Emergence of Flat-Band Magnetism and Half-Metallicity in Twisted Bilayer Graphene

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Evidence of flat-band magnetism and half-metallicity in compressed twisted bilayer graphene is provided with first-principles calculations. We show that dynamic band-structure engineering in twisted bilayer graphene is possible by controlling the chemical composition with extrinsic doping, the interlayer coupling strength with pressure, and the magnetic ordering with external electric field. By varying the rotational order, the interplay between electronic and geometric degrees of freedom leads to an unbalanced distribution of charge density resulting in the spontaneous apparition of localized magnetic moments without disrupting the structural integrity of the bilayer. Weak exchange correlation between magnetic moments is estimated in large unit cells. External electric field applied perpendicularly to the bilayer plane switches the local magnetic ordering from ferro- to anti-ferromagnetic. Half-metallicity is achieved with substitutional doping by shifting the chemical potential of one spin distribution leaving unaltered the localized character of the electronic states. Flakes of compressed twisted bilayer graphene exhibit spontaneous magnetization, demonstrating that correlation between magnetic moments is not a necessary condition for their formation.

I. INTRODUCTION

Progress in assembling multilayered two-dimensional (2D) materials has come with a rich array of physics arising from the van der Waals (vdW) forces that hold together parallel layers[1]. Owing to the geometrical degrees of freedom allowed by the vdW interactions, flat structures can easily change the layers’ mismatch by rotating the planes, and also to vary the interlayer distance by applying compression. As a result, compounds with physical properties that are fundamentally distinct from those of the constituent layers can be created.

Special attention deserves twisted bilayer graphene (tBLG), an extended crystalline planar structure composed of two vdW bonded graphene sheets where one sheet is twisted with respect to the other. At specific rotational angles, known as magic-angles, the Moiré patterns that emerge as a result of the offset in the relative orientation of the sheets create an atomic-scale periodic potential able to modify the linear dispersion of graphene[2]. The flat bands created at the twist angle of 1.05° allow tBLG to exhibit an unconventional superconducting phase not observed in monolayer or AB stacked bilayer graphene [3–6]. MIT’s Jarillo-Herrero’s group reported an insulating state when injected electrons reside in a Moiré unit cell, relating this behavior to an example of Mott physics[3, 4]. Padhi et al. ascribed this physical effect to a Wigner crystallization[7]. Strongly correlated states in compressed tBLG far from the flat-band angle were measured by Yankowitz et al.[8, 9], pointing out to an avenue to creating partially filled flat bands at higher twist angles. In all cases, hints of strong-coupling behavior appears at twist angles less than 2°. The possibility of creating magnetic structures in compressed tBLG with a larger twist angle was suggested by Ynduráin[10].

The existence of intrinsic magnetism in graphitic layers is still debated and generally related to the presence of topological defects such as zigzag edges, grain boundaries, vacancies or adatoms[11, 12], which break the sublattice symmetry and creates a magnetic moment of $1\mu_B$ per isolated $p_z$ orbital removed[13]. Hitherto, the possibility of inducing magnetism in 2D bilayer graphene without disrupting the hexagonal network has been suggested [14] and remain poorly characterized[3]. Parametrized tight-binding calculations within the Hubbard model of non-relaxed small-twist angle tBLG suggested that antiferromagnetism and spiral ferromagnetism may arise[14]. However, the uncertainty of the on-site repulsion term that eventually leads to magnetism in model Hamiltonians often yield ambiguous results. It is therefore highly desirable to clarify the conditions for observing magnetism in bilayer graphitic networks within an ab initio approach to treat realistic systems in their detailed complexity using a minimal set of tuning physical parameters.

