





Resonant magnetic proximity hot spots in Co/hBN/graphene

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(Received 12 January 2026; revised 8 June 2026; accepted 10 June 2026; published 23 June 2026)

Magnetic proximity effects in Co/hBN/graphene heterostructures are systematically analyzed via first-principles calculations, demonstrating a pronounced localized spatial variation of the induced spin polarization of graphene's Dirac states. The proximity-induced exchange coupling, magnetic moments, and tunneling spin polarization (TSP) are shown to depend sensitively on the atomic registry at the interfaces. We analyze more than 20 distinct stackings—including high- and low-symmetry configurations—and reveal that the spin splittings of graphene's Dirac bands span a wide range from 1 to 100 meV, depending on the local hybridization of Co d_{z^2} , hBN p_z , and graphene p_z orbitals. The strongest proximity effects emerge at geometric resonances, or “proximity hot spots”, where the three orbital states overlap maximally. The local spin polarization also depends sensitively on energy: Dirac states aligned with resonant Co orbitals experience the most pronounced exchange interaction. At these energies, the pseudospin Hamiltonian description of magnetic proximity effects breaks down. Outside these resonances, the pseudospin picture is restored. Our findings highlight the intrinsically local nature of proximity effects, governed by the spectral resonance and interlayer wave function overlap. We further quantify how additional hBN layers, interlayer twist, and multilayer graphene modify the proximity exchange and TSP, offering microscopic insight for designing spintronic van der Waals heterostructures with engineered interfaces and optimized spin transport.

DOI: [10.1103/PhysRevB.113.235142](https://doi.org/10.1103/PhysRevB.113.235142)

I. INTRODUCTION

Spintronics aims to utilize the spin degree of freedom of electrons in addition to their charge, enabling novel paradigms in information storage, processing, and transport with potentially lower energy consumption and higher operational speed [1–3]. Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDCs), are particularly promising for spintronic applications due to their high mobility, tunable band structures, and the ability to form van der Waals (vdW) heterostructures. However, most pristine 2D materials lack intrinsic magnetism or significant spin-orbit coupling (SOC), which are essential for active spin control. As such, an important research avenue involves engineering spin-dependent phenomena in 2D systems via proximity effects, i.e., by placing them in contact with functional materials such as ferromagnets or materials with strong SOC [4].

This interfacial engineering enables magnetic and spin-orbit interactions to propagate from substrates into adjacent 2D layers. The beauty of vdW engineering lies in the fact that spin interactions can be transferred without direct chemical bonding or crystal structure modification. Thus, the *proximity-induced (magnetic) exchange interaction* endows graphene with magnetism, when it is placed on ferromagnetic metals through insulating barriers such as hexagonal boron nitride (hBN) [5–7]. Indeed, first-principles calculations predict proximity-induced spin splittings in the graphene Dirac bands

on the order of tens of meV [5], which has been corroborated experimentally by nonlocal spin transport measurements and tunneling magnetoresistance [8]. These proximity-induced phenomena are key to enabling efficient spin injection and manipulation in 2D materials, and they form the basis for a new generation of vdW spin valves, magnetic tunnel junctions, and spin transistors.

Among the tunable parameters of 2D heterostructures, the twist angle between adjacent layers plays a key role, giving rise to moiré patterns and allowing control over interlayer coupling and proximity effects. For instance, it has been theoretically predicted that twisting graphene on a $\text{Cr}_2\text{Ge}_2\text{Te}_6$ (CGT) substrate can reverse the sign of the proximity exchange interaction [9]. Similarly, in TMDC/CrI₃ heterostructures, the valley splitting can be tuned by more than an order of magnitude via twisting, which directly modulates the orbital hybridization at the interface [10]. These findings point to the importance of local atomic arrangements in determining proximity-induced properties.

In this work, we use density functional theory to study how the proximity-induced exchange coupling varies locally in Co/hBN/graphene heterostructures. These stacks are commonly used in spin-injection devices—both in conventional lateral geometries [4,11,12] and, more recently, in one-dimensional edge-contact setups [13]—as well as in magnetic tunnel junctions [14]. Previous theory [5,15] has shown that graphene can acquire a sizable (10 meV) exchange field from cobalt even through one or two layers of hBN, due to the alignment of Co d-states with graphene's Dirac point. What has been missing so far is a systematic study

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of how this exchange effect varies across the atomic structure, and how it depends on twisting, particularly in light of the recently introduced concept of pseudospin-preserving versus pseudospin-breaking proximity effects (see Ref. [16]), demonstrated in graphene/Cr₂Ge₂Te₆ slabs by some of the present authors.

We analyze more than 20 high- and low-symmetry Co/hBN/graphene stacking configurations to quantify the impact of local atomic registries on Dirac band spin splittings, induced magnetic moments, and tunneling spin polarization (TSP). Our results reveal that even nominally uniform heterostructures may exhibit spatial inhomogeneity in spin injection and transport. These effects can be understood as emerging from spatially varying hybridization across the moiré unit cell, leading to position-dependent spin splittings and anisotropies. In particular, we demonstrate that the induced spin splittings in graphene can vary from 1 to 100 meV, with local magnetic moments and tunneling spin polarizations (TSPs) also displaying strong spatial dependence. Regarding TSPs, specific local geometries can give rise to spin-filtering regions of strongly enhanced polarization in realistic device structures.

