Ferromagnetism in a (001), (110), and (111)-Oriented Ru Monolayer on Ag, Au, and Cu-Substrates

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Abstract

We have studied the magnetic behavior of a 4d transition metal Ru monolayer (ML) on different substrates and orientations. In the ground state, a Ru-ML is expected to be ferromagnetic on Ag(001) and Au(001) with a magnetic moment ($\mu$) of 1.73 Bohr magnetons ($\mu_B$) in both cases. On Cu(001), a Ru-ML is not magnetic. In this paper, we study the magnetic behavior of a Ru-ML at other orientations, i.e., (110) and (111). We found magnetism on Au (111), and Ag (111) ($\mu \sim 1.3 \mu_B$ for both) but no magnetic activity on a Cu substrate in any orientation. Further, we found that on Ag(110), a Ru-ML is ferromagnetic with $\mu = 1.3 \mu_B$. On Au(110), a Ru-ML is not magnetic. Since on the (001) and (111) orientations a Ru-ML has about the same magnetic activity on Ag as on Au, we found surprising the behavior in the (110) orientation. We analyze it in detail in the final part of the paper. We found that there exists a metastable ferromagnetic state, in this case, and that a Ru-ML becomes ferromagnetic under a small expansion of the Au-lattice. This is not the case for Cu.

I. INTRODUCTION

In the 4d transition metal series, itinerant magnetism in three dimensions (3D) was studied by Gunnarsson [1] and Janak [2] using the qualitative Stoner criterion for ferromagnetism which is never satisfied for any metal in the 4d series [3]. Electronic structure calculations using state-of-the-art methods gave the interesting result that elements might be forced to conserve their atomic magnetism, if synthesized at the nanometer scale [4]. In 2D, the coordination number is reduced and, consequently, the d-band width changes and the local density of states (LDOS) at the Fermi level, $\varepsilon_F$, increases [5,6]. Furthermore, the exchange integral, $J$, might in general, not be lower in 2D as compared to 3D [7]. For these reasons, itinerant 2D ferromagnetism is not restricted to the elements that exhibit it in 3D [8–10]. In the past few years, several groups presented ab-initio calculations on the ferromagnetism of 4d transition metal monolayers (ML) on Ag(001) and Au(001) substrates. For the 4d transition metals, ML magnetism was predicted for Ru, Tc and Rh. For a Ru-ML a large magnetic moment of 1.7 Bohr magnetons was predicted [3,11]. No experimental evidence of Ru-ML magnetism was given until Pfandzelter, Steierl and Rau [4] reported the first observation of 2D ferromagnetism on a Ru-ML grown by epitaxy on a C(0001) substrate. Recently, García et al., [12] studied Cu(001) as a substrate and obtained that a Ru-ML on Cu(001) could become magnetic upon expansion of the Cu-lattice. They have studied two factors to decide on whether the ML has or has not magnetic activity. One is the lattice constant of the substrate which is adopted by the ML grown on top of it. The other is the ML-substrate interaction of the existing d-states. They have studied in detail the influence of expansion and contraction of the ML-substrate distance. They have shown that when it is contracted, and the interatomic distance of the Ru atoms on the monolayer, consequently, enhanced, magnetism appears on the monolayer.

In this work, we study further the Ru-monolayer. We report the results obtained for the magnetic moment on Ag, Au and Cu substrates in the (110) and (111) orientations.
The rest of the paper is organized as follows. Section II is devoted to a brief review of the main highlights of the theory. Section III is devoted to our results. In the first part of it we report the magnetic moment resulting for a Ru-ML from our calculations in the (110) and (111) orientations. We have included the results in the (001) orientation from references [3] and [12], for completeness. Since the results in the (110) orientation are somehow surprising, we include at the end of this section a detailed discussion of them and study the effect of pressure and expansion in this case. In the last section IV, we present our conclusions.

II. THEORY

We use the known surface Green function matching (SGFM) method [13] to calculate the LDOS for the ML. To calculate the magnetic moment, we use both the Hubbard [14] method and a Stoner Hamiltonian [15]. They both lead to the same result for ferromagnetism.