In this paper we study the physical properties of tBLG with twist angles in the range of 5.05° to 2.0°. Theoretical evidence of the emergence of magnetism under hydrostatic pressure and doping is provided, and the tunability of the bilayers’ magnetic properties considered. We find that the transient distortions in the distribution of charge density between vdW bonded layers are overwhelmed by the enhanced hybridization of AA stacked C atoms under compressing strain, which leads to a sudden flattening of the dispersive bands and to an unbalanced occupation of the localized states. The spontaneous emergence of localized magnetic moments is analyzed by rotating systematically one of the layers, observing that magnetism is induced only within a small range of twist angles. The magnetic arrangement of the localized states is determined by subtle differences in energy with a competition between ferro- and anti-ferromagnetic ordering between moments at AA stacking zones.

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II. COMPUTATIONAL METHODS

Self-consistent calculations of the electronic structure of pristine and doped tBLGs were performed with the localized atomic-like orbital basis set of the SIESTA density functional theory (DFT) based code [15, 16]. A double-ζ basis set within the local density approximation (LDA) approach for the exchange-correlation functional was used. Although vdW functionals are known to describe accurately the interaction between the parallel layers of pristine graphene sheets [17], LDA was considered a suitable functional since the dominating effects here are the new states coupling the graphene layers upon compression and chemical modifications. Also, within the LDA, the required level of accuracy in the description of large unit cells can be obtained at an affordable computational cost, which is 10 times less expensive than van der Waals functionals [17]. Atomic positions of vdW-distance bonded bilayers were relaxed with a force tolerance of 1 meV/Å. Integration over the Brillouin zone (BZ) of the smaller tBLGs was performed using a Monkhorst sampling of $18 \times 18 \times 1$ k-points. The number of k-points used in larger cells were reduced accordingly to the length of the unit cell vector. The radial extension of the orbitals had a finite range with a kinetic energy cutoff of 50 meV to ensure a good overlap between parallel sheets. The numerical integrals were computed on a real space grid with an equivalent cutoff of 300 Ry.

III. RESULTS AND DISCUSSION

Moiré lattices are created by choosing a twist angle between two graphene layers so that a unit cell with coincidence site lattice points is created [18–20]. Commensurate angles are parameterized by an integer $i$ where the twist angle $\theta_i$ is given by $\cos \theta_i = \frac{3i^2 + 3i + 5}{3i^2 + 3i + 1}$ [6, 19]. We start by considering four tBLG geometries in which one layer of AA-bilayer graphene is rotated an angle $\theta_i$ with respect to the other layer. Twist angles $\theta_{i=6} = 5.09^\circ$, $\theta_{i=8} = 3.89^\circ$, $\theta_{i=10} = 3.15^\circ$, and $\theta_{i=16} = 2.0^\circ$ were considered. Internal coordinates of pristine and doped tBLGs separated by the vdW distance of 3.3 Å were fully relaxed. Hydrostatic pressure is simulated by reducing the separation between fully-relaxed parallel layers. Electronic and magnetic properties of compressed tBLG structures were computed with atoms at fixed positions, which is known to introduce minor changes upon additional relaxation [21]. To avoid interactions between neighboring cells in the perpendicular-to-the-plane direction, tBLGs were modeled within planes separated in $z$-direction by 33.0 Å.

Fig. 1a shows the band structure the fully relaxed $i=6$ tBLG. The two degenerate bands observed in the $\Gamma \rightarrow K \rightarrow M$ high-symmetry path of the BZ exhibit the linear dispersion of graphene and can be related to the absence of short-range correlation between layers, similarly to turbostratic bilayer graphene [22, 23]. After a rigid approach of one sheet to the other so that the vertical separation is reduced to $\Delta z = 2.7 \AA$, the massless fermion character of the bilayer vanishes, as shown in Fig. 1b. This effect is a consequence of the enhanced hybridization between layers which induces localization, while preserving band degeneracy due to the lack of symmetry breaking. This localization mechanism is a consequence of the potential introduced by the Moiré pattern and can be described by tight-binding calculations in low-twist angles [24, 25].

