Magnetic states of linear defects in graphene monolayers: effects of strain and interaction

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The combined effects of defect-defect interaction and of uniaxial or biaxial strains of up to 10% on the development of magnetic states on the defect-core-localized quasi-one-dimensional electronic states generated by the so-called 558 linear extended defect in graphene monolayers are investigated by means of ab initio calculations. Results are analyzed on the basis of the heuristics of the Stoner criterion. We find that conditions for the emergence of magnetic states on the 558 defect can be tuned by uniaxial tensile parallel strains (along the defect direction) at both limits of isolated and interacting 558 defects. Parallel strains are shown to lead to two cooperative effects that favor the emergence of itinerant magnetism: enhancement of the DOS of the resonant defect states in the region of the Fermi level and tuning of the Fermi level to the maximum of the related DOS peak. A perpendicular strain is likewise shown to enhance the DOS of the defect states, but it also effects a detuning of the Fermi level that shifts away from the maximum of the DOS of the defect states, which inhibits the emergence of magnetic states. As a result, under biaxial strains the stabilization of a magnetic state depends on the relative magnitudes of the two components of strain.

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I. INTRODUCTION

Technological applications of two-dimensional (2D) nanomaterials require the ability to control their mechanical, electronic, and magnetic properties. In the last decade, graphene in the 2D monolayer form has become an important subject of research, motivated by its mechanical strength and the rich electronic phenomenology connected with the Dirac-fermion nature of its electronic structure near - within a scale of ~1 eV - the Fermi level. The origin of magnetism in graphene is not fully understood, being usually associated with the presence of vacancies or adsorbates that tend to bind to vacancies. In bipartite lattices, these defects lead to an imbalance in the electronic occupation of the two sub-lattices, which leads to stabilization of magnetic ground states, as predicted by the Lieb theorem. In a 2D material such as graphene, vacancies and topological point defects can be created in non-equilibrium densities by electron-beam irradiation. However, full control over such magnetic states is hampered by the random placement of vacancies.

Judicious introduction of structural defects presents an alternative for manipulating the electronic and magnetic properties in 2D materials. Besides the tilt GBs that inevitably occur in polycrystalline graphene, a so-called 558 extended line defect was shown to occur in graphene layers grown on Ni substrates as the interface across which the stacking of the graphene layer with respect to the Ni substrate shifts from AB to AC (in the usual convention for layer stacking in close-packed lattices). Furthermore, recent experimental work has introduced a protocol for the synthesis of this 558 extended defect in a controllable fashion in a graphene monolayer, which shows that the possibility of manipulating the electronic and magnetic properties of graphene and other two-dimensional materials, by controllable introduction of defects, is a realistic prospect for the near future.

The morphology of the 558 extended defect, shown in Fig. consists of a periodic unit composed of two side-sharing pentagonal rings connected to an octagonal ring. Alexandre et al. employed ab initio calculations to show the development of itinerant ferromagnetism in the quasi-one-dimensional (q1D) electronic states that are strongly localized on the core of the 558 defect. The ferromagnetic state obtained by Alexandre et al. requires n-type doping in order for the Stoner criterion for a ferromagnetic instability to be met. Electron doping shifts the Fermi level to the maximum of the peak in the electronic density of states (DOS) associated with the extended van Hove singularities that appear at and near the Fermi level, that are characteristic of the q1D electronic states generated by the 558 extended defect.

The extended van Hove singularities, related to the large flat portions of the defect electronic states crossing the Fermi level, signal a strong localization of the q1D defect states that leads to an enhancement of exchange and correlation effects. Tuning the Fermi level to the region of the maximum of the related DOS peak leads to the onset of the magnetic states. Large periodic supercells were employed in Ref. with negligible couplings between the 558 defect in the home cell and its periodic images, meaning that conditions for the emergence of the magnetic state apply to the case of an isolated and unstrained 558 defect in that study. One is naturally led

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to consider the formation of magnetic states in the 558 defect in graphene under less restrictive conditions.

Two-dimensional materials grown on mismatched substrates are commonly subject to strain. Moreover, strain engineering opens up the possibility of tailoring electronic and magnetic functionalities in 2D materials by the intentional application of strain. Graphene is known to withstand strains as high as 20-25% without failure [14, 29, 30], being one of the 2D systems of choice for strain engineering [31]. Generally, tensile strains lead to reduced band widths and extended van Hove singularities, and thus to enhanced exchange and correlation effects, as exemplified by the case of palladium, which displays paramagnetic states that are very close to magnetic instabilities that can be triggered by quantum confinement and strain in low-dimensional structures [32, 33, 35, 36].

