Spectral properties and the Kondo effect of cobalt adatoms on silicene

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In terms of the state-of-the-art first principle computational methods combined with the numerical renormalization group technique the spectroscopic properties of Co adatoms deposited on silicene are analyzed. By establishing an effective low-energy Hamiltonian based on first principle calculations, we study the behavior of the local density of states of Co adatom on external parameters, such as magnetic field and gating. It is shown that the Kondo resonance with the Kondo temperature of the order of a few Kelvins can emerge by fine-tuning the chemical potential. The evolution and splitting of the Kondo peak with external magnetic field is also analyzed. Furthermore, it is shown that the spin polarization of adatom’s spectral function in the presence of magnetic field can be relatively large, and it is possible to tune the polarization and its sign by electrical means.

I. INTRODUCTION

The discovery of graphene, a two-dimensional (2D) honeycomb lattice of carbon atoms, in 2004 [1] spurred an interest in other 2D materials, especially those sharing graphene’s crystal structure. The search was motivated by the hope that such materials would also share the defining feature of graphene, i.e. the presence of Dirac cones in their electronic structures [2]. The suppression of backscattering characteristic of Dirac fermions should then lead to similarly high carrier mobilities [3–6] and possible use of graphene siblings in ultra-fast electronic devices [7–11]. The continuously growing list of elements and compounds for which the existence of such graphene analogues was predicted theoretically and in some cases confirmed experimentally includes: Si (so called silicene) [12–18], Ge (germanene) [12, 13], Sn (stanene) [19, 20], Al (aluminene) [21, 22] and hexagonal BN (white graphene) [23].

Of these, silicene is particularly interesting thanks to its compatibility with the current Si-based electronic technology. The first proof of the concept field effect transistor made out of silicene has already been demonstrated [24]. Many of the characteristic properties of graphene are predicted to be present also in its silicon counterpart. The band structure of the free-standing silicene exhibits the expected Dirac cones [12], which can be preserved also on suitably selected substrates [25]. The zigzag edges of silicene nanoribbons are predicted to be spin-polarized [12, 26, 27] just like in the case of graphene [2]. However, some notable differences also exist between the two materials. While graphene is planar, in silicene the two sublattices are shifted vertically (buckling) because of larger in-plane lattice constant (weaker π bonds) and the element’s preference for forming sp³ hybrids (no graphite analogue exists for Si). Consequently the π and σ bands are hybridized. The spin-orbit (SO) interaction in silicene is three orders of magnitude stronger than in graphene and is responsible for a small 1.5 meV gap in the electronic structure [28, 29]. This may lead to the realization of the spin Hall effect in experimentally accessible temperatures. The symmetry breaking effect due to buckling opens an interesting possibility of fine tuning the gap using vertical electric field [30, 31].

Another way of affecting the properties of 2D materials is by deposition of magnetic adatoms on the surface. In fact, the presence of impurities has been invoked to explain the spin relaxation time in graphene [32]. Besides modification of material properties, individual magnetic adatoms themselves can pose very interesting objects to study. This is because strong coupling between localized states of adatoms and the band of 2D material can result in various nontrivial effects. One of such effects, which has been widely studied in the context of quantum dots and molecules, is undoubtedly the Kondo effect [33]. In this effect the magnetic moment of confined electrons, either in an adatom or a quantum dot, becomes screened by surrounding mobile electrons. This results in the formation of a resonance in the local density of states at the Fermi level [34]. The Kondo effect due to the presence of magnetic adatoms has already been considered in the case of graphene [35, 36]. Moreover, the spectroscopic properties of Co adatoms on graphene have also been examined [37], and recently the presence of the Kondo effect has been reported [38]. Thus, while there are several considerations of spectroscopic properties of magnetic adatoms on graphene, not much is known about the spectral features and, in particular, the Kondo effect for other 2D materials, such as silicene. The aim of this paper is therefore to shed light on the physics of Co adatoms on silicene, with an emphasis on the Kondo regime.

The paper is organized as follows. In Sec. II we discuss the first principles methods used to determine the lowest energy geometry and the density of states (DOS) of silicene with Co adatom. Section III is devoted to numerical renormalization group calculations. First, we formulate the effective Hamiltonian, describe the method and then discuss the numerical results. The paper is summarized...
in Sec. IV.

