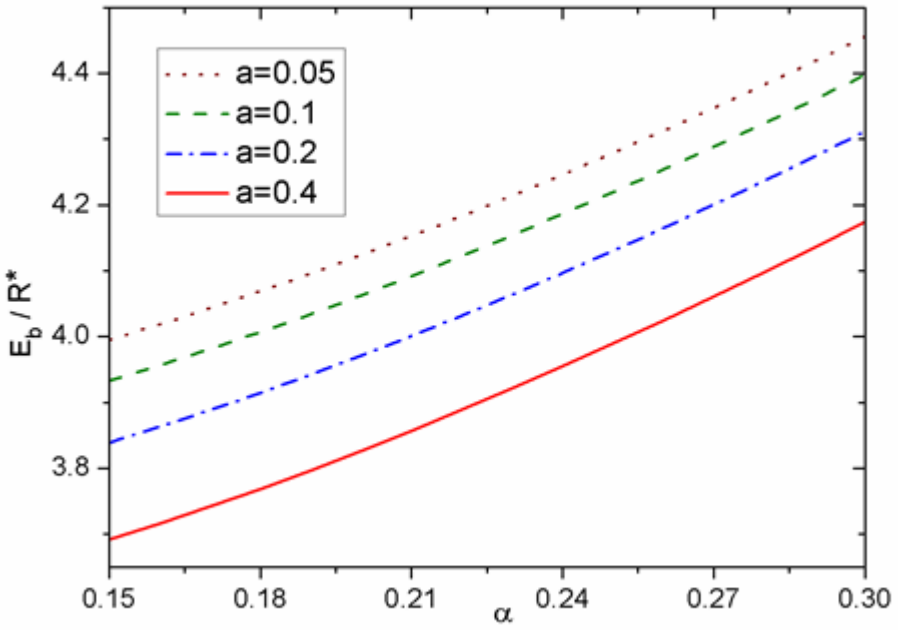
$$\left((\tilde{E}^2 - \frac{\tilde{U}^2}{2})\phi + \frac{2\tilde{E}}{\pi}\int\int \frac{k' dk' \phi(k') d\varphi}{\sqrt{k^2 + k'^2 - 2kk'\cos\vartheta}}\right)\phi(k) = k^2\left(\frac{4}{\alpha^2} + \left(\frac{\mu}{m}\right)^2 k^2\right)\phi(k),$$

Numerical results for monolayer graphene



The binding energy of hydrogen- like impurity in doped SLG in effective Rydberg as function of parameter $a = q_s a_B$ *for different values of dielectric constant.*