Additional compression reducing the interlayer distance to $\Delta z = 2.5 \AA$ leads to a completely different sce-
FIG. 2. Real-space spatial distribution around the AA stacking region of four spin configurations. a) Compressed $\theta_{i=6} = 5.09^\circ$ tBLG creates a circular distribution of unbalanced charge. b) A four-times extended unit cell (blue-line polygon) an anti-ferromagnetic ordering of magnetic moments across the AA sites is observed. c) Ferrimagnetic ordering of magnetic moments in a hexagonal supercell containing three- AA-sites (blue-line polygon). Dashed lines is a guide to the eye. d) Application of an electric field perpendicular to the tBLG plane leads to a local anti-ferromagnetic ordering distributed circularly around the AA site. Isosurfaces correspond to a charge density of $\sim 5 \times 10^{-3} \text{e}^{-}/\text{Å}^3$.

The dispersive twofold-degenerate bands accommodating two electrons apiece collapse in two groups (one for each spin quantum number) of four nearly flat states (see Fig.1c). Minority and majority spin flat-bands are completely empty and filled respectively. A small fraction of charge that is held in the dispersive bands at lower energies prevents the bilayer from exhibiting half-metallicity. The tBLG becomes magnetic and a total magnetic moment of 3.91 $\mu_B$ emerges centered on the AA stacking region, exhibiting a ferromagnetic ordering between neighboring atoms and a spatial extension of $\sim 1\text{Å}$, as displayed in Fig.2a. Smaller distances between parallel virtual planes were observed to introduce substantial variations in the total energy and magnetic moments of the bilayers. A configuration with a magnetic moment of 3.7$\mu_B$ was obtained in a unit cell with a vertical separation of 25 Å between repeated images.

To observe a possible AFM ordering across AA stacked regions, additional unit cells must be included in the simulation. Spin-polarized calculations on tBLGs containing four $i=6$ unit cells (2032 atoms) were conducted considering both restricted and unrestricted values of the total magnetic moment of the supercell. The result is shown in Fig2b, where a network of magnetic moments exhibits stripes aligned ferromagnetically but with an anti-ferromagnetic ordering across $\pm 60^\circ$ direction. The structure factor of this configuration would give one Bragg peak out of the three $M$ points of the BZ. This so-called 'single-Q' state with alternating magnetic oscillations in two directions was obtained by fixing the supercell magnetic moment to 0. The formation energy of this configuration is 1 meV lower than a configuration with 16$\mu_B$, namely $4\mu_B$ per AA site. Multiple other metastable configurations were obtained conducting restricted and unrestricted calculations, which yield spin configurations of 12 and 10.75 $\mu_B$, both with higher formation energies.

Within a colinear model, a more conclusive analysis involves the inspection of a hexagonal lattice composed of three AA stacking regions. The resulting supercell (1524 atoms) exhibits a ferrimagnetic ordering where two AA regions are anti-ferromagnetically aligned with the third one, as displayed in Fig.2c. The total magnetic moment of this configuration is 3.77 $\mu_B$, and its formation energy is 9 meV lower than a configuration with all spins aligned ferromagnetically. The total magnetic moment of the latter is 11.8 $\mu_B$, namely 3.9 $\mu_B$ per AA site, which recovers the result of Fig.1c. Considering that in the supercell containing three AA regions the magnetic moments are allowed to interact with more degrees of freedom, and due to the exchange-correlation energy favoring the ferrimagnetic alignment, one can conclude that the alignment of Fig.2c is preferred.

Within the anti-ferromagnetic Heisenberg model (in which neighboring spins can antialign with any possible angle) tBLG is ripe for frustration owing to the triangular arrangement of neighboring magnetic moments. Not existing a physical way to maximally satisfy all three bonds
in the triangular lattice simultaneously, a possible solution would entail a non-collinear spin alignment where spins would form a triangular formation at 120°. This possibility is typical of materials hosting highly localized magnetic moments on d- or f-orbitals and less likely on delocalized C atom p-orbitals. Without an ad hoc on-site Coulomb repulsion term added in the DFT calculations, non-collinearity or spirals were not observed[14, 26].

