Hybrid super-lattices of graphene and hexagonal boron nitride: Ferro-magnetic semiconductor at room temperature

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Carbon(C) doped hexagonal boron nitride(hBN) has been reported to be ferromagnetic at room temperature. Substitution by C in hBN has been reported to preferably form islands of graphene. We have developed a mechanistic understanding of ferro-magnetism with graphene islands in hBN from first principles and propose a refinement to the tight-binding framework to access the observed scenarios. We find a general property, that bipartite lattices like hBN, where the sub-lattices differ in on-site energies, inherently mediate anti-ferromagnetic order between neighbouring local magnetic moments irrespective of whether they are in same or different sub-lattices, unlike in graphene. The mechanism is rooted at spatial separation of lone-pairs (of nitrogen(N)) and back transferred electrons (on boron(B)) of opposite spins due to Coulomb repulsion, and naturally implies a net non-zero moment with odd number of local moments. Accordingly, we propose a class of ferri-magnetically ordered inter-penetrating super-lattices of magnetic graphene islands in hBN, which can be chosen to be a ferromagnetic semiconductor or a half-metal, and retain a net non-zero magnetic moment at room temperature.

I. INTRODUCTION

Possibility of ferro-magnetism exclusively due to electrons in 2p orbitals, particularly in the functionalized three coordinated bipartite networks [1, 2] of boron(B), carbon(C) and nitrogen(N), has opened up a new direction in pursuit of magnetic materials, which are lighter and thinner than those made of traditional metals, and thus also have large spin relaxation time due to weaker spin-orbit coupling, and yet magnetically as well as structurally stable at room temperature. Magnetism in half-filled bipartite systems [3, 4] is primarily sourced at functionalizations which impact the two sub-lattices unequally, leading to ferri-magnetic (FeM) order between them, implying a net non-zero magnetic moment, accompanied by finite density of states (DOS) for the minority spin at Fermi energy. Many such scenarios of functionalization of graphene(Gr), [5, 6] particularly in ribbons [7, 8] and finite segments with magnetic edges [9, 12], have been widely proposed in the last decade or so. Howver, presence of finite DOS near Fermi energy due to the inherent semimetallic nature of graphene and spurious edge states, tend to undermine the effects of functionalization, unless precisely cut into ribbons of systematic band gap, which poses its own experimental challenge. On the other hand Hexagonal boron nitride(hBN), being a wide band gap due to difference in electronegativity of the two sub-lattices, would not interfere with transfer of charge involving the spin polarized DOS of graphene islands embedded in it. Magnetic Gr-hBN hybrids that have been wide proposed [13, 14] as well in last few years as magnetic material, alongside reports of success in synthesis of robust hybrid structures which can facilitate magnetism [20, 23] particularly at the Gr-hBN interfaces. Recent experimental finding [24] of ferro-magnetism at room temperature in C doped hBN has rekindled efforts in this direction. However, this result, along with the fact that substitution by C in hBN forms arrays of graphenic islands(Gr-islands) in hBN [22, 23], poses a new question: how magnetic order between two Gr-islands propagates through hBN and how does it lead to the observed FM. Answering these questions and making systematic proposals for Gr-hBN hybrid ferro-magnets and half-metals is the key motivation for our work.

Triangular Gr-islands offer the largest magnetic moments (Lieb’s theorem), since the zigzag edges in all its sides belong to the same sublattice [10]. FM ordering of free standing triangular Gr-islands through odd members C chain has been shown possible due to the nearest neighbour AFM ordering of the bridge sites [11, 12] between Gr-islands. Triangular graphene islands with zigzag edges embedded in hBN is expected to be a stable motif [23, 25, 26] for devices. However, neighbouring magnetic Gr-islands embedded in hBN have been reported to prefer anti-ferromagnetic (AFM) order [27, 28], in contrast to the observed [24] ferromagnetism in C doped hBN. Thus the true nature of interaction between of localised magnetic moments in hBN needed to be thoroughly understood to make a systematic progress in this direction. Accordingly, we began our work with deriving an atomically resolved understanding of the mechanism of mediation of AFM order by -B-N- pathway connecting two Gr-islands, and subsequently show how to switch the order to FM, which leads to systematic proposals of half-metal or FM semiconductor possible at room temperature, besides offering explanations to existing reports [18, 24] of ferro-magnetism in these systems. Our study is based on analysis of spin polarized electronic structures calculated from first principles [29], as well as within the mean field approximation of Hubbard model [4] (MFH) in a tight-binding (TB) framework. Effective strength of exchange interaction (J) and transition temperatures (T) are estimated within the Ising model of
spin Hamiltonians \[^{[30]}\]. Orbital resolved understanding of the underlying mechanisms have been developed based on Wannier functions \[^{[31]}\], which are spatially localized linear combination of kohn-Sham eigen states, and are known to unambiguously divide the charge density into bonding and atomic orbitals.