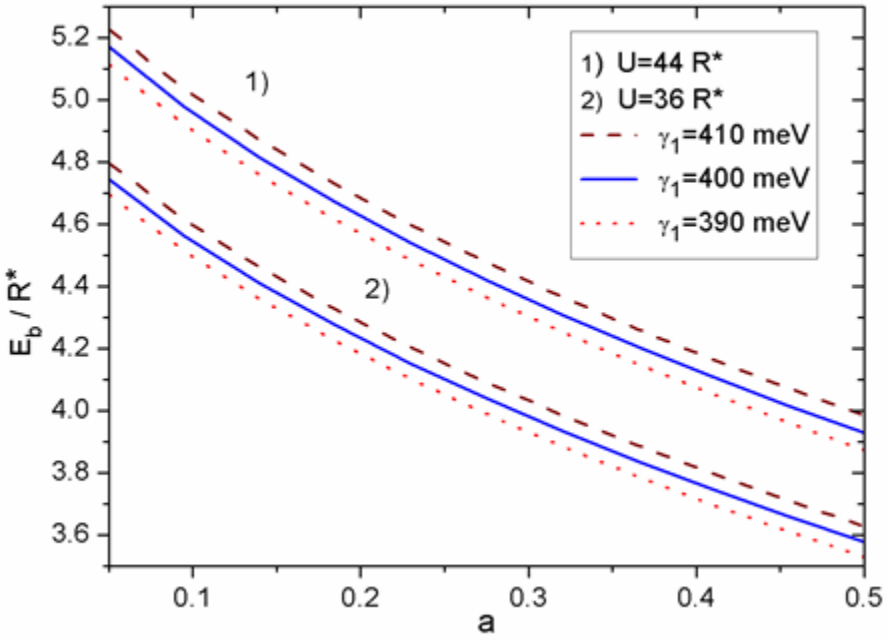
Numerical results



The binding energy of hydrogen- like impurity in doped SLG in effective Rydberg as function of effective fine structure constant for different values of parameter $a = q_s a_B$:

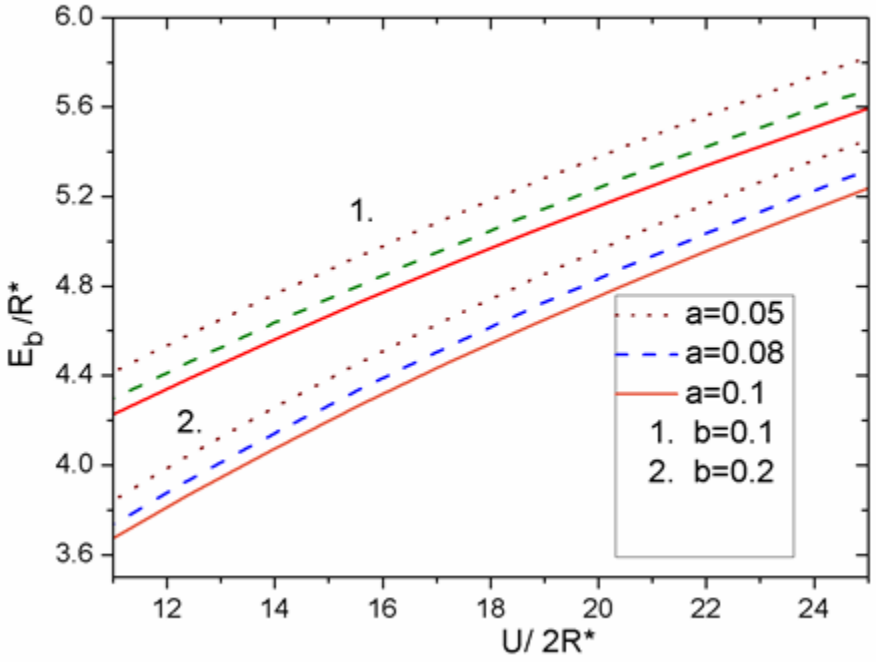
$$q_s = 4\alpha k_F \qquad k_F = \sqrt{\pi n}$$

Numerical results for bilayer graphene



Dependence of the binding energy of an impurity electron in BLG (in effective Rydberg) on the parameter a for two values of the gap:1) U=44R 2) U=36R and for different values of parameter gamma1.

$$R^* = 6.5\ meV$$



Dependence of the binding energy of an impurity electron in BLG (in effective Rydberg) on the gap U for different values of the parameter a : solid line corresponds to a=0.1, dashed line is for a=0.08, and dotted line is for a=0.05.

$R^* = 6.5\ meV$

Conclusion

- In this work we investigate the binding energy of hydrogen like impurity states in doped SLG and BLG with opened energy gap.
- We suggest an analytical method based on the variational approach in the momentum space for the Coulomb problem in graphene systems.
- The suggested method is more appropriate for systems with complicated dispersion law of charge carriers, e.g. for a graphene bilayer.
- The binding energy of an impurity electron in doped SLG and BLG is studied by this method and it is shown that the energy is tunable by the gate voltage, dopants concentration and is in the region of few ten meV.
- The possibility of impurity energy tuning by external fields and by changing band structure parameters can be promising for applications in nano- and optoelectronics for construction of new devices.

Thank you for your attention