In the present study, we employ ab initio calculations to address the combined effects of defect-defect interaction and of uniaxial or biaxial strains of up to 10% on the development of magnetic instabilities on the q1D electronic states generated by the 558 extended defect on graphene monolayers.

Our calculations indicate that conditions for the development of magnetic instabilities on the core-localized q1D defect states can be tuned by tensile uniaxial strains, along the defect direction, at both limits of isolated and interacting 558 defects. A tensile strain along the defect axis, which we refer to as a parallel strain, leads to two cooperative effects that favor the emergence of itinerant ferromagnetic in the 558-defect states: (i) enhancement of the DOS of the q1D states in the region of the Fermi level and (ii) tuning of the Fermi level to the maximum of the related DOS peak.

On the other hand, an uniaxial tensile strain in the direction perpendicular to the defect line (perpendicular strain) is shown to be detrimental to the development of magnetic states on the 558 defect, because in this case, while we still obtain an enhancement of the DOS of the q1D as in the case of a parallel strain, the Fermi level is found to shift away from the maximum of the defect DOS, i.e., a perpendicular strain leads to a detuning of the Fermi level that inhibits the emergence of the magnetic states. As a result, under biaxial strains we find that the stabilization of a magnetic state depends on the relative magnitudes of the two components of strain, parallel and perpendicular.

Regarding the meaning of our DFT-theory mean-field results, it must be stressed that, because of their 1D nature, these correlated magnetic states do not show long range order [37]. Instead, they present algebraic correlation functions, and the magnetic states we find in our calculations should manifest themselves in experimental samples as magnetic domains with a null average macroscopic magnetization.

II. METHODOLOGY

In our calculations we employ the SIESTA code implementation of Kohn-Sham density functional theory (DFT), within the generalized-gradient approximation (GGA) for the exchange and correlation functional. Interactions between valence electrons and ionic cores are treated using norm-conserving pseudopotentials in the Kleinman-Bylander factorized form. A double-zeta LCAO basis set, augmented with polarization orbitals, is used to expand the electronic wave functions. In all calculations, an equivalent real-space mesh cutoff of 250 Ry is used, and meshes of up to 64 k-points along the extended-defect direction are used to converge the electronic density and the density of states.

Full structural relaxation is performed, with forces on atoms reaching values of 0.01 eV/Å or lower in all cases. For the equilibrium (unstrained) geometries, the residual pressure on the supercell is lower than 1 kBar in all cases. In a few selected cases, convergence of energies...
and magnetic moments is verified with calculations employing larger k-point sets and a mesh cutoff of 300 Ry, to ensure that our results are converged with respect to calculational parameters.

The supercells we employ, as shown in Fig. 1, contain a single 558 extended defect, and the supercell vector in the direction perpendicular to the defect (the x-axis of the cell) determines the nearest defect-defect distance \( R \) in the periodic array of defects generated by our use of periodic boundary conditions, as shown in Fig. 3. Supercells containing 558 defects may be classified by the number \( N \) of “buffer” zigzag chains of carbon atoms in the bulk part of the cell, as suggested in Ref. [12].

In our analysis, we find it more expedient to classify the supercells by the distance \( R \) between the 558 defect in the home cell and its closest periodic images. We consider a total of six different supercells: \( R = 5.7 \text{ Å} \) (\( N = 0 \)), \( R = 10.0 \text{ Å} \) (\( N = 2 \)), \( R = 14.3 \text{ Å} \) (\( N = 4 \)), \( R = 18.7 \text{ Å} \) (\( N = 6 \)), \( R = 23.0 \text{ Å} \) (\( N = 8 \)), and \( R = 27.3 \text{ Å} \) (\( N = 10 \)). These supercells cover the range of defect-defect distances between \( R = 5.7 \text{ Å} \), the smallest possible distance between adjacent 558 defects, and \( R = 27.3 \text{ Å} \), a value at which defect-defect interaction is negligible and the electronic properties of the defect are characteristic of isolated defects.

The geometry of the supercell with \( R = 18.7 \text{ Å} \), with six buffer chains between defects, is shown in Fig. 1. The inset in Fig. 1(b) shows a 2x2 frame of the supercell with \( R = 5.7 \text{ Å} \), with no buffer chains between the 558 defect in the home cell and its closest periodic images.