### II. COMPUTATIONAL DETAILS

Equilibrium configurations and spin polarized energetics are calculated within the framework of density functional theory (DFT) in plane wave basis \[^{[32]}\], using ultrasoft pseudopotentials \[^{[33]}\] and gradient corrected Perdew-Burke-Ernzerhof (PBE) exchange-correlation \[^{[34]}\] functional. PBE results have been refined using the hybrid HSE \[^{[32]}\] approximation of exchange-correlation for better representation of exchange-interaction. However, given the computationally intensive nature of HSE calculations, only a representative variety of calculations have been refined using HSE. Total energies minimized using the BFGS \[^{[36]}\] scheme, are converged with plane-wave cutoff over 800 eV, k-mesh equivalent to 30×30 for a hBN primitive cell and forces per atom less than 10⁻⁴ Rydberg/Bohr. Wannier functions are constructed \[^{[37]}\] by maximally aligning the Kohn-Sham states with a template of \(2p_z\) atomic orbitals on C and N atoms and bonding orbitals between nearest neighbours. Electronic structure of \(2p_z\) electrons has been calculated using MFH-TB, wherein \(H_{MF} = \sum_{i,s} \varepsilon_i c_i^{\dagger} c_i + \sum_{< i, j>, \sigma} t_{ij} c_i^{\dagger} c_j + \sum_{i, \sigma} U_i n_i n_{i'}\), where \(\varepsilon_i\) are the onsite energies \((\varepsilon_B, \varepsilon_N, \varepsilon_C)\), \(t_{ij}\) are nearest-neighbour hopping parameters \((t_{CC}, t_{BN}, t_{CN}, t_{CB})\) and \(U(U_B = U_N = U_C)\) are the strength of on-site Coulomb repulsion. Parameters have been obtained by comparing DOS calculated using MFH-TB and DFT, and are in good agreement with reported values \[^{[39]}\].

### III. RESULTS AND DISCUSSIONS

We begin by considering \[^{[Fig.1(a,e)]}\] two islands separated by a single site (N or B), in the middle of a large hydrogen passivated hBN chunk, as well as constituting a honeycomb super-lattices \[^{[Fig.1(b,f)]}\] in an infinite hBN sheet. We considered two type of Gr-islands: 3B1N (C4a) and 3N1B (C4b), where \(m\)B\(n\)N implies substitution of \(m\) and \(n\) numbers of B and N atoms by C respectively. Each of the islands thus host a net magnetic moment of \(2(=3-1)\) \(\mu_B\) \[^{[3]}\] owing to different coverages of the B and N sub-lattices. In agreement with previous reports \[^{[27, 28]}\], we also find AFM ordering of sub-nanometer length-scale between neighbouring Gr-islands. Effective J estimated using HSE approximation of exchange correlation confirms that -B-N- zigzag connectivity between neighbouring Gr-islands favour their AFM ordering, more than that due to -B-N- armchair connectivity \[^{[27]}\]. Confirmation of AFM order by HSE approximation is our basis to accept it as the true order of the ground state. Strength of AFM order, as measured by J between the Gr-islands, is found more if mediated by B than by N, and reduces