A key insight revealed in our study is that proximity effects are inherently local. Because they depend on orbital hybridization, particularly between out-of-plane orbitals (graphene p_z , N p_z , and Co d_{z^2}), the atomic registry and relative alignment between layers become critically important. Even small variations in stacking—induced by lattice mismatch or intentional twist—can lead to dramatic modulations of the proximity-induced interactions. The degree of this hybridization, and therefore the strength and character of the proximity effect, depends sensitively on the exact stacking configuration and interlayer distances. Our results have direct implications for the design of spintronic devices and suggest new strategies for tuning interfacial magnetic interactions at the atomic scale.

The manuscript is organized as follows. In Sec. II, we introduce the structural setup of the graphene/hBN/Co heterostructures that we consider in our first-principles calculations. In Sec. III, we summarize the DFT calculation details we employ to unveil different band-structure effects and tunneling conductances, based on different local atomic stacking configurations. Exemplary input files are listed in the Supplemental Material [17]. In Sec. IV, we compare band structure and density of states of selected stacking configurations and highlight the impact of the local atomic registries on proximity physics. These results are mapped to a more spatially extended supercell of graphene/hBN/Co. Section V provides insights into the relationship between tunneling spin polarization and the associated local atomic stacking. In Sec. VI, we analyze the overlap of atomic orbitals in three-layer atomic structures as a function of the twist angle using geometric modeling. Finally, in Sec. VII we summarize the main findings of our research and conclude the manuscript.

II. STRUCTURAL SETUP

The graphene/hBN/Co heterostructures are set up with the atomic simulation environment (ASE) [18] and the

CellMatch code [19], implementing the coincidence lattice method [20,21]. We consider small, medium-sized, and large-scale atomic structures, to illustrate the effects of local atomix registries on the magnetic proximity effects.

Small structures are shown in Fig. 1. In total, we consider 18 high-symmetry lattice-matched commensurate stacks S , and six additional stackings—derivatives of geometries $S_{1,1}$ and $S_{1,2}$ —with reduced symmetry that may appear in moiré superlattices. The lattice constant of graphene is $a = 2.46 \text{ \AA}$ [22], the one of hBN is $a = 2.504 \text{ \AA}$ [23], and the one of hcp-cobalt is $a = 2.507 \text{ \AA}$ [24]. Here, we fix an effective average lattice constant of $a = 2.4903 \text{ \AA}$ for this well lattice-matched system, as a compromise to make the lattices commensurable and to keep the unit cells small to be considered as representative atomic registries which can be identified within larger systems. The corresponding strain is about $\pm 1.2\%$ for the individual material components.

In all structures, the individual monolayers are barely strained, so the extracted band offsets and magnetic proximity effects are representative when compared to those in experiment. To simulate quasi-2D systems, we add a vacuum of about 20 \AA to avoid interactions between periodic images in our slab geometries.

III. COMPUTATIONAL DETAILS

For reproducibility, we provide representative input files for all calculations done on the $S_{1,2}$ configuration, in the Supplemental Material [17].

A. DFT calculations

The electronic structure calculations and structural relaxations of the graphene/hBN/Co heterostructures are performed by DFT [25] with Quantum ESPRESSO v7.2 [26–28]. Self-consistent calculations are carried out with a dense k -point sampling of $300 \times 300 \times 1$. We use an energy cutoff for charge density of 800 Ry and the kinetic energy cutoff for wave functions is 75 Ry for the scalar relativistic pseudopotentials with the projector augmented wave method [29] with the Perdew-Burke-Ernzerhof exchange correlation functional [30]. Open shell calculations provide the spin polarized ground state. For the self-consistent calculation, we employ a threshold of 1×10^{-8} Ry and Fermi-Dirac smearing of 5×10^{-4} Ry. For the relaxation of the heterostructures, we add DFT-D2 vdW corrections [31–33] and use quasi-Newton algorithm based on trust radius procedure. To get proper interlayer distances and to capture possible moiré reconstructions, we allow all atoms to move freely within the heterostructure geometry during relaxation. Relaxation on the high-symmetry structures is performed until every component of each force is reduced below 1×10^{-4} Ry/ a_0 , where a_0 is the Bohr radius. In the case of reduced-symmetry stackings, the atoms are only allowed to relax in z direction, otherwise the atoms would rearrange to a high-symmetry stacking.

In all calculations, we consider collinear Co. Noncollinear effects, which may arise due to spin-orbit coupling and the interface with hBN, are expected to be secondary. While small local canting may occur at the atomic scale, the relevant chiral spin textures driven by such interactions typically develop on