II. FIRST PRINCIPLES CALCULATIONS

The first principles calculations were performed using the generalized gradient approximation (GGA) of density functional theory (DFT). The specific method applied was full potential linearized augmented plane wave (FLAPW) [39] as implemented in the WIEN2K package [40]. The Perdew-Burke-Ernzerhof parametrization [41] of the exchange potential was used in all the cases. The 2D Brillioun zone (2D BZ) integration was performed using suitably dense mesh corresponding to several hundreds k-points (or more) in the single unit 2D BZ. The convergence criteria for energy, charge per atom and forces were set to $10^{-4}$ Ry, $10^{-3}$ e and 2 mRy/a.u., respectively. In all the calculations the silicene planes were separated by 14 Å ensuring the lack of hopping between the neighboring planes.

In the first step the lattice constant and the sublattices’ displacement of bulk silicene were optimized. For the lowest energy configuration we have found the in-plane lattice constant and the vertical displacement to be equal to $a = 3.86$ Å and $\Delta = 0.46$ Å [42], respectively, in good agreement with the previous calculations [12, 28]. When the spin-orbit interactions were included in the calculations the small band gap of $\Delta E \approx 1.5$ meV separating the tips of the Dirac cones appeared in the band structure, also in good agreement with the literature [28].

Next we compared three possible high symmetry locations of the Co adatom over the silicene. These are indicated in Fig. 1 and include the locations over two non-equivalent lattice sites (“1” and “3”) and also the position over the center of the hexagon (“2”). The calculations were performed using 3x3 supercells with the full relaxation of the atomic positions within the supercell. It has been found, in agreement with earlier works [43, 44], that the order of the total energies is as follows

$$E_2 < E_1 < E_3$$

that is the central position “2” is the most favorable energetically, followed by the position over the “lower” sublattice A. The ground state is separated from the other two configurations by $\Delta E_{Tot} \approx 0.17$ Ry. These conclusions were additionally confirmed by 4x4 calculations for “1” and “2” cases with the same overall results.

In order to make sure that the size of the supercell used is sufficiently large so that the limit of the single impurity is reached we next studied the convergence of the magnetic moment and the local density of states (LDOS) of the Co adatom against the size of the supercell. Because of the huge computational costs involved, the structural relaxation was not performed during these calculations. Instead we adopted the geometry obtained in 4x4 calculations for Co and its surroundings (up to $R = 8$ Å radius, corresponding to 4 coordination zones) embedding so defined “cluster” into the bulk silicene. As the deviations of Si atoms from bulk positions were found to be negligible at this distance from Co, the procedure is reasonable. We have found that both quantities stopped changing meaningfully when 7x7 (corresponding to the supercell lattice constant $a_{sc} = 27$ Å) or larger supercells were used. The total magnetic moment, located predominantly on Co, equals 1 $\mu_B$. We conclude therefore that the impurity can be effectively treated as a spin one-half in the Anderson model.

In the final step we have calculated global and local DOS using 7x7 supercell and including the spin-orbit coupling. The 2D BZ integration was performed at this point using suitably dense mesh corresponding to $10^4$ k-points in the original 1x1 2D BZ. The results for the total DOS of the structure, together with the DOS of pure silicene,
are presented in Fig. 2. In the vicinity of the adatom the hybridization effect comes into play, and it drastically rebuilds the LDOS. In consequence, the DOS of the system with an adatom follows the same general outline as the DOS of pure silicene but with additional modulations visible in Fig. 2. The most notable of these is perhaps the sharp peak located exactly at the Fermi energy in the minority spin channel. Analysis of the orbital contribution to the local density of states of cobalt shown in Fig. 3 indicates that the peak at the Fermi energy in the total DOS of the structure originates mainly from the $d_{3z^2-r^2}$ orbitals of the adatom.

III. NUMERICAL RENORMALIZATION GROUP CALCULATIONS

A. Effective model

Based on the first-principle results we can now establish an effective Hamiltonian for the Co adatom on silicene. The calculated magnetic moment of the adatom justifies usage of a spin one-half single impurity Anderson model [45]. In order to find the parameters of the effective single-orbital model we follow the procedure described in Ref. [46]. From the calculated occupancy of Co orbitals, $n_d \approx 7.8$ (in agreement with Ref. [44]), we conclude that charge fluctuations can occur between the states with 7, 8 and 9 electrons. Starting with the Anderson model with full five-fold degeneracy of the d-shell electrons, we note that in the mean field approximation the energies of the respective charge states enumerated by $j$ can be expressed as, $E(j) = j\epsilon + Uj(j-1)/2$, where $\epsilon$ is an adatom on-site energy and $U$ denotes the Coulomb correlations. Following Ref. [44], the latter parameter will be set equal to $U = 4$ eV. From the minimum energy condition with respect to $j$ we can estimate the on-site energy $\epsilon = (1/2-n_d)U$. Focusing on consecutive energies of the states with 7, 8 and 9 electrons (with respect to the lowest energy), we can find from $\tilde{\epsilon}_d = E(8) - E(7)$ and $2\tilde{\epsilon}_d + \tilde{U} = E(9) - E(7)$, the parameters for the effective impurity Hamiltonian, $\tilde{\epsilon}_d = -1.2$ eV, $\tilde{U} = U$, which has the following form