A. The Green’s function

The SGFM surface Green’s function, $G_s$, is given by

$$G_s^{-1}(\epsilon, \mathbf{k}) = \epsilon I - H_{00}(\mathbf{k}) - H_{10}(\mathbf{k})T$$  \hspace{1cm} (1)

where $H_{00}$ and $H_{01}$ are the in-layer (surface) and interlayer interaction Hamiltonians, respectively, in the customary description in terms of principal layers. The $T$ matrix is defined as $G_{10} = TG_{00}$. $G_{10}$ is the propagator from the principal layer 0 to the first one. $G_{00} \equiv G_s$ is the propagator within the surface principal layer. $I$ is the unit matrix and $\epsilon$ is the energy. $\mathbf{k}$ is the wave vector defined in the First Brillouin Zone (FBZ). A quickly converging algorithm for the $T$ matrix allows a very effective use of this and other SGFM formulae [16].

We use Eq. (1) to calculate the LDOS for the (001)-, (111)- and (110)- free surface. The SGFM surface Green’s function, Eq. (1), has been used to describe a substrate-ML system as well [17–20]. Here, we rather use the following formula for the Green’s function, $G_{ML}$, of the substrate-ML system [12].

$$G_{ML}^{-1}(\epsilon, \mathbf{k}) = G_{s(A)}^{-1}(\epsilon, \mathbf{k}) + (\epsilon I - H_{00(B)}(\mathbf{k})) - I_A H^z I_B - I_B H^z I_A$$  \hspace{1cm} (2)

In this supersupermatrix form, the expression is very transparent. The supersupermatrix, $G_{ML}$, is labeled with the indices describing the two media $A$ and $B$. The upper diagonal part describes a semi-infinite medium $A$ with a surface (see Eq. 1); the lower diagonal part describes a free-standing monolayer of $B$ atoms. Both interact through the supersupermatrix Hamiltonian $I_M H^z I_N, (M, N = A, B)$. These matrices $H_{00(A)}, H_{10(A)}, H_{00(B)}$ and $I_M H^z I_N$ are readily written in the two-center approximation within the Slater-Koster description [21].

The LDOS for the entire ML-substrate system is obtained from

$$N_{ML}(\epsilon) = -\frac{1}{\pi} \int \text{Im} [\text{Tr} G_{ML}^{-1}(\epsilon, \mathbf{k})] d\mathbf{k}$$  \hspace{1cm} (3)

We use the method by Cunningham to perform the numerical integration in the 2D FBZ [22].
B. The magnetic moment

The magnetic moment is calculated using first the Hubbard and then the Stoner model. They both gave us the same result for a ferromagnetic system. The magnetization, in units of Bohr magnetons, $\mu_B$, is given by

$$\mu(\Delta) = \int_{-\infty}^{\epsilon_F} \left[ n_d^+ (\varepsilon) - n_d^- (\varepsilon) \right] d\varepsilon$$

where $\Delta$ is the magnetic band splitting, $n_d^\pm (\varepsilon)$ indicates $n_d (\varepsilon \pm \frac{\Delta}{2})$ and, $n_d (\varepsilon)$ is $d$-band contribution to the paramagnetic density of states per spin, per eV, per atom.

We conserve the total $d$-band electronic occupation, $N_d$, at each step,

$$N_d = \int_{-\infty}^{\epsilon_F} \left[ n_d^+ (\varepsilon) + n_d^- (\varepsilon) \right] d\varepsilon$$

so that charge transfer from the $p$- or $s$- sub-band is neglected.

The total energy, $E$, of the system, in this approximation, is calculated from

$$E(\Delta) = \int_{-\infty}^{\epsilon_F} \left[ n^+ (\varepsilon) + n^- (\varepsilon) \right] \varepsilon d\varepsilon + \frac{J\mu^2}{4}$$

where $n^\pm (\varepsilon) = n_s (\varepsilon) + n_p (\varepsilon) + n_d^\pm (\varepsilon)$, where $n_s (\varepsilon)$ and $n_p (\varepsilon)$ are the contributions to the LDOS from the $s$ and $p$ states, respectively, and $J$ the Stoner parameter. In these equations the only independent variable is $\Delta$. We get the magnetic moment from the value of the magnetic band splitting, $\Delta_0$, that minimizes $E(\Delta)$ in Eq.(6) with $\mu(\Delta)$ defined in Eq. 4.