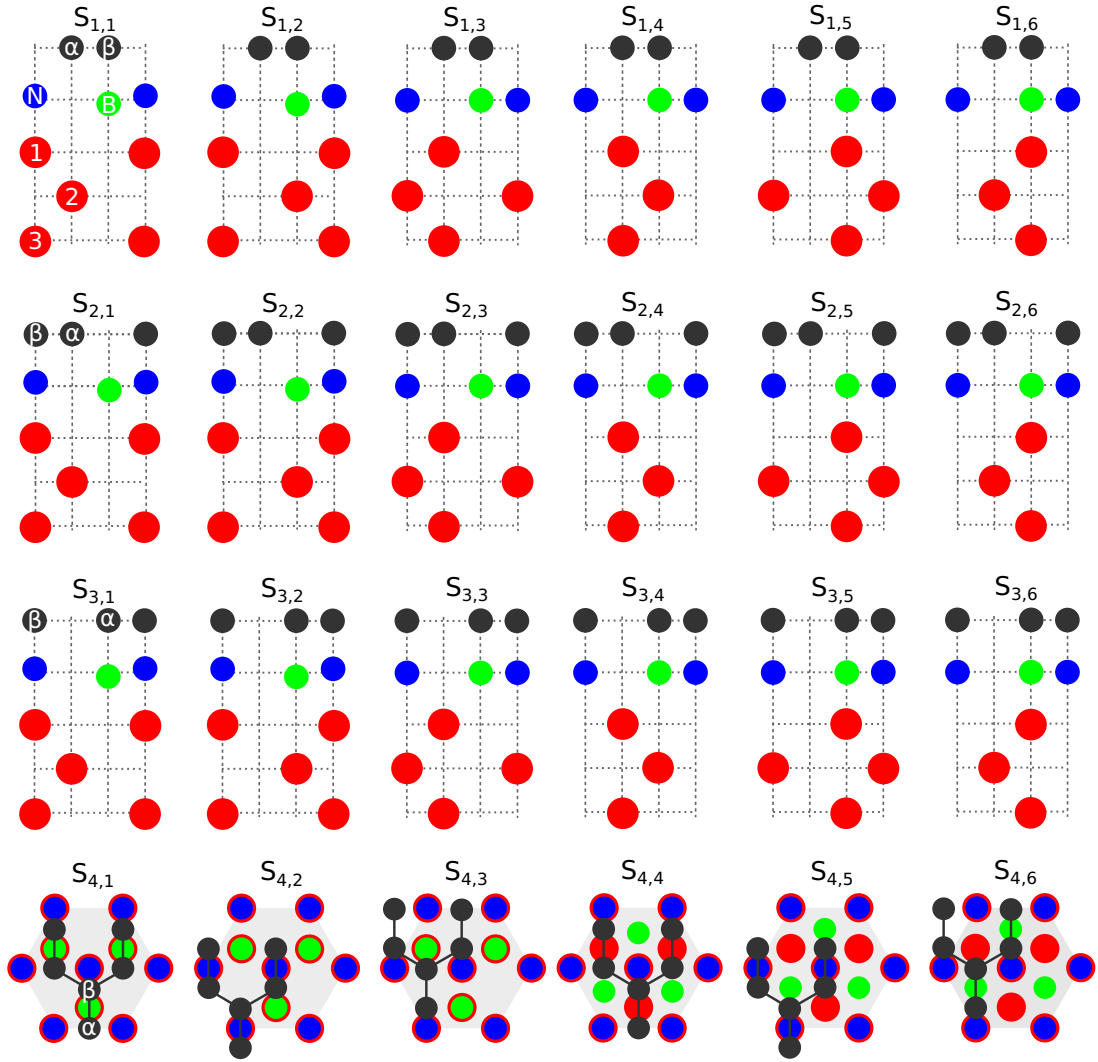


FIG. 1. Sketch of the geometries, showing the different stacking configurations $S_{1,1} - S_{3,6}$, of the 18 lattice-matched high-symmetry commensurate structures. The colors of the spheres correspond to different atoms (black = C, green = B, blue = N, red = Co). Within each row, the graphene/hBN stacking is fixed. Within each column, the hBN/Co stacking is fixed. Labels α and β represent the graphene sublattices, while labels 1 – 3 represent the different Co layers. The rippling of hBN, if present, is indicated. Structures $S_{4,1} - S_{4,6}$ in the last row have lowered symmetry and are derived from geometries $S_{1,2}$ and $S_{1,1}$. Further details are summarized in Table I.

much larger length scales than those accessible in our DFT supercells and are more appropriately described within micro-magnetic simulations. For example, Co/hBN interfaces were predicted to exhibit a sizable Dzyaloshinskii-Moriya interaction, which can stabilize nontrivial magnetization textures, such as complex domain patterns and skyrmionlike states [34]. Indeed, spin-orbit coupling shows negligible impact compared to the exchange coupling, justified on exemplary calculation results shown in SM [17].

The density of states (DOS) is calculated with the optimized tetrahedron method [35] and magnetic moments are calculated via Löwdin population analysis [36] as implemented in Quantum ESPRESSO. For each structure, we calculate the total energy, average interlayer distances, induced magnetic moments, and the rippling of the hBN layer (deviation of B/N z positions from the average). Note that the

hBN rippling is always such that the B atom is closer to the Co interface than the N atom.

B. Transmission calculations

The transmission calculations are performed by PWCOND implemented in Quantum ESPRESSO package [27]. By considering a lead/scattering-region/lead setup, the code solves the quantum mechanical scattering problem and calculates the ballistic conductance. We consider symmetric tunneling geometries schematically shown in Fig. 2, which are based on the stacking configurations in Fig. 1. The atomic positions of the scattering regions are fully relaxed prior to transmission calculations. The magnetizations of the Co leads are parallel, as we are interested in the variation of the spin-dependent transmission across different atomic registries.