\[ H = H_{\text{band}} + H_{\text{imp}} + H_{\text{tun}}. \]  

Here, $H_{\text{band}} = \sum_{\sigma} \int d\varepsilon c_{\varepsilon}^\dagger(\varepsilon)c_{\varepsilon}(\varepsilon)$ describes the electrons in silicene with the corresponding density of states, see Fig. 2. The second term models adatom and is given by $H_{\text{imp}} = \sum_{\varepsilon} \tilde{\epsilon}_d d_{\varepsilon}^\dagger d_{\varepsilon} + \tilde{U} d_{\varepsilon}^\dagger d_{\varepsilon}^\dagger + g\mu_B S_z B$, where $\tilde{\epsilon}_d$ is the energy of an electron occupying the impurity and $\tilde{U}$ denotes the Coulomb correlation energy. The last term accounts for the Zeeman splitting, with $B$ being the external magnetic field and $S_z$ denoting the spin of the adatom. The operator $d_{\varepsilon}^\dagger$ creates a spin-$\sigma$ electron on the adatom, and $c_{\varepsilon}^\dagger(\varepsilon)$ is the corresponding creation operator for spin-$\sigma$ electrons in silicene. Finally, the coupling between the substrate and adatom is modeled by the tunneling Hamiltonian $H_{\text{tun}} = \sum_{\varepsilon} \int d\varepsilon V(\varepsilon)\rho(\varepsilon)[c_{\varepsilon}^\dagger(\varepsilon)d_{\varepsilon} + d_{\varepsilon}^\dagger c_{\varepsilon}(\varepsilon)]$, where $V(\varepsilon)$ denotes the tunnel matrix elements assumed to be equal to $V = 0.65$ eV and $\rho(\varepsilon)$ is the density of states of bulk silicene, cf. Fig. 2. The parameter $V$ has been evaluated by Harrison’s scaling method [47] for the average Si-Co bond length $r = 2.45$ Å.

Since we are interested in nonperturbative effects resulting from the hybridization of Co adatom and silicene, to get the most accurate information about system’s spectral properties we employ the numerical renormalization group (NRG) method [48–50]. In NRG, the band is first discretized in a logarithmic way with a discretization parameter $\Delta$. Then, such discretized Hamiltonian is tridiagonalized numerically and transformed to a tight-binding Hamiltonian of the following form

\[ H_{\text{NRG}} = H_{\text{imp}} + \sum_{\sigma} V(d_{\varepsilon}^\dagger f_{\varepsilon\sigma} + f_{\varepsilon\sigma}^\dagger d_{\varepsilon}) \]

\[ + \sum_{n=0}^{\infty} \sum_{\sigma} \left[ \epsilon_n f_{n\sigma}^\dagger f_{\varepsilon\sigma} + t_n (f_{n+1\sigma}^\dagger f_{\varepsilon\sigma} + f_{n\sigma}^\dagger f_{n+1\sigma}) \right], \]  

where $f_{n\sigma}^\dagger$ is the creation operator of an electron with spin $\sigma$ on the $n$th site of the chain, $t_n$ denotes the hopping integral and $\epsilon_n$ is the on-site energy. In NRG calculations we assumed $\Delta = 1.7$ and kept at least 1500 states at each iteration. To obtain the most accurate results for the spectral functions, we also optimized the broadening parameter appropriately [51].

B. Discussion of numerical results

We now focus on the behavior of the spectral function of Co adatom, $A_\sigma(\omega) = -\text{Im}G_R^\sigma(\omega)/\pi$, where $G_R^\sigma(\omega)$ is the Fourier-transform of the corresponding retarded Green’s function, $G_R^\sigma(t) = -i\theta(t)\langle \{ d_{\varepsilon\sigma}(t), d_{\varepsilon\sigma}^\dagger(0) \} \rangle$. The total spectral function, $A(\omega) = A_\uparrow(\omega) + A_\downarrow(\omega)$, corresponds to the local density of states of adatom, which

![Figure 3. The local density of states of Co adatom. Both total and partial, orbital resolved contributions are indicated.](image)

![Diagram](image)
$U = 4$ are indicated in the legend of panel (b). The parameters are: at half maximum of the resonance in the spectral function, associated Kondo temperatures, obtained from the halfwidth low-energy behavior where the Kondo effect can emerge. The arithmic scale. The inset in (a) presents the zoom onto the total spectral function exhibits Hubbard resonances for on the case of no gating, $\tilde{\epsilon}_d$.