III. RESULTS AND DISCUSSION

Our results are analyzed in terms of the Stoner criterion (SC) for itinerant magnetic instabilities:

\[
IN(\epsilon_F) \geq 1 \quad ;
\]

where \( I \) is the exchange integral and \( N(\epsilon_F) \) is the DOS at the Fermi level. [We denote the DOS at energy \( \epsilon \) as \( N(\epsilon) \).]

Our focus is to address the effects of defect-defect interaction and strain on the development of magnetic states on the q1D electronic states of the 558 defect in graphene, based on the heuristics of the SC. While the strong localization of the q1D defect states favors both factors in the left-hand side of the SC inequality, in Ref. [11] it was shown that, in the isolated-defect limit, tuning the Fermi level with \( n \)-type doping is required for the ferromagnetic instability to set in, which means that the SC is not met for an isolated 558 defect in a neutral and unstrained graphene layer.

We consider ferromagnetic (FM) and antiferromagnetic (AFM) couplings between defects [12], as well as the spin-unpolarized non-magnetic case (NM). Figure 1 shows schematically the starting spin distribution for the initial states of the FM and AFM states in our DFT calculations. After electronic self-consistency is achieved, we obtain the corresponding FM and AFM states for the 558 defect. We have also attempted several other initial spin configurations, such as an antiferromagnetic coupling between the two zigzag chains on the core of the 558 defect (as considered in Ref. [12]), as well as other initial antiferromagnetic arrangements of initial spin states for the atoms along the core of the 558 defect. At the GGA level, these converge either to the FM or to the AFM states shown in Fig. 1.

In our calculations, we have imposed isotropic and anisotropic biaxial strains as well as parallel and perpendicular uniaxial strains. In the following discussion we concentrate our analysis first on the effects of tensile parallel strains, followed by a discussion on the effects of tensile perpendicular strains and biaxial strains.

A. Energetics

We start by addressing the combined effects of defect-defect interaction and a homogeneous parallel strain on the energetics and magnetic states of the defect in the neutral (undoped) case. Figure 2 shows the difference in total energy per defect periodic unit, with respect to the energy of the NM state, for the FM \( (\Delta E^{\text{FM}}_{\text{tot}} = E^{\text{FM}}_{\text{tot}} - E^{\text{NM}}_{\text{tot}}) \) and AFM states \( (\Delta E^{\text{AFM}}_{\text{tot}} = E^{\text{AFM}}_{\text{tot}} - E^{\text{NM}}_{\text{tot}}) \) of the 558 defect as functions of the defect-defect distance \( R \). The figure shows \( \Delta E_{\text{tot}} \) for the equilibrium (unstrained) as well as for the uniaxially-strained cases, at a parallel strain of 10%.

Figure 2 shows that the equilibrium FM and AFM states are nearly energy-degenerate for all values of \( R \).
A discernible trend is that, for both the FM and AFM states, $\Delta E_{\text{tot}}$ increases in magnitude as the defect-defect interaction is reduced with increasing $R$. A small energy difference of $\sim 2.5$ meV (per defect periodic unit), favoring the AFM state is observed for $R = 18.7$ Å, while for $R = 23.0$ Å the FM state is favored by $\sim 3.4$ meV. At the largest distance of $R = 27.3$ Å, defect-defect interaction effects are negligible and the two phases are degenerate, with $E_{\text{tot}}$ values that are smaller than the NM case by 24 meV per defect periodic unit.

The energetics of the magnetic states of the strained 558 defect shows a richer structure. The AFM state is favored for all values of $R$, except for the case of $R = 23.0$ Å, and the FM-AFM split in energy is much larger at small defect-defect separations than in the unstrained case, with the AFM state being favored by 20 meV at the smaller distance of $R = 5.7$ Å. At larger defect-defect distances, the FM and AFM states become nearly degenerated, with energies that are lower than the NM case by $\sim 55-62$ meV, compared with the unstrained results of 24 meV. Generally, a parallel uniaxial strain enhances the stability of the magnetic states with respect to the NM state.