![FIG. 1: LSDA Spin-density of a pair of C4a(3B1N) islands at their closest approach \((d = 0)\) embedded in (a): a finite hBN chunk, and (e): as a part of a honeycomb super-lattices in hBN sheet. Their C4b(3N1B) counterparts are shown in (b) and (f) respectively. Planar projection of Wannier functions representing \(2p_z\) orbital of C along (c): C-N and (g): C-B bonds for honeycomb super-lattices made of C4a and C4b islands respectively. Spin-resolved Wannier function of \(2p_z\) orbital of (d): the bridging N atoms between C4b islands and (h): of the outer C atoms of the C4a islands connected through a B atom](image)

![FIG. 2: (a): Schematic representation of spin-dependent hopping mechanism. Contour plot of total magnetization of the ground state calculated as function of \(t'(t)\) and onsite energy \(E_{on-site}\) for a pair of (b): C4a(3B1N) and (c): C4b(3N1B) islands with \(d = 0\) (closest approach of identical islands) in a finite hBN patch at three different U values(eV). For U=4.0eV and U=2.0eV the FM-AFM boundary is shown by black dotted line.](image)
Notably, spin selective back transfer in effect indicates spin dependent hopping of electrons within a tight-binding (TB) framework. We resort to MFH-TB model to test the relevance of spin dependent hopping in determining the correct magnetic ordering of the ground state. Spatial separation of spins suggest symmetric opposite displacement of orbitals of opposite spins away from the host atom, as depicted in the schematic model[Fig.2(a)], which implies similar increase in the orbital energies (on-site term) for both the spins. Accordingly, we consider a pair of C4 defects in close proximity (d=0) in the middle of a large hBN chunk whose edges are sufficiently away from the C4 islands, and calculate AFM, FM and non-magnetic(NM) ground states as a function of spin-asymmetry of hopping $\Delta t = t_\uparrow - t_\downarrow$ applied to all the (B/N)-C bonds around the C4 islands, and on-site term of the (B/N) atoms connected to the C4 islands, and look for the true magnetic ordering of the ground state by comparing total energies calculated in FM, AFM and NM conditions. We chose an isolated hBN chunk in order to avoid the dependence of the magnetic ordering on the choice of periodic unit-cell. As evident from the TB-MFH based phase diagram shown in Fig.2(b,c), the ground state with spin independent hopping and standard parameters[39], is FM ordered with total 4\(\mu_B\) magnetic moment due to the two FM ordered C4 islands, in disagreement to DFT results. The AFM ordering of the ground state, emerges only beyond a threshold value of rapidly beyond $d = 3$, where $(2d + 1)$ is the total number of B and N atoms in the shortest -B-N- pathway connecting the islands. Spin densities in the vicinity of the intermediate B(N) atom between two C4b(C4a) islands suggest[Fig.1(e,f,a,b)] spatial separation of electrons of two spins on opposite sides of the B(N) atom towards the Gr-islands on two sides. To trace the origin of this spin separation we looked at the spatially localized Wannier functions[37] representing the $2p_z$ orbitals of C and N. As evident in Fig.1(d), the two unpaired $2p_z$ orbitals of N with opposite spins extend spatially in opposite directions, resulting into back transfers of opposite spins to the C atoms on its two sides. Similarly on B atom between two C4b islands[Fig.1(h)], the back transferred electrons from the $2p_z$ orbitals of the two neighbouring C atoms are of opposite spins, implying spin separation about B as observed in the spin-densities[Fig.1(e,f)]. Furthermore, Fig.1(c,g) imply that the back transfer from C to B is more than that to N, which is consistent with the fact that the effective $J$ is more for B mediated AFM than N mediated AFM. These observations appear to imply connection between the spin separation of lone pairs and back transferred electrons in the -B-N- pathway, to the observed AFM order of the Gr-islands it connects.

FIG. 3: Schematic model of (a): AFM ordered C4a(3B1N) islands with spin-dependent hopping. (b): Inherent AFM order between two local moment shown by C. (c): FM ordered C4a(3B1N) islands due to the extra local moment(C) at B site between the C4a islands. LSDA spin density plot of honeycomb super-lattice of C4a islands with $d = 1$ in (c): absence and (d): presence of C in the intermediate B sites. Wannier function representing the $2p_z$ orbitals of (e): the two N atoms back traiferring to the C in the middle, and (f): of the C atom itself, in the -N-C-N- zigzag pathway between C4a islands. (g): Occupancy of spin due to $2p_z$ electrons at sites along the C-N-C-N-C zigzag path due -N-C-N- connectivity between C4a islands calculated using PBE, HSE and from MFH at U=2.0 eV and 6.0 eV.