One can consider if it is possible to reinstate the Kondo resonance by changing the chemical potential via gating. First of all, it can be seen that, quite naturally, by tuning $\mu$ the position of the Hubbard resonances changes accordingly, see Fig. 4. Moreover, by adjusting the Fermi energy, one can also considerably affect the low-energy behavior of the system. In fact, for values of $\mu$ selected in Fig. 4, a pronounced Kondo resonance develops. This can be clearly seen in Fig. 4(b), which shows the spectral function plotted on logarithmic scale, as well as in the inset of Fig. 4(a), which presents a zoom into the low energy behavior of $A(\omega)$. For the considered values of gating, there is sufficient number of states at the Fermi energy to screen the adatom’s spin. One can then observe the Kondo effect with relatively large Kondo temperature, of the order of up to a few Kelvins, as estimated from the halfwidth at half maximum of the Kondo peak, see Fig. 4(b).

To gain a deeper understanding of the effect of gating on the local density of states, we also analyze the behavior of the spectral function by continuously tuning the chemical potential. This is presented in Fig. 5, which shows the energy and chemical potential dependence of the local density of states, with the bottom panel zooming into the low-energy behavior of $A(\omega)$. First, we note that for $\mu \approx -1.2$ eV and $\mu \approx 2.8$ eV, the spectral func-
tential dependence of the occupation a spin one-half, see Fig. 6(a) presenting the chemical po-

ture, since then the empty and doubly occupied states of the 

earlily relevant, values of temperature. By looking at the 

Kondo peak is nicely visible in the inset of Fig. 7(c). We 

Kondo correlations in the presence of magnetic field is in 

strongly affects the behavior of the spectral function. An 

an important observation is a strong spin polarization of 

Hubbard resonances: \( A_{\uparrow} (A_{\downarrow}) \) becomes suppressed for 

\( \omega > 0 \) (\( \omega < 0 \)). Moreover, magnetic field also has a 

strong effect on the low-energy behavior of \( A(\omega) \): the 

Kondo resonance becomes split if the Zeeman energy \( E_Z \) 

becomes larger than \( k_B T_K \), \( E_Z = g_\mu_B B \gtrsim k_B T_K \). The 

spin polarization of the spectral function can be clearly 

seen in Figs. 7(a) and (b), while the splitting of the 

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note that the largest suppression of the Kondo peak oc-

\( k_B T_K \approx 0.32 \) K, which is smaller than for the case of \( \mu = 2 \) 

eV and \( \mu = -0.78 \) eV. Consequently, larger suppression of 

the Kondo resonance is observed for smaller \( T_K \), since 

the condition \( E_Z \gtrsim k_B T_K \) is then better satisfied. We 

also notice that the effect of splitting and suppression of 

the Kondo peak in the presence of magnetic field is in 

fact similar to the effect of an exchange-field splitting of 

orbital level caused by the presence of ferromagnetic cor-

relations [52–56]. Thus, if due to proximity effect with 

magnetic substrate, the density of states of silicene be-

comes spin-polarized, the Kondo effect may be also split 

and suppressed even in the absence of magnetic field.

It is also interesting to analyze the energy and chemical

4. Effect of external magnetic field

Let us now consider how external magnetic field af-

fects the behavior of the local density of states of Co 

adatom. The energy dependence of the spin-resolved 

and total spectral function calculated in the presence of 

external magnetic field \( B = 2 \) T is depicted in Fig. 7, 

where the insets show the zoom into the low-energy be-

havior of \( A(\omega) \). First of all, one can see that magnetic 

field strongly affects the behavior of the spectral function. 

An important observation is a strong spin polarization of 

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It is also interesting to analyze the energy and chemical
Figure 7. The zero-temperature (a) spin-up, (b) spin-down and (c) total spectral function for different values of chemical potential, as indicated in the figure, calculated in the presence of external magnetic field $B = 2$ T. The insets present the zoom into the low-energy behavior of the spectral function. Parameters are the same as in Fig. 4 and we assumed the $g$-factor, $g = 2$.