TABLE I. Total energies with respect to the lowest energy reference structure $S_{1,2}$, averaged interlayer distances between the layers, $d_{\text{Co/hBN}}$ and $d_{\text{hBN/Gr}}$, rippling of the hBN layer, δ_z , and the induced atomic magnetic moments on boron (B), nitrogen (N), and carbon atoms at α and β sublattice sites in graphene.

| config. | $E_{\text{tot}} - E_0$ [meV] | $d_{\text{Co/hBN}}$ [Å] | δ_z [Å] | $d_{\text{hBN/Gr}}$ [Å] | B [$10^{-3}\mu_B$] | N [$10^{-3}\mu_B$] | α [$10^{-3}\mu_B$] | β [$10^{-3}\mu_B$] |
|-----------|------------------------------|-------------------------|----------------|-------------------------|----------------------|----------------------|-----------------------------|----------------------------|
| $S_{1,1}$ | 4.305 | 2.040 | 0.059 | 3.071 | -41.99 | 15.38 | 0.43 | 0.25 |
| $S_{1,2}$ | 0 | 2.039 | 0.060 | 3.072 | -45.14 | 13.15 | 0.36 | 0.31 |
| $S_{1,3}$ | 281.824 | 2.992 | 0.007 | 3.121 | -1.92 | 0.79 | 0.08 | -0.18 |
| $S_{1,4}$ | 282.429 | 2.994 | 0.007 | 3.120 | -2.07 | 0.12 | 0.02 | -0.14 |
| $S_{1,5}$ | 300.364 | 3.102 | 0.003 | 3.122 | -1.83 | 5.51 | -0.25 | 0.18 |
| $S_{1,6}$ | 302.107 | 3.107 | 0.003 | 3.122 | -1.33 | 4.78 | -0.25 | 0.16 |
| $S_{2,1}$ | 30.700 | 2.038 | 0.060 | 3.210 | -42.38 | 14.79 | 3.89 | -3.33 |
| $S_{2,2}$ | 26.175 | 2.035 | 0.061 | 3.208 | -45.48 | 12.51 | 3.81 | -3.20 |
| $S_{2,3}$ | 310.869 | 2.994 | 0.007 | 3.301 | -1.90 | 0.48 | -0.09 | 0.08 |
| $S_{2,4}$ | 311.467 | 2.995 | 0.008 | 3.299 | -2.11 | -0.14 | -0.09 | 0.07 |
| $S_{2,5}$ | 328.462 | 3.104 | 0.004 | 3.298 | -1.95 | 5.51 | -0.12 | 0.05 |
| $S_{2,6}$ | 330.295 | 3.109 | 0.003 | 3.295 | -1.44 | 4.77 | -0.12 | 0.04 |
| $S_{3,1}$ | 32.916 | 2.038 | 0.060 | 3.236 | -43.18 | 16.23 | 3.37 | -3.45 |
| $S_{3,2}$ | 28.804 | 2.035 | 0.061 | 3.239 | -46.41 | 13.95 | 3.23 | -3.43 |
| $S_{3,3}$ | 315.285 | 2.992 | 0.008 | 3.354 | -2.09 | 0.60 | -0.18 | 0.08 |
| $S_{3,4}$ | 316.028 | 2.993 | 0.008 | 3.355 | -2.25 | -0.08 | -0.15 | 0.04 |
| $S_{3,5}$ | 334.027 | 3.103 | 0.004 | 3.359 | -1.78 | 5.42 | 0.03 | -0.02 |
| $S_{3,6}$ | 335.895 | 3.109 | 0.003 | 3.358 | -1.25 | 4.62 | 0.02 | -0.02 |
| $S_{4,1}$ | 17.419 | 2.036 | 0.060 | 3.163 | -45.87 | 13.50 | 1.35 | -1.09 |
| $S_{4,2}$ | 25.126 | 2.036 | 0.061 | 3.208 | -45.92 | 13.31 | 0.11 | 0.14 |
| $S_{4,3}$ | 16.215 | 2.036 | 0.060 | 3.152 | -45.52 | 12.96 | 1.48 | -0.97 |
| $S_{4,4}$ | 21.632 | 2.039 | 0.060 | 3.163 | -42.68 | 15.75 | 1.42 | -1.10 |
| $S_{4,5}$ | 29.439 | 2.038 | 0.060 | 3.208 | -42.75 | 15.59 | 0.13 | 0.14 |
| $S_{4,6}$ | 20.587 | 2.039 | 0.060 | 3.152 | -42.37 | 15.22 | 1.50 | -0.99 |

When performing the self-consistent calculation for the scattering region (leads), we employ the same parameters and pseudopotentials as above, but a k -point grid of $60 \times 60 \times 1$ ($36 \times 36 \times 24$). The specific input for PWCOND is given in the Supplemental Material [17]. From the spin-dependent transmissions, $T_{\uparrow/\downarrow}$, we extract the tunneling spin polarization (TSP) as

$$P_T = \frac{T_{\uparrow} - T_{\downarrow}}{T_{\uparrow} + T_{\downarrow}}. \quad (1)$$

This polarization is a function of the electron energy and, as we show below, depends strongly on the atomic registries.