A magnetic moment at an AA region can be slightly modulated by engineering the tBLG with biaxial strain, which induces a symmetric lattice deformation without breaking the system symmetry. Increasing the length of the hexagonal unit cell vector by 3%, an enhanced chemical potential misalignment for both spin distributions is obtained. Fig.1d shows that the two majority-spin bands that were partially filled become fully filled, while two of the flat states become partially empty. In the minority spin channel, one of the flat bands is slightly populated receiving the transferred charge. As a result the tBLG reduces its net magnetic moment to 3.85 $\mu_B$.

Application of an electric field to bilayer AB graphene is a well-established method for opening an electronic band gap[27]. Cao et al. [4] proposed the application of perpendicular electric fields by means of differential gating to tune interactions in magic-angle tBLG. Here, it was observed that local ferromagnetic ordering at an AA site can be further tuned by applying a displacement field of 0.5 V/Å perpendicularly to the tBLG plane. The total magnetic moment decreases to 0.5$\mu_B$ by equalizing the charge distribution across electronic states of both spin channels. Both the minority and majority spins exhibit at Fermi level (see Fig. 1e) some of the valence bands partially filled and one fully empty, but with a misalignment in the chemical potential. Fig.2d shows the local magnetic moments extended anti-ferromagnetically at in-plane first-neighboring C atoms over the vicinity of the AA stacking region. The local moments align ferromagnetically with the closest atoms in the opposite layer. Increasing the electric field up to 1 V/Å, or decreasing it down to almost zero slightly modifies the total magnetic moment. Removing completely the external field leaves the bilayer in the local anti-ferromagnetic configuration with a total magnetic moment of 0.4$\mu_B$, and a formation energy 20 meV above the ferromagnetic configuration discussed above (Fig.2a).

Decreasing the twist angle to $\theta = 3.89^\circ$, the twofold degenerate bands of the paramagnetic vdW-bonded tBLG collapse at the Fermi level in four nearly flat bands of identical shape across the two spin channels when the layers are separated by 2.5Å. An energy misalignment of some meV yields a net magnetic moment of 2.5$\mu_B$ (see Fig.3a). Note the similarity of the bands at Fermi level with those of ordinary AB stacked bilayer graphene [22], namely only two bands touch each other at $K$ point with non-linear dispersion. The spatial distribution of the magnetic moment is similar to the one shown for $i=6$ tBLG in Fig.2a. Biaxial strain equivalent to increasing the unit cell vector in a 3% modulates the electronic states of both charge distributions and reduces the magnetic moment to 2.0$\mu_B$ (Fig.3b).

Interestingly, a slight decrease of the twist angle to $\theta = 3.15^\circ$ in compressed tBLG leads to a paramagnetic spin distribution with no band misalignment. Reducing the interlayer distance to $\Delta z = 2.5\text{Å}$, the dispersion of the vdW-bonded bilayer bands is reduced from 0.5 eV to $\sim 0.15\text{ eV}$ (Fig.3b). No disruption of the bands other than spanning a reduced energy range and some hybridization with flat bands in the zone center is observed. A linear crossing is observed at $K$ point and a set of two bonding and antibonding flat states emerges at $\pm 60$ meV. Therefore no magnetic moment is created upon compression of an $i=10$ tBLG.

For the same interlayer distance of 2.5Å, the electronic spectrum of a smaller twisted-angle bilayer such as $\theta = 2.0^\circ$ (3268 atoms) exhibits no linear dispersion at Fermi level and a zero net magnetic moment. Considering that additional calculations on $\theta = 6.0^\circ$ showed that hydrostatic pressure causes the apparition of magnetism, it can be concluded that spontaneous magnetism in compressed tBLG arises for relatively large twist angles where $\theta > 10^\circ$ is a lower limit.