FIG. 4: (a):Representation of inter-penetrating C4a-X honeycomb-Kagome super-lattices for various intermediated substitution by C at X (B or N) sites for $d = 3$. Energy difference ($E_{FM} - E_{AFM}$) for different X different separations of C4a islands.(b):$d=1$, (c):$d=2$, (d):$d=3$ and (e):$d=4$. $E_{FM} - E_{AFM} < 0$ implies FM order in hexagonal super-lattice.
$\Delta t$, and the threshold $\Delta t$ itself decreases with decreasing $U$ as well as increase in on-site term. Therefore with standard on-site terms and $U$ for B, C and N, spin dependent hopping is crucial for the ground state to have AFM ordering of Gr-islands, in agreement with DFT result. The fact that the $\Delta t$ threshold decreases with decreasing $U$, reiterates the role of $U$ at B and N sites in mediating the AFM order. In agreement with the fact the B mediated AFM is stronger than N mediated AFM, the onset of AFM order in the ground state indeed occurs at a lesser threshold for $\Delta t$ in case of B mediated AFM. Fig(3a)], schematically summarizes the mechanism of propagation of AFM order through -B-N- zigzag pathway between Gr-islands. This mechanism thus implies a generic refinement of tight binding model for bipartite lattices if the sub-lattices have different on-site energies. In fact, the mechanism point to a general property, that magnetic order mediated by such bipartite lattices between two neighbouring magnetic local moments, would inherently be anti-ferromagnetic irrespective of whether the local moments are located in the same of different sub-lattices, as represented in Fig(3b). Notably, this is different than in graphene, where the nature of magnetic interaction depends on whether the local moments are in the same or different sub-lattices. In hBN, interaction between local moments weaken if the connecting -B-N- pathways allow an equal number of B and N atoms implying an integer number of B-N bonds, since along the bonds back transfer of electrons of both spins can occur on similar footing to reduce kinetic energy. This is also the reason why -B-N- armchair connectivity is less effective than zigzag connectivity in mediation of AFM order.

The mechanism[Fig3(a)] also readily suggests that the AFM order can be switched to FM if an unpaired electron is present in the pathway, as proposed in Fig(3c)]. Such an unpaired electron can arise from a single substitution by C, or from another magnetic Gr island, on or close to the -B-N- pathway between the neighboring Gr-islands of the honeycomb lattice. Spin density in Fig3(e), compared to that in Fig3(d) without the intermediate C between the two C4 islands, indeed clearly confirms the anticipation of FM order of Gr-islands(C4a) connected by N-C-N- zigzag pathway. Facilitation of FM order due to spin separation of the N lone pairs is evident in Fig3(f), where the two N atoms on two sides of C is seen to back transfer electrons of same spin (spin1) to C due to presence of a $2p_z$ electron of spin2 at C[Fig3(g)], which appears to open a half-metallic bridge connecting the two Gr-islands. Hybrid HSE exchange correlation functional increases the effective J beyond its PBE value, implying robustness of the observed FM order in the ground state. Since Hubbard Hamiltonian in effect evolves into a spin exchange Hamiltonian at high U, it was possible to match PBE and HSE spin densities along the -N-C-N pathway [Fig3(h)] with TB-MFH spin densities at $U=2.0$ eV and $U=6.0$ eV respectively with $\Delta t$ along (N/B)-C bonds as parameter, thus confirming the central role of of nonzero $\Delta t$ in rationalizing the FM ordering of Gr-islands mediated -N-C-N- pathway. Since even membered -B-N- pathway is expected to suppress mediation of magnetic order, the generalization of the -N-C-N- pathway for strong FM ordering is -(2d+1 B,N)-C-(2d+1 B,N)-. These results suggest that in general an odd number of magnetic Gr-islands (single C atom(C1) or patch(Cm)), if located within nanometers of each other in hBN, can be ferri-magnetically ordered amounting to a net magnetic moment, which is what might have been experimentally observed.