IV. LOCAL VARIATIONS OF PROXIMITY EXCHANGE

We wish to convey the idea that the precise atomic stacking registry has a significant impact on both proximity-induced magnetic exchange coupling, which modifies the Dirac bands of graphene, and on the tunneling spin-injection efficiency.

The following analysis should be generally applicable to vdW interfaces.

A. Monolayers of graphene and hBN

We start with the simplest scenario, considering monolayers of graphene and hBN. As shown above, we can already form 18 different high-symmetry stacking configurations when considering lattice-matched constituents. Depending on the precise atomic stacking registry, strong variations in interlayer distance and induced magnetic moments occur, see Table I. Note, that the magnetization of bulk Co atoms is $1.69\mu_B$ and the spin polarization at the Fermi level is $P_N = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}} = -0.556$.

The lowest energy configuration is $S_{1,2}$, with interlayer distances of about 2.0 Å, between Co and hBN, and about 3.1 Å, between hBN and graphene. Additionally, the hBN is rippled by about 0.06 Å, in agreement with Ref. [5]. Depending on the stacking registry, interlayer distances between

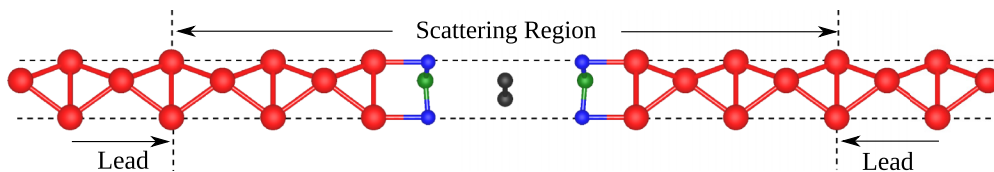


FIG. 2. Setup for the transmission calculations. For the transmission calculations with PWCOND, we consider a Co/hBN/graphene/hBN/Co stack as the scattering region, with semi-infinite bulk Co leads.