Cao et al. [4] proposed electrostatic gating for changing the charge carrier density and induce superconductor-metal transition in magic-angle tBLG. Substitutional B and N chemical doping is an efficient method to introduce hole and electrons in graphitic layers, at the expense of creating defect sites that may disrupt the local geometry of the sheets. Fig.4 shows the band diagrams of a $i=6$ tBLG with one B/N atom at a position far from the AA stacked C atoms. Geometries were fully relaxed prior to decreasing the interlayer distance. Across the two spin channels, both types of doping atoms generate an identical distribution of electronic states but with different energy alignment with respect to the Fermi level. B doping removes one electron out of the bilayer and decreases

![Figure 3: Spin-resolved band diagrams of tBLG with a vertical separation of the graphene sheets of 2.5Å. a) $\theta = 3.89^\circ$ exhibits a total magnetic moment of 2.5$\mu_B$. Both b) $\theta = 3.15^\circ$ and c) $\theta = 2.0^\circ$ exhibit a paramagnetic configuration.](image-url)
the total magnetic moment to $3.28 \mu_B$, while adding some dispersion to the flat valence bands. Interestingly, despite the donor behavior of an N atom, the magnetic moment of the bilayer decreases to $3.0 \mu_B$, enhances the localized character of the valence bands, and turns the bilayer into a half-metal, with one spin channel metallic while the other spin channel features a 40 meV insulating band gap. The real-space representation of the unbalanced charge distribution show two different scenarios. Single N atom doping changes the local ferromagnetic ordering of the magnetic moment to anti-ferromagnetic. Fig.4c shows that, even though the foreign atom sits far from the AA stacking region, the magnetic moments remain centered at the AA stacked C atoms with a triangular shape Magnetic moments of both types of doping have a spatial extension similar to the one of pristine tBLG in Fig2a, and are practically insensitive to external electric fields.

Empirical-free DFT-based calculations of systems containing hundreds of atoms requires one to assume some approximations that might compromise the accuracy of the results. An insufficient number of k-points may introduce a bias in the Fermi level alignment and, therefore, in the exact value of the magnetic moment on spin-unrestricted calculations. Also, a reduced basis set in the SIESTA code calculation may describe poorly the C atoms orbital hybridization at the AA stacking region. Results presented above for pristine tBLG were reproduced with the more precise double-\(\zeta\) polarized basis set and no significant differences were found, with the exception of the magnetic moment of compressed $i = 6$ tBLG that was estimated in $2.8 \mu_B$. The all-spin-up three-AA site $i = 6$ tBLG computed with the same basis set yields an average magnetic moment of $3.6 \mu_B$, close to the $3.9 \mu_B$ obtained above.

An analysis of the magnetic properties of tBLG flakes was conducted to obtain a description of isolated magnetic moments, namely without possible coupling with neighboring moments in virtual cells, and to avoid a possible lack of accuracy derived from an insufficient sampling of the BZ. \(\Gamma\)-point calculations of isolated AA stacked regions were conducted on $\theta_{i=6}$ and $\theta_{i=10}$ tBLGs created by repeating two times the unit cell along each in-plane cell vectors. Armchair edges were terminated with H atoms to remove chemically reactive dangling bonds. Only H atoms were relaxed in the pristine and doped bilayer configurations.

Spin-unrestricted calculations on a $i=6$ tBLG flake yield a total magnetic moment of $3.0 \mu_B$ whose spatial extension increases with respect to the periodic arrangement to $\sim 1.5 \AA$. Fig.5a shows the circular arrangement of the magnetic moment in the vicinity of the central AA region with a six-vertex star shape ending as approaching the neighboring AA regions at the flake edges. Substitution of a C atom at the center of the flake with a B atom (one electron less than C) reduces the magnetic moment to $2.0 \mu_B$. The B atom and its 2nd and 4th neighboring C atoms are anti-ferromagnetically aligned to the rest of the network atoms, which contributes to changing the spatial extension of the magnetic moment to a three-vertex star shape (Fig5b). A second B atom in the same layer at 4th neighboring position yields a total magnetic moment of $2.1 \mu_B$, whereas if it is in substitution of a C atom in the layer below (14 meV lower in the formation energy) the moment is of $1.0 \mu_B$.