III. RESULTS

A. The density of states

We have considered three different fcc substrates (Ag, Au, Cu) on top of which a ML of the 4$d$-transition metal Ru, is grown. We consider the substrate to be grown on three possible orientations, i.e., (001), (110) and (111). A Ru-ML grown on Ag and Au in the (001) orientation has been considered previously by Blügel and by García et al., on a Cu substrate. We quote below their results for completeness. The (110) and (111) cases are new.

First, we have calculated the total Ru-ML paramagnetic density of states for each system and each orientation considered. In Table I, we give its value, $N(\varepsilon_F)$, at the Fermi level. Magnetism is attributable to the behavior of the $d$-electrons, and, therefore, their contribution to $N(\varepsilon_F)$, should be, in principle, more significant. We quote this value in Table I, as well. The trend is the same as expected and goes as follows. The highest value is, in all the cases considered, the one for the (001) orientation. For the (110) we get the smallest.
Cu(001) is an exception though, since \(N(\varepsilon_F)\) is highest in the (111) orientation, instead. But since a Ru-ML is not magnetic on Cu in any orientation (see below), we concentrate on the trend based on Ag and Au. For any particular orientation, the system Ru/Ag presents the highest value of \(N(\varepsilon_F)\), Ru/Au follows, and Ru/Cu is the last.

### B. The magnetic moment

As we stated above, the magnetic moment (\(\mu\)) is calculated from the value of the magnetic splitting, \(\Delta_0\), that minimizes \(E(\Delta)\) in Eq. (6). Our results appear in Table II. The magnetic splitting, \(\Delta_0\), obtained in this way correlates directly with \(N(\varepsilon_F)\) and with the corresponding \(d\)-contribution \((d - N(\varepsilon_F))\) for any orientation, i.e., it is highest for Ru/Ag, smaller for Ru/Au, and the smallest for Ru/Cu, where we get actually zero. So, for a Ru-ML, \(N(\varepsilon_F)\), the \(d - N(\varepsilon_F)\), and \(\Delta_0\), have a common trend.

The Ru-ML spin discriminated total density of states (SLDOS) appears in Figs. 1-3 for all the cases considered. On Table II, we give its value at the \(\varepsilon_F\) for the majority and minority spin.

From the results presented in Figs. 1-3 and Eq. 4, we have calculated the magnetic moment (\(\mu\)) at the Ru-ML. We give our results in Table III. We use for the Ru-ML the Stoner parameter from Sigalas and Papaconstantopoulus \[23\], \(J = 0.560\) eV. From Table III, we see that \(\mu\) follows the same trend as \(N(\varepsilon_F)\), \(d - N(\varepsilon_F)\), and \(\Delta_0\). Indeed the highest moment is for Ru/Ag, Ru/Au follows and Ru/Cu is last. Within each system, \(\mu\) is highest in the (001) orientation and lowest in the (110) one. For the (001)-orientation, we find 1.73\(\mu_B\) for Ru/Ag and Ru/Au, reproducing the results by Blügel \[3\]. For Ru/Cu we find zero \[12\]. For (111), the magnetic moment on Ru/Ag and Ru/Au are about the same, roughly 1.3\(\mu_B\) (See Table III). For Ru/Cu we find zero. These results are to be expected on the grounds of the lattice constant value for these isoelectronic noble transition metal substrates. The lattice constant for Ag and Au is approximately equal, \(i.e., 4.8\) Å, while Cu has a lattice constant equal to 3.61 Å. Therefore Cu, in general, in any orientations shrinks the space between the Ru-atoms, at the ML atomic layer, an effect that is against the magnetic activity as it is discussed in Ref. \[12\]. The Ru-atoms on Cu have an interatomic distance which is shorter than the one on the corresponding Ru-surface (the Ru-lattice constant is 3.81 Å). The Ru-surface is not magnetic in any orientation, according to our calculation.

The trend that within each system \(\mu\) is highest on the (001) orientation and lowest in the (110) one, seems, at first sight, to be easily related to a geometric property. But this is not actually the case. Let us try, for example, to find a simple relation that agrees with the result that \(\mu\) is smaller in the (111)-orientation than in the (001) one. In an fcc-lattice the first-nearest neighbors (FNN) distance is \(\frac{a}{\sqrt{2}}\), with \(a\) the lattice constant. When a monolayer is grown on top of a substrate, the number of FNN that an atom on the ML has, varies with the crystallographic orientation. Some of these neighbors are on the ML-atomic layer and others belong to the substrate. Table IV summarizes these observation. The numbers are presented following the trend that we got for the magnetic moment value. We see from this Table that neither the total number of FNN, nor the number of them on the ML-atomic layer or in the substrate correlate with the magnetic moment. The last column line in Table IV is the distance between the ML-atomic plane and the first substrate atomic plane. This parameter does not correlate with \(\mu\), as well. It seems that there is no simple
geometric parameter to correlate with the trend of the value that \( \mu \) takes in the different crystallographic directions.