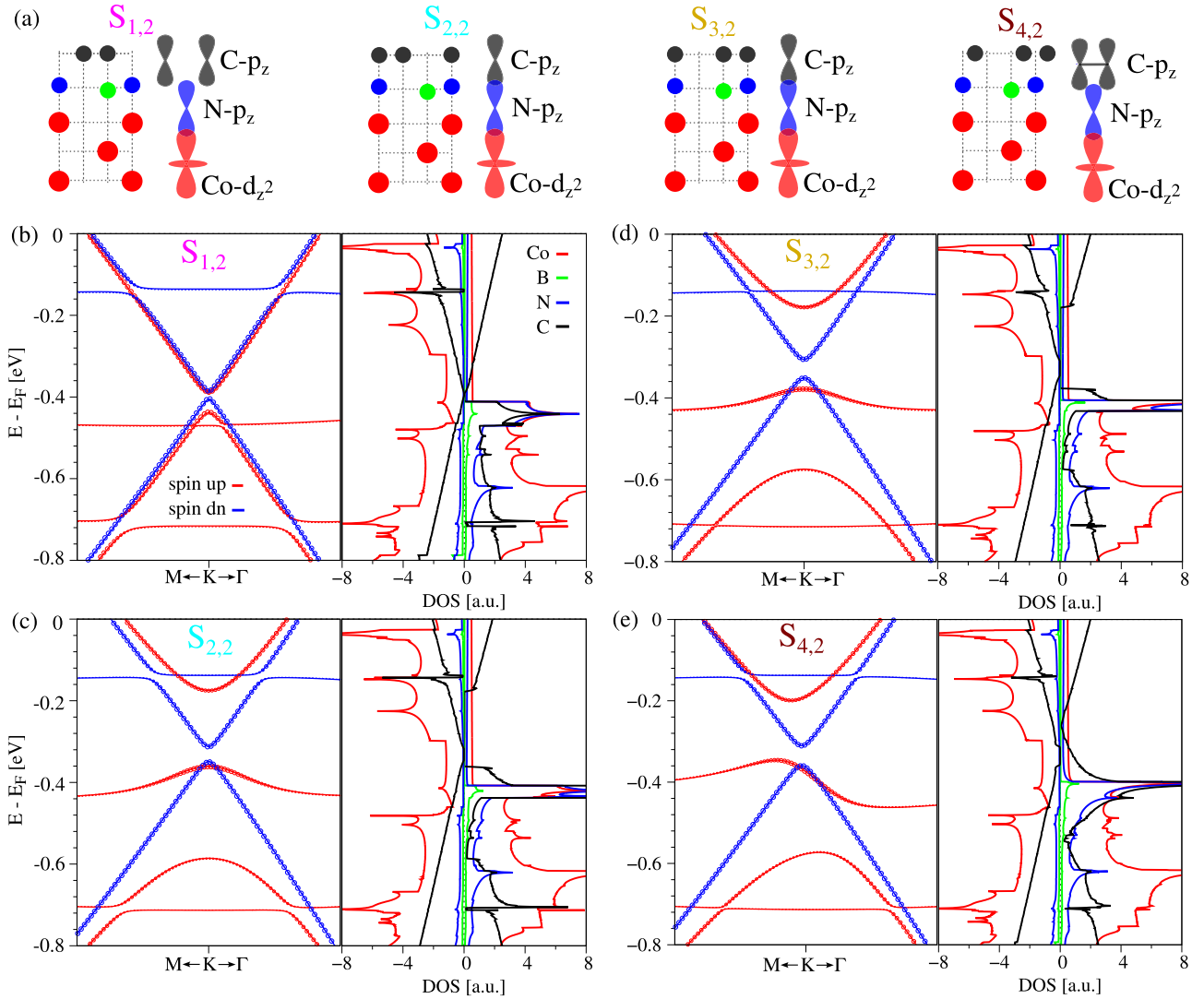


FIG. 3. (a) Side views of exemplary high-symmetry stacking configurations $S_{1,2}$, $S_{2,2}$, $S_{3,2}$, and $S_{4,2}$. The hybridization channels from Co d_{z^2} to C p_z orbitals via N p_z orbitals are sketched. (b) Enlargement of the proximitized low-energy Dirac bands ($E_F = 0$) and the corresponding spin- and atom-resolved density of states of the $S_{1,2}$ configuration. The open circles on the bands represent the projection on graphene orbitals. Positive (negative) DOS corresponds to majority (minority) spin channels. The PDOS of hBN (graphene) atoms is enhanced by a factor of 10 (100). (c), (d), (e) The same as (b), but for the corresponding stacking configuration as labeled in the dispersion.

Co and hBN vary in the range of 2.03 – 3.11 Å, while the interlayer distance between hBN and graphene varies between 3.07 – 3.36 Å. Significant rippling of the hBN layer occurs only when the N atom is directly above the top Co atom. From Table I, it is also evident that the proximity-induced magnetic moments are strongly dependent on the registry.

For all 24 registries in Fig. 1, we have calculated the proximitized low-energy Dirac bands and the corresponding spin and atom-resolved DOS, see SM [17]. Representative low-energy Dirac bands, for the $S_{1,2}$, $S_{2,2}$, $S_{3,2}$, and $S_{4,2}$ stackings, are shown in Fig. 3. We find that the registry dictates the overlap of the wave functions and thereby the hybridization of C p_z orbitals with Co d_{z^2} orbitals, mediated by N p_z orbitals, as sketched in Fig. 3(a). Already, the four selected dispersions demonstrate that the Dirac bands can experience vastly different spin splittings, band alignments, and even anisotropies. For example, the $S_{1,2}$ configuration shows very well preserved Dirac bands, moderate proximity-induced

exchange splittings, as well as moderate anticrossings with the flat bands originating from Co d orbitals. In contrast, for the $S_{2,2}$ configuration, in particular the spin-up Dirac cone is not recognizable anymore as strong hybridization occurs. The reason is the direct hybridization channel, as sketched in Fig. 3(a). Across the stacking configurations we studied, the proximity-induced exchange spin splitting in the Dirac cone ranges from 1 to 100 meV, with systematically larger splittings observed for holes. As already mentioned, a key factor in the hybridization is the position of the N atom, as we explicitly demonstrate by calculating the integrated local DOS for two stacking configurations [17]. Also the energetic position of the Dirac point is quite different for the stackings shown in Fig. 3. Overall, we find the Dirac point in the range of 0.2 – 0.4 eV below the individual heterostructure Fermi level, indicating the possibility of strong doping variations across the configurations. When low-symmetry registries are considered, such as $S_{4,1}$, we additionally find a strong anisotropy of the