B. Magnetic States: Effects of Tensile Parallel Strain

Shifting gears now to the onset of magnetic states, we show in Fig. 3 the magnetic moment per defect unit $\mu$ (in units of the Bohr magneton, $\mu_B$) as a function of uniaxial tensile parallel strain for different values of $R$. For the unstrained cases (0% strain), we observe that $\mu$ decreases with increasing $R$, with the exception of the anomalous case of $R = 5.7$ Å, that shows a very small value of $\mu$. Magnetic moment values at the largest defect-defect separations in our study, $\mu = 0.007 \mu_B$ for $R = 23.0$ Å and $\mu = 0.003 \mu_B$ for $R = 27.3$ Å, are very small for the unstrained defects. Figure 3 also shows that the rate of increase of $\mu$ with strain increases with $R$.

Indeed, at a 4% parallel strain the values of $\mu$ are nearly the same for all values of $R$ (with the exception of the anomalous case of $R = 5.7$ Å that we discuss in more detail below), and for a strain of 10% the behavior of $\mu$ as a function of $R$ is reversed, and the magnetic moment becomes an increasing function of the defect-defect separation, for the range of $R$ values we consider. Note that for the larger defect-defect distances ($R = 23.0$ Å and $R = 27.3$ Å), for strains between 1% and 2% the $\mu$ values increase by two orders of magnitude and become comparable to those for smaller values of $R$. The case of $R = 5.7$ Å is anomalous, with very small values of $\mu$ for strains up to 5%. In this case, strains larger than a critical value between 5% and 6% are needed for $\mu$ to reach values of 0.1-0.2 $\mu_B$.

In order to facilitate the visualization of these trends, in Fig. 4 we plot the data from Fig. 3 as a function of $R$ for three different values of tensile parallel strain: unstrained, 4%, and 10%. Generally, from Figs. 3 and 4 we conclude that defect-defect interaction favors the emergence of itinerant magnetism in unstrained 558 defects, with the exception of the case of defects at their closest possible separation ($R = 5.7$ Å). In its turn, a tensile parallel strain also leads to the onset of magnetism, and supersedes the effect of interaction, starting at about a 4% parallel strain, as shown in Fig. 4. At 4% parallel strain, the magnetic moment per defect unit is nearly independent of $R$ (for $R \geq 10.0$ Å), and for larger strains $\mu$ increases with distance, in stark contrast with the behavior of the unstrained defects.

The mechanisms behind these trends, and also behind the behavior of the anomalous case of defects at a distance of $R = 5.7$ Å, can be understood from the perspective of the Stoner criterion. Figure 5 shows the DOS, $N(\epsilon)$, in the Fermi level region, for the six defect-defect...
distances we consider. For each case, we show $N'(\epsilon)$ for the unstrained state, and for the cases of 4% and 10% parallel strain.

Starting from the anomalous $R = 5.7$ Å case in Fig. 5(a), we observe that application of a tensile strain does not enhance the defect-related peak in the DOS near the Fermi level. This indicates that strain does not enhance the localization of the defect electronic states at the Fermi level, and its only effect in this case is a better tuning of the Fermi level, that shifts closer to the maximum of the DOS peak in Fig. 5(a). Thus, the only factor in Eq. 1 that is affected by application of a tensile parallel strain in this case is the value of the DOS at the Fermi level, $N'(\epsilon_F)$, and the exchange integral remains essentially unchanged.

At larger distances this picture changes, as shown in Figs. 5(b)-(f) where we observe that a parallel tensile strain induces two effects in the electronic structure of the 558 defect. The first one is a better tuning of the Fermi level, that shifts closer to the peak of defect states in the DOS, as in the $R = 5.7$ Å case, but we also observe an enhancement of the height of the DOS peak, connected with a stronger localization of the electronic states of the 558 defect in the Fermi level region. Note that at the two largest distances in our study ($R = 23.0$ Å and $R = 27.3$ Å), the evolution of the DOS and also of the Fermi level position with strain is more complex due to the presence of two DOS peaks of defect states near the Fermi level in the unstrained state, that merge into a single peak at larger strains.

Regarding the anomalous $R = 5.7$ Å case, we speculate that when 558 defects are separated by a distance $R = 5.7$ Å, the lack of a bulk region (as shown in the inset in Fig. 1) onto which the defect-related electronic states can relax, inhibits the enhancement of the localization of the defect states induced by the parallel strain, that we observe at larger distances where the defects are surrounded by bulk material.