As a first conclusion, we can say that the magnitude of the magnetic moment on a Ru-ML grown on a noble metal depends strongly on the lattice constant. It is about the same on Ag and Au and it is zero on Cu in any orientation. Within each system the magnitude of \( \mu \) is higher in the (001) orientation and smallest on the (110). The trend of \( \mu \) correlates with the ML-total-paramagnetic density of states at the Fermi-level \( N(\varepsilon_F) \), with the corresponding \( d^- \)-band contribution to it, and with the corresponding magnetic band splitting, \( \Delta_0 \).

There is an exception to this picture worth looking at. For a Ru-ML/Au(110), \( \mu = 0 \), while \( \mu = 1.3\mu_B \) for a Ru-ML/Ag(110). We devote next sub-section to examine this point in more detail.

### C. The (110) orientation

The null value for the Ru-ML/Au system in the (110)-orientation deserves some attention. On general grounds the behavior of a Ru-ML on a Au or a Ag substrate should not present a big difference in what the magnetic activity is concerned. Actually a Ru-ML has essentially the same value of \( \mu \) on Au and on Ag in the (001)- and (111)-orientation. For this reason, the big difference that we find in the (110) orientation for Ru/Ag and Ru/Au is striking. The fact that the Ru-ML shows no magnetic activity on a Cu-substrate in any orientation whatsoever is not, since, in this case, the Ru atoms are brought together too closely by the substrate potential for any magnetic activity to appear. But this argument does not hold true in the case for Ru-ML/Au.

To further explore the difference between a Ru-ML/Au and a Ru-ML/Ag in the (110) orientation, we have produce Fig. 4. It shows the difference curve between the \( d^- \)-band contribution to the Ru-ML total paramagnetic density of states, \( N(\varepsilon_F) \), comparing a Ru-ML/Cu(110) to a Ru-ML/Ag(110) (upper curve) and a Ru-ML/Au(110) to a Ru-ML/Ag(110) (lower curve). In both cases, it is evident that the number of \( d^- \)-electrons, in the vicinity of the \( \varepsilon_F \), is much higher for the Ru-ML/Ag (the difference curve is strongly negative) which is the only one that shows magnetic activity in this direction. So the effect is due to the presence of \( d^- \)-electrons much more nearby \( \varepsilon_F \). Notice that the Stoner criterium for ferromagnetism is fulfilled by Ru-ML/Ag(110) but it is not neither by the Ru-ML/Au(110) nor by the Ru/Cu(110). Actually Ru on a Cu substrate does not fulfill the Stoner criterium in any orientation whatsoever. (See Table I and recall that, \( J = 0.560 \text{ eV} \))

### D. The Effect of pressure and expansion in the (110)-orientation

As a last point in this paper, we study the effect on the ML magnetism of pressure and expansion of the Ru/Au (110) system. First, we present in Fig. 5 the total paramagnetic LDOS for the three systems considered. On the top-graph the Ag(110) surface LDOS is compared to the Ru(110) surface LDOS and to the Ru-ML/Ag (110) LDOS. The middle and lower graphs deal in the same way with the Ru/Au(110) and Ru/Cu(110) cases. The case of interest here is the Ru/Au(110). The other two are presented for completeness.
Let us refer to the middle graph (Ru/Au(110)). At $\varepsilon_F$ (the origin in the graph), the Ru-ML/Au(110) LDOS is well below that the corresponding value for Ru-ML/Ag(110). Notice, nevertheless, that the peak, just below $\varepsilon_F$, in the Ru-ML/Au(110) LDOS is almost as high as the one on the corresponding curve for the Ru-ML/Ag(110) LDOS at $\varepsilon_F$. So the question arises: can pressure or expansion bring this peak to the $\varepsilon_F$ and turn on the magnetic activity of the Ru-ML on a Au (110) substrate?