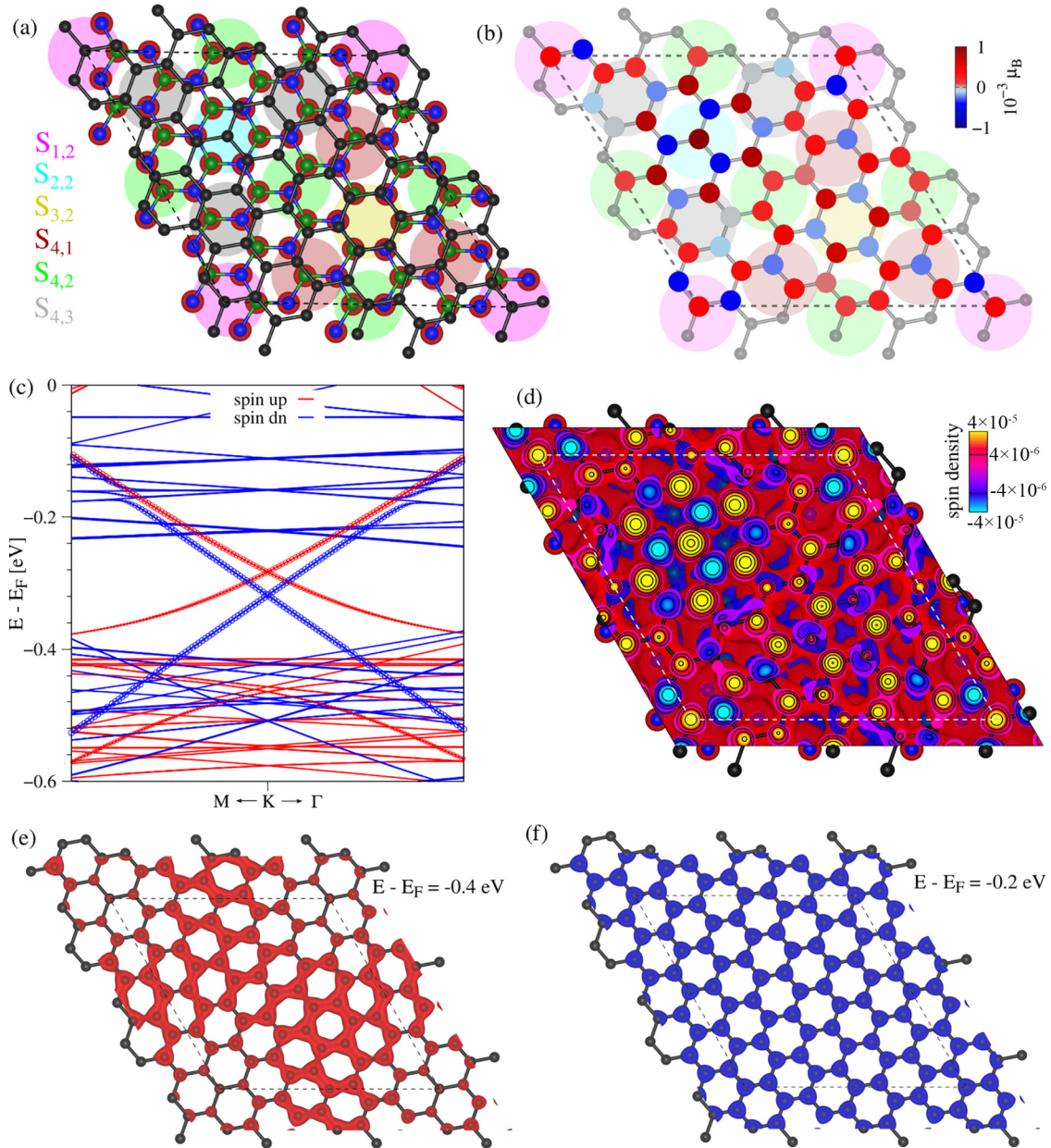


FIG. 4. (a) Medium-sized Co/hBN/graphene supercell. The different colored spheres emphasize the different local high-symmetry stackings. The dashed line represents the unit cell. (b) The proximity-induced calculated magnetic moments on C atoms, overlaid on the geometry. (c) DFT-calculated spin-resolved band structure in the vicinity of the K point. The open circles on the bands represent projections onto graphene orbitals. (d) DFT-calculated spin density, $\rho_{\uparrow} - \rho_{\downarrow}$, in units $e/\text{\AA}^3$. We cut through the p_z orbitals slightly above the C atoms. Yellow/red corresponds to isovalues with positive density, while cyan/blue corresponds to isovalues with negative density, in line with the magnetic moments shown in (b). (e) Spin density, taking into account states below the Dirac point at $E - E_F = -0.4$ eV and energy window of ± 10 meV. The density is positive, highly nonuniform, and mainly localized around the $S_{3,2}$ configuration. The color bar is the same as in (d). (f) Same as (e), but above the Dirac point at $E - E_F = -0.2$ eV. The density is negative and uniformly distributed.

low-energy Dirac band spin splittings. This is demonstrated in Fig. 3(e) and in the SM [17], where we calculate the low-energy dispersion along two different Brillouin zone paths.

When considering more realistic experimental heterostructure setups, strain is minimized, twist angles can be arbitrary, and many local stacking configurations may occur, due to the moiré structure from the lattice mismatch. For simplicity, we consider lattice-matched hBN and Co, and place graphene on top at different twist angles, minimizing strain. One of such possible geometries is shown in Fig. 4. This supercell has 191

atoms, built by considering an aligned energetically favorable Co/hBN interface from the $S_{1,2}$ geometry of Fig. 1, but with a lattice constant of 2.5051 Å. The graphene layer is placed at a twist angle of 10.89° above the hBN/Co interface and has a lattice constant of 2.46 Å. The strains for Co and hBN are -0.076% and 0.044% . This medium-sized structure is still computationally manageable, but the local stacking registries are less comparable to those in small lattice-matched cells due to the rather large twist angle involved. For the medium-sized structure, we have calculated the low-energy Dirac dispersion,

DOS, and the local magnetic moments on the C atoms, see Fig. 4 and SM [17].

The low-energy Dirac bands for this geometry, see Fig. 4(c), are almost gapless, in contrast to those Dirac bands from the individual stackings. This results from an averaging effect of the graphene sublattice asymmetry on the various stacking configurations. Furthermore, a rather uniform proximity exchange splitting of about 35 meV arises near the Dirac point, again due to the averaging effect. We emphasize that the observed averaging should be understood as a consequence of the medium-sized supercell band structure capturing contributions from multiple local stacking registries. A comprehensive moiré band structure analysis is beyond the scope of this work, which instead focuses on the registry dependence of the proximity-induced exchange.

The induced magnetic moments in carbon in this supercell vary strongly within $\pm 1 \times 10^{-3} \mu_B$, see Fig. 4(b). In fact, starting at the $S_{2,2}$ configuration, magnetic moments on C atoms are largest and opposite on A and B sublattice. Moving away towards the $S_{1,2}$ configuration, the polarizations gradually decrease. Furthermore, the sublattice polarizations even reverse sign. Finally, in $S_{4,2}$ and $S_{4,3}$ the sublattice arrangements are very different. This variety nicely demonstrates the very local character of proximity exchange coupling and the influence of the atomic registry on spin properties.