The parallel-strain induced enhancement of localization, hence of the exchange integrals in Eq. 1, is connected with the changes in the 558-defect electronic states. In Fig. 6, we show the band structures for the unstrained and 10% parallel-strained cases, for three differ-
different values of $R$. Figure 6(a) shows the $R = 5.7$ Å case, where extended van Hove singularities do not appear in the band structure of the unstrained defect. At this defect-defect distance, even for the 10%-strained case in Fig. 6(b) we observe no extended van Hove singularities in the band structure, and the only effect of strain is the tuning of the Fermi level, as discussed in the previous paragraph. This explains why for $R = 5.7$ Å the system develops only a moderate value of $\mu$, even for such large value of strain, and generally the behavior of $\mu$ with strain does not follows the trends we observe at larger defect-defect distances.

When 558 defects are separated by $R = 10.0$ Å, extended van Hove singularities, connected to the large flat portions of the defects bands at the Fermi level, appear in the band structure for the unstrained defect, as shown in Fig. 6(c). This observation, along with the fact that the Fermi level in this case is very near the maximum of the DOS peak, are the reasons behind the development of a large value of $\mu$ already for the unstrained defects in this case. For the strained states, a better tuning of the Fermi level to the maximum of the resonant defect peak in the DOS [shown in Fig. 6(b)], coupled with an enhancement of the extended van Hove singularities, due to an enlargement of the flat portions of the bands at the Fermi Level, and a reduction of the band widths of the defect bands, shown in Figs. 6(d), explain the increase of $\mu$ with increasing strain displayed in Fig. 6.

Strain plays an even more decisive role in the limit of non-interacting defects ($R = 27.3$ Å). As indicated above, the unstrained defect shows a borderline behavior, with a very small value of $\mu$. Given the presence of quite wide van Hove singularities in the band structure of the unstrained defect, as displayed in Fig. 6(c), it is to be expected that tensile strains in this case should drive the system towards a more robust magnetic state. Indeed, for a critical parallel tensile strain between 1% and 2% the system develops a sizeable value of $\mu = 0.24 \mu_B$. Further increase in the value of $\mu$ for larger strains is explained along the same reasoning as the $R = 10.0$ Å case, i.e., better tuning of the Fermi level and an enhancement of the flat portions of the defect bands that leads to more localized states and enhanced exchange effects. For this non-interacting case, Fig. 6(f) shows a marked increase in the extent of the extended van Hove singularities lying at the Fermi level, at 10% parallel strain, along the $\Gamma-Y$ and $L-X$ lines in the Brillouin zone [both are parallel to the defect direction, as shown in Fig. 1(c)].

C. Magnetic States: Effects of Perpendicular and Biaxial Tensile Strains

The above discussion shows that a parallel tensile strain favors the emergence of magnetic states in the 558 defect in graphene, by enhancing both factors encoded in the Stoner criterion in Eq. 1. In the present section, we consider the effects of biaxial and perpendicular tensile strains, analyzing in detail the strongly interacting $R = 10.0$ Å case, that displays the largest value of $\mu$ for the unstrained defects, and the non-interacting $R = 27.3$ Å case. These two examples suffice to highlight the general trends and the generality of the results will be pointed out as we proceed with the discussion.

1. Perpendicular Tensile Strain

Filled black circles in Fig. 7 show the effect of perpendicular uniaxial tensile strains from 1% to 5% on the magnetic states of the $R = 10.0$ Å case. At a 5% strain the magnetic moment of the defect states has dropped to zero, indicating at a first sight that a perpendicular tensile train does not favor the emergence of magnetic states in the 558 defect. The issue, however, calls for a more detailed analysis.

Figure 8(a) shows the evolution of $\mathcal{N}(\epsilon)$ with strain for this case. The first observation to be drawn from Fig. 8(a) is that a tensile perpendicular of up to 5% enhances the peak related to the defect states in the DOS, i.e., a perpendicular strain may actually enhance the localization and thus the exchange integral of the defect states. However, the figure also shows a fast detuning of the Fermi level, connected with the overall changes in the band structure induced by the application of the perpendicular strain. Note that the height of the defect peak in $\mathcal{N}(\epsilon)$, at 2% perpendicular strain, is greater than that of the unstrained defect, while the value of $\mu$ decreases in

![Graph](image-url)
Fig. 7, the reason being the smaller value of $N(\epsilon_F)$ that results from the shift in the position of the Fermi level.

Therefore, quenching of the magnetic moment in this case is connected to a low value of $N(\epsilon_F)$, and not to a delocalization effect that would impact the exchange integral. This is an important observation, because the Fermi level can be tuned by doping, and we can anticipate that magnetic states in graphene samples under perpendicular tensile strains, containing 558 defects, may be induced by proper Fermi-level tuning.