As evident in Fig4a), the Gr-islands(C4), and the sites(X) of the unpaired electron, which can be a B or a N site, describe a system of two inter-penetrating super-lattices: one being the honeycomb super-lattice made by the C4 islands, while the other one is a twisted Kagome super-lattice made by X sites. The -B-C-B- or -N-C-N- mediated FM order of Gr-islands suggest a ferrimagnetic order between the super-lattices. We now survey the variation in strength of the FM order in the hexagonal super-lattice as a function of location of the X site,
which determines the twist of the Kagome lattice, as depicted in Fig.4(a). The energy difference $E_{FM} - E_{AFM}$ plotted in Fig.4(b) for C4a-X honeycomb-Kagome (H-K) super-lattices, suggest a systematic emergence of strong FM ordering in the hexagonal super-lattice, if the X site allow an odd membered -B-N- pathway connecting the Gr-islands. As evident in Fig.4(b), this is possible only with X:B(N) for the honeycomb lattice made of C4a(b). That even membered -B-N- pathway suppress propagation of magnetic order, is reiterated by the observation that strong FM order between C4a islands occurs only for X:B, since such X connects to nearest C4a island through odd membered -B-N- pathway. X should also be typically within 7Å from the shortest -B-N- zigzag pathway connecting two neighbouring C4a islands. Similar results exist for C4b islands as well as bigger C9(6B3N) islands in the hexagonal super-lattice. In fact, these results are valid for a general Cm-Cn H-K super-lattices where Cm and Cn are two magnetic Gr-islands constituting the two lattices, and can be chosen to be same of dissimilar. The corresponding $T_C$ estimated as $2J/ln(2+\sqrt{3})$, where $-6J = (E_{FM} - E_{AFM})$, indicates existence of FM order at room temperature. Fig.4(b) also suggests a d dependence of strength of the FM order, which can be understood in terms of the competition between the inherent AFM order of the Gr-islands in the honeycomb lattice and the FM order induced by the Kagome lattice of X sites. With increasing d the strength of the AFM order reduces, leading to a peak of the FM order which reduces with further increase of d beyond 4, implying in effect a length-scale of nanometer.

FM ordering in the honeycomb super-lattice leads to FM-semiconducting(FM-Sc) [Fig.5(b)] to half-metallic [Fig.5(a)] phases depending on X being a B site or an N site in C4a-X H-K super-lattices. Emergence of FM-Sc or half-metallic phases can be understood in terms of the difference in their localization owing to their different size(C4 and X) and distribution(honeycomb and Kagome). Fig.5(e,f) and Fig.5(c,d) suggests that the properties of the C4b-X:(B,N) and C4a-X:(N,B) H-K super-lattices will be similar. Fig.5(c) and (d) explains emergence of half-metallic and FM-Sc phases due to X:N and X:B in agreement with DFT results shown in Fig.5(a) and (b). Fig.5(c) and (f) explains emergence of half-metallic windows at Fermi energies due to X:N and X:B respectively, and suggests that the key to make the half metal window broader is to make spins at X more delocalized. This is possible if either the X sites are closer due to a twisted Kagome X super-lattice, or the X sites are replaced by Gr-islands, as evident in the DOS of C9-C4 H-K super-lattices [Fig.5(g)] calculated from first principles.

IV. CONCLUSION

To conclude, we show that Coulomb repulsion driven spatial separation of lone-pairs and back transferred electrons of opposite spins on N and B, to be the primary mechanism for the anti-ferromagnetic order mediated by -B-N- pathway between neighbouring magnetic Gr-islands in hexagonal boron nitride. The mechanism suggests a spin dependent hopping with increasing U to access the anti-ferromagnetic ground state suggested from first principles (PBE,HSE). The mediated magnetic order becomes ferromagnetic if an odd number of unpaired spin interjects the -B-N- pathway, implying in general a finite net magnetic magnetic moment due to odd number of magnetic islands in proximity. An inter-penetrating system of honeycomb and twisted Kagome super-lattices of magnetic Gr-islands in hBN has been proposed, wherein, the two ferri-magnetically ordered super-lattices should retain a net non-zero magnetic moment at room temperature, besides constituting a ferromagnetic semiconductor or a half-metal depending on the nature of Gr-islands in the two lattices.

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