The answer to this question appears in Fig. 6 and Table V. Pressure does not turn on the magnetic activity but expansion does (enhancement of the Au lattice constant). In this figure we present the total energy (Eq. 6) as a function of the magnetic band splitting $\Delta_0$. Notice first that, according to our results, a metastable magnetic state does exist for a Ru-ML/Au(110) at zero expansion (see the minimum in Fig. 6(a)). The corresponding magnetic moment is $\mu = 0.69 \mu_B$ and the magnetic splitting is $\Delta_0 = 0.386$ eV. This state is somehow premonitory of the magnetic activity under expansion. In the rest of Fig. 6, we present the magnetic activity of Ru/Au(110) under hydrostatic expansion up to 4% of the lattice constant of the substrate. We give, for completeness, a broader account of our results in Table V. This kind of expansion might be possible by applying pressure perpendicular to the sample since according to the strain tensor this will enhance the distance between the Ru-atoms on the ML atomic layer.

IV. CONCLUSIONS

We have studied the magnetic activity of a Ru-ML grown on three different substrates, i.e., Ag, Au and Cu in three crystallographic orientations, (001), (111), and (011). In the (001) orientation, we reproduced the results already obtained by Blügel [3] and by García et al., [12]. The results for the other two directions are new. We get a higher magnetic moment, $\mu$, for Ru/Ag, next Ru/Au and last Ru/Cu. For each system, $\mu$ is highest on the (001) orientation and lowest on the (110)-one. The Ru/Cu system has no-magnetic activity in any orientation. For Ru/Ag, $\mu = 1.73 \mu_B$ in the (001), $\mu = 1.3 \mu_B$ in the (111), and $\mu = 1.3 \mu_B$ in the (110). For the Ru/Au, $\mu = 1.73 \mu_B$ in the (001), $\mu = 1.29 \mu_B$ in the (111), and $\mu = 0$ in the (110). See Table III and Figs. 1-3. The non existence of magnetic activity for the Ru/Au (110) contrasts strongly with the Ru/Ag (110) magnetic moment value of $\mu = 1.3 \mu_B$. To better understand this fact, we have explored the behavior of the Ru/Au (110) system and found that a metastable state does exist at zero pressure and that it becomes magnetic under expansion (enhancement of the in-layer lattice constant). See Figs. 4-6 and Table V.

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Table I

| Orientation | \( N(\varepsilon_F) \text{[states/spin/eV/atom]} \) |
|-------------|--------------------------------------------------|
|             | \( \text{Ag total } d \) | \( \text{Au total } d \) | \( \text{Cu total } d \) |
| 001         | 2.7042 | 2.6601 | 2.5824 | 2.5440 | 1.5132 | 1.4516 |
| 111         | 2.6029 | 2.5899 | 2.5128 | 2.4948 | 1.5521 | 1.5235 |
| 110         | 2.3390 | 2.3152 | 1.7469 | 1.7303 | 1.1665 | 1.1231 |

Table II

| Orientation | \( N(\varepsilon_F) \text{[states/spin/eV/atom]} \) |
|-------------|--------------------------------------------------|
|             | \( \text{Ag maj. min. } \Delta_0 \text{ (eV)} \) | \( \text{Au maj. min. } \Delta_0 \text{ (eV)} \) | \( \text{Cu maj. min. } \Delta_0 \text{ (eV)} \) |
| 001         | 0.509 | 1.899 | 0.969 | 0.531 | 1.723 | 0.972 | 1.513 | 1.513 | 0.000 |
| 111         | 0.701 | 1.744 | 0.725 | 0.644 | 1.687 | 0.718 | 1.547 | 1.547 | 0.000 |
| 110         | 1.082 | 3.036 | 0.725 | 1.715 | 1.715 | 0.000 | 1.130 | 1.130 | 0.000 |

Table III

| Orientation | The Magnetic Moment [\( \mu_B \)] |
|-------------|-----------------------------------|
|             | \( \text{Ag } \) | \( \text{Au } \) | \( \text{Cu } \) |
| 001         | 1.73 | 1.73 | 0.00 |
| 111         | 1.30 | 1.29 | 0.00 |
| 110         | 1.30 | 0.00 | 0.00 |
### Table IV

| Orientation | ML Substrate | ML-first plane distance |
|-------------|--------------|-------------------------|
| 001         | 4            | $\frac{a}{2}$           |
| 111         | 6            | $\frac{a}{\sqrt{3}}$   |
| 110         | 2            | $\frac{a}{2\sqrt{3}}$  |