2. Biaxial Strain

Now that we have analyzed the effects of parallel and perpendicular uniaxial tensile strains, we conclude by addressing the effects of biaxial tensile strains. From the foregoing discussion, we know that both parallel and perpendicular strains tend to enhance the extended van Hove singularities of the defect states, hence both lead to an enhancement of the associated exchange integrals. On the other hand, they produce opposite effects in $N(\epsilon_F)$, the value of the DOS at the Fermi level, with parallel strains of up to 10% leading to larger values of $N(\epsilon_F)$, while perpendicular strains lead to a fast detuning of the Fermi level and hence to rather low values of $N(\epsilon_F)$.

We have performed calculations of isotropic biaxial strains of up to 10% for all defect-defect distances in our study. We obtain a ferromagnetic state under isotropic biaxial strain only for the $R = 10.0\,\text{Å}$ case. For the other five values of $R$, magnetic moments were either null or negligible for all values of biaxial strain from 1% to 10%.

The behavior of $\mu$ with strain for the $R = 10.0\,\text{Å}$ case is shown by the filled squares in Fig. 7. We obtain that for biaxial strains of up to 5% the tuning and detuning effects of the two components of strain nearly cancel each other, and $\mu$ remains nearly constant, but a downwards trend can be observed already for strains between 4% and 5%.

For a 10% tensile biaxial strain, $\mu$ vanishes, due to the Fermi-level detuning associated with the perpendicular component of strain. In Fig. 8(b) we show the evolution of the DOS with biaxial strain for this case.

We have also addressed the case of nonisotropic biaxial strains. Filled red triangles in Fig. 7 show the combined effects of a 10% parallel strain coupled with perpendicular tensile strains of 5%, 8%, and 10%, for the $R = 10.0\,\text{Å}$ and $R = 27.3\,\text{Å}$ cases. For both values of $R$, a homogeneous biaxial strain of 10% produces an unpolarized spin state, due to a rather low value of $N(\epsilon_F)$, as shown for $R = 10.0\,\text{Å}$ in Fig. 8(b). Note that a substantial enhancement of the defect-related peak in $N(\epsilon)$, with respect to the unstrained state, is observed, but the value of $N(\epsilon_F)$ is rather small due to the Fermi-level detuning effect prompted by the perpendicular component of strain. These observations also apply to the $R = 27.3\,\text{Å}$ case.

For smaller values of perpendicular strains, we obtain that: (i) for the more robust magnetic state of the $R = 10.0\,\text{Å}$ case, $\mu = 0.47\,\mu_B$ for a 5% perpendicular strain and $\mu = 0.29\,\mu_B$ for an 8% perpendicular strain, both combined with a 10% parallel strain. For the non-interacting defects at $R = 27.3\,\text{Å}$, full quenching of the magnetic moment is observed when the parallel strain is combined with an 8% perpendicular strain, and $\mu = 0.49\,\mu_B$ for a 5% perpendicular strain. As with the case of isotropic biaxial strains, competition between the Fermi-level tuning and detuning effects, due respectively to the parallel and perpendicular components of strain determine the fate of the magnetic states of the 558 defect under anisotropic biaxial strains.

D. Conclusions

In this work, we have addressed the combined effects of defect-defect interaction and of uniaxial or biaxial strains of up to 10% on the development of magnetic instabilities on the quasi-one-dimensional (q1D) electronic states generated by the 558 extended defect on graphene monolayers, by means of ab initio calculations. We have considered uniaxial strains along the defect direction (parallel
strain) and along the perpendicular direction (perpendicular strain), and isotropic and anisotropic biaxial strains. We frame our results on the basis of the Stoner criterion for itinerant magnetism, and analyze the effects of the various strain states on the basis of their impact on the two ingredients encoded in the Stoner criterion: localization of the defect-generated electronic states in the region of the Fermi level and the magnitude of the DOS of the defect states at the Fermi level.

We obtain that conditions for the development of magnetic instabilities in the defect states can be tuned by tensile uniaxial parallel strains at both limits of isolated and interacting 558 defects. Parallel strains are shown to lead to two cooperative effects that favor the emergence of itinerant magnetism in the 558-defect states: enhancement of the DOS of the defect states in the region of the Fermi level and tuning of the Fermi level to the maximum of it.

Given the tuning and detuning of the Fermi level promoted, respectively, by parallel and perpendicular uniaxial strains, under biaxial strains we find that the stabilization of a magnetic state depends on the relative magnitudes of the two components of strain.

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