One should expect that if doping with an acceptor atoms reduces the magnetic moment of the bilayer flake in $1 \mu_B$, doping with a donor N atom should have the opposite effect. However, substitution with an N atom at the AA site, and additional substitution with a second atom at 4th neighboring position, the same total magnetic moment as in B doping is obtained. A weak charge of opposite sign with ferromagnetic alignment between the N atom and its 4th nearest neighbors barely modifies the shape of the unbalanced charge distribution around the defect with respect to the pristine configuration (see Fig.5c). A $i=10$ tBLG, that in the periodic configuration was paramagnetic, exhibits a $1 \mu_B$ magnetic moment. The AA region is isolated in a bilayer flake where edges were cut back so only one AA site is present. Fig.5d shows the distribution of the magnetic moment over a flake demonstrating that the absence of periodicity con-
FIG. 5. H atom-terminated flakes of compressed twisted bilayer graphene show that magnetism arises in non-periodic systems. Flakes are created by repeating four unit cells of \(i=6\) and \(i=10\) twisted bilayers. a) For a rotation angle of \(\theta_{i=6}=5.09^\circ\) the spatial extension is larger than for a periodic system. Doping with B atoms b) change the shape of the magnetic moment to triangular. N doping c) reduces the spatial extension for the same isosurface of \(10^{-3}\) e\(^{-}\)/\(\AA^3\). d) shows the unbalanced charge distribution for \(\theta_{i=10}=3.15^\circ\).

tributes to the modulation of magnetism in tBLG.

IV. CONCLUSIONS

Combining uniaxial vertical pressure with precise twist of the graphene sheets, dynamic band-structure engineering in graphene Moiré superlattices is possible, demonstrating that tBLG is a rich ground for hosting emergent flat-band magnetism and half-metallicity. The multiple degeneracies of the single-particle energy spectrum of tBLG that are due to inherent symmetries are broken when hydrostatic pressure enhances electronic localization at AA stacking sites and creates magnetic ordered states. A hexagonal lattice of AA sites has a preference for ferromagnetic ordering hosting an anti-ferromagnetic ordered magnetic moment in the center. In the light of the small differences in energy observed (9 meV of exchange-correlation energy with respect to the ferromagnetically aligned configuration), it would be adventurous to select one spin ordering over another to remove the observed practical degeneracy of the system’s ground state.

Even though the magnetic state of a tBLG can be sensitive to the accuracy of the simulation parameters (i.e., extension of the basis set, orbitals’ energy cutoff, sampling of the BZ, etc), corrections to conducted DFT calculations, without particular assumptions about interactions among the charge carriers, is not expected to modify the ground state towards an anti-ferromagnetic order. Experimental observation are expected to shed light on the long-range ferromagnetic ordering of tBLG magnetic states. A critical conclusion, though, leads us to note that, owing to accuracy limitations of DFT calculations with large number of atoms, this result must be taken cautiously and the all-up spin configuration must not be totally discarded as the ground state of the system.

The artificial injection of electrons into the sheets of experimental realizations was mimicked here in compressed tBLG by chemical doping with B and N atoms which modulates the magnetic moments and induces flat-band half-metallicity. Time-reversal symmetry breaking with an external electric field allows for local ferro- to anti-ferromagnetic ordering transition of spatially localized states of periodic systems, similarly to N atom doping. The vanishing bandwidth (flat states) of periodic magnetic arrangements was reproduced on finite-size bilayer flakes resulting on different magnetic moments depending on the twist angle. The emergence of magnetism on compressed tBLG is not related directly to the periodicity of the system but to the enhanced hybridization of the stacked C atoms.

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