### Table V.

| % Expansion | Magnetic moment [$\mu_B$] |
|-------------|--------------------------|
| 0           | 0.00 (0.69 metaestable state) |
| 1           | 0.97                     |
| 2           | 1.04                     |
| 3           | 1.11                     |
| 4           | 1.18                     |
| 5           | 1.19                     |
| 6           | 1.32                     |
| 7           | 1.38                     |
| 8           | 1.43                     |
| 9           | 1.47                     |
Fig. 1 Our results for the Ru-ML/Ag in the three different orientations. We present the Ru-ML spin discriminated total density of states (SLDOS). In this case $\Delta_0 \neq 0$ for all the three orientations and, consequently, $\mu$ is also different from zero. See text and Tables II and III.

Fig. 2 A Ru-ML/Au (See caption of Fig.1). Notice that, in this case $\Delta_0 = 0$ for the substrate grown in the $(110)$ orientation and therefore $\mu = 0$. Compare with the previous case. (See text).

Fig. 3 A Ru-ML/Cu. (See caption of Fig.1). $\Delta_0 = 0$ ($\mu = 0$) for all the orientations in this case.

Fig. 4 Here we show the difference-curve between the $d$–band contribution to the Ru-ML paramagnetic density of states for the Ru/Cu and Ru/Ag (upper curve) and for the Ru/Au and Ru/Ag (lower curve) in the $(110)$ orientation. See text.

Fig. 5 We present three sets of graphs, one for each of the three cases considered here [Ru-ML/Ag(110), Ru-ML/Au(110), and Ru-ML/Cu(110)]. For each case we compare three curves that represent the total paramagnetic local density of states (LDOS) for

i) The Ru-ML.

ii) The $(110)$-oriented surface of the substrate.

iii) The $(110)$-oriented Ru surface.

Fig. 6 The total energy, $E(\Delta)$, (Eq. 6) as a function of the magnetic band splitting, $\Delta$, for a Ru-ML/Au(110) under expansion of the Au lattice constant. See text for details.
TABLES CAPTIONS

Table I. We present here the Ru-ML total paramagnetic density of states at the $\varepsilon_F$, $N(\varepsilon_F)$, in the orientations considered. The largest is for Ag, then for Au and the smallest is for the Cu substrate. Also, for a given substrate, the highest $N(\varepsilon_F)$, is in the (001) -orientation and the smallest in the (110)-one. In the second column, we also quote the corresponding contribution of the $d$-band. The trends are the same. Notice that for the Cu-substrate, the trend is not followed in the (111)-orientation. Ru/Cu is not magnetically active in any orientation.

Table II. In the first column, we present the corresponding direction of growth of the substrate. Next, we quote our values for the Ru-ML spin discrimated total density of states (SLDOS) at the Fermi level for majority and minority spin. The next column gives the corresponding magnetic band splitting, $\Delta_0$. See text.

Table III. We give the magnetic moment (in units of Bohr magnetons, $\mu_B$), on the Ru-ML in different orientations for the three substrates considered.

Table IV. We give here the number of first nearest neighbors (FNN) of a Ru-ML atom that lie on the ML and in the substrate. The last column gives the ML- first plane distance in each case. None of these parameters follows the magnetic moment trend.

Table V. We present here the magnetic moment for a Ru-ML/Au(110) under expansion of the Au lattice constant. See text for details.
1 ML Ru/Cu [hkl]

Energy (eV)

spin dep. LDOS[states/spin/eV/atom]

Fermi level

maj.

min.

(001)  (111)  (111)

-10  0  10  -10  0  10 -10  0  10
metastable state
0%
\( \mu = 0.69 \mu_B \)
\( \Delta = 0.386 \text{ eV} \)

1%
\( \mu = 0.97 \mu_B \)
\( \Delta = 0.54032 \text{ eV} \)

2%
\( \mu = 1.04 \mu_B \)
\( \Delta = 0.58124 \text{ eV} \)

3%
\( \mu = 1.11 \mu_B \)
\( \Delta = 0.62112 \text{ eV} \)

4%
\( \mu = 1.18 \mu_B \)
\( \Delta = 0.65815 \text{ eV} \)