The effect of external magnetic field can be better revealed when one considers the spin polarization of the spectral function, which is defined as, $P = \frac{A(\omega)}{A(\omega)}$. The dependence of the spin polarization on energy $\omega$ and chemical potential $\mu$ for a few values of magnetic field is shown in Fig. 9. This figure is generated for the same values of $B$ as those considered in Fig. 8, again focusing on the low-energy behavior. When the impurity is either empty or doubly occupied, the spin polarization is suppressed and approaches zero. Its behavior, however, becomes completely changed in the local moment regime, see Fig. 9. One can notice that for higher energies the spectral function becomes fully spin-polarized, $P \approx 1$ for $\omega < 0$ and $P \approx -1$ for $\omega > 0$. Interestingly, it can be also seen that the interplay of finite Zeeman splitting and the density of states for several values of external magnetic field. This is presented in Fig. 8, which shows $A(\omega)$ for $B = 1, 2, 5$ T. In this figure we focus on the low-energy regime, where Kondo effect can emerge, and the interplay between the Zeeman splitting and Kondo correlations is most revealed. One can see that, depending on the value of external magnetic field and gating, the Kondo resonance can become split and suppressed. This is especially visible for $\mu = 1.5$ eV, where with increasing $B$, one shifts the position of the split Kondo peaks. Moreover, there are such values of $\mu$, especially those close to the mixed valence regime, where the magnetic field is not strong enough to suppress the Kondo resonance, see Fig. 8.
Figure 9. The energy and chemical potential dependence of the spin polarization of the spectral function, $P = \frac{A^\uparrow(\omega) - A^\downarrow(\omega)}{A(\omega)}$, calculated for different values of external magnetic field: (a) $B = 1$ T, (b) $B = 2$ T and (c) $B = 5$ T. The other parameters are the same as in Fig. 4.

Figure 10. The spectral function plotted as a function of energy and magnetic field for selected values of chemical potential for which pronounced Kondo peak develops in the absence of magnetic field: (a) $\mu = 2$ eV, (b) $\mu = 0.65$ eV and (c) $\mu = -0.78$ eV. The dotted lines mark the Zeeman energy $E_Z = \pm g\mu_B B$. The other parameters are the same as in Fig. 4.

states of silicene, can result in a sign change of the spin polarization at $\omega = 0$ around $\mu = 0.5$ eV, which is most visible for $B = 5$ T, see Fig. 9(c). At low energies and for $\mu \lesssim 0.5$ eV ($\mu \gtrsim 0.5$ eV), $P$ becomes positive (negative).

Finally, in Fig. 10 we study the evolution of the splitting of the Kondo peak with external magnetic field. This figure is calculated for selected values of the chemical potential, the same as considered in Fig. 7. It can be seen that the Kondo peak becomes suppressed when magnetic field is so strong that the condition $E_Z \gtrsim k_B T_K$ is fulfilled. Thus, the suppression occurs first for the case of $\mu = 0.65$ eV, while larger field is needed to destroy the Kondo resonance for the other two cases, see Fig. 10. When magnetic field is large enough such that $E_Z \gtrsim k_B T_K$, $A(0)$ becomes suppressed and the spectral function shows only side peaks, which occur exactly at the spin-flip excitation energy $\omega = \pm E_Z$. The position of those side peaks depends thus linearly on magnetic field, which can be nicely seen in Fig. 10, where the dotted lines mark the Zeeman energy $E_Z$.

### IV. CONCLUSIONS

We have theoretically considered the spectroscopic properties and the Kondo effect of Co adatoms on silicene. By using the first principle calculations, we have determined the total density of states of Co-silicene system and estimated the orbital level occupancy together with the magnetic moment of Co. Our DFT results allowed us to formulate an effective low-energy Hamiltonian for spin one-half impurity, which was further used to analyze the spectral properties of Co adatoms. This analysis was performed by employing the numerical renormalization group method with a non-constant density of
states. We focused on the behavior of the local density of states (spectral function), which can be probed experimentally by using the scanning tunneling spectroscopy. The analysis involved the effects of external magnetic field and gating of silicene. We showed that by appropriately tuning the parameters one can obtain clear signatures of the Kondo effect. We also analyzed the evolution and splitting of the Kondo resonance with an external magnetic field. Finally, we studied the spin polarization of the spectral function in the presence of magnetic field, whose magnitude and sign were found to greatly depend on the position of chemical potential.

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