Even though the low-energy Dirac dispersion resembles a uniform proximity-induced exchange coupling, see Fig. 4(c), the local nature of the coupling is clearly visible in the magnetic moments. To further support this picture, we have also calculated the local density of states (LDOS), at different energies, see SM [17]. From the LDOS map at the Fermi level, we find a rather uniform charge density distribution on graphene. At lower energy, $E - E_F = -0.4$ eV, roughly near the strong anticrossing in the spin-up channel of the dispersion, the charge density concentrates around regions where C and N atoms are vertically stacked. This picture is in line with the dispersions of the high-symmetry stackings, i.e., the coupling between layers, and the associated band anticrossing, is concentrated to specific regions in real space.

In Fig. 4(d), we also show the DFT-calculated spin density, which is in line with the magnetic moments. The spin density is calculated as the difference between the spin-up and spin-down electron densities, integrated up to the Fermi level. In contrast, in Figs. 4(e) and 4(f), we show spectrally resolved local spin densities, taking into account the states at ± 100 meV above or below the Dirac point. Below the Dirac point near the anticrossing, the spin density is positive, highly nonuniform, and mainly localized around the $S_{3,2}$ configuration, similar to the LDOS. Such regions form *proximity hot spots*. Above the Dirac point, the spin density is negative and uniformly distributed across graphene. This demonstrates the dependence of the local nature of proximity physics on energy.

We even generated a much larger supercell (1619 atoms), see SM [17], which further serves to illustrate the spatial variation of magnetic proximity effects arising from different local registries S .

B. Additional graphene and hBN layers

In experiments, often more than one monolayer of the same material is considered when building heterostructures. The

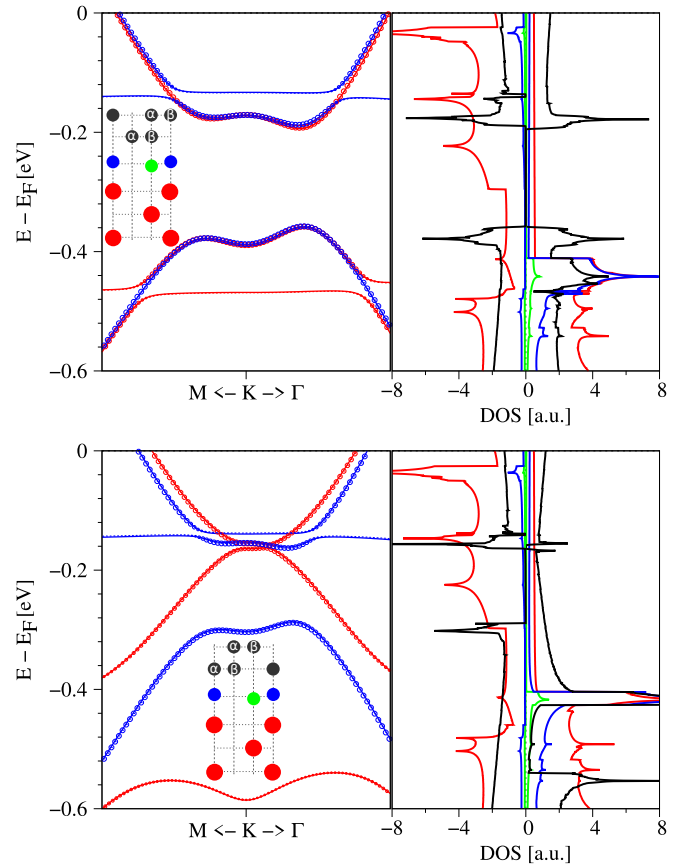


FIG. 5. Enlargement of the proximitized low-energy bilayer-graphene bands ($E_F = 0$) and the corresponding spin- and atom-resolved density of states of selected configurations of bilayer-graphene/hBN/Co. The open circles on the bands represent the projection on bilayer-graphene orbitals. Positive (negative) DOS corresponds to the majority (minority) spin channels. The stackings are sketched in the inset.

results for bilayer graphene and bilayer hBN are summarized in the SM [17]. Here, we briefly discuss the main findings.

With two hBN layers, the proximity coupling is strongly suppressed, as evident from the proximity-induced magnetic moments on C atoms and the low-energy Dirac band splittings. Nevertheless, a pronounced coupling between Co and C orbitals can still arise, which is now mediated by a consecutive coupling via N orbitals from the first hBN layer and B orbitals from the second hBN layer. In particular, the low-energy dispersions show that band topologies are still strongly affected by the local stacking configuration. More precisely, spin splittings vary in sign and can still range up to tens of meV for specific atomic configurations.

In the case of bilayer graphene, the short-rangeness of proximity effect is at play. While the first graphene layer still shows pronounced proximity-induced magnetic moments, up to about $\pm 4 \times 10^{-3} \mu_B$ for some stackings and in line with the monolayer graphene results, the magnetic moments in the second graphene layer are further suppressed by one order of magnitude. The band gap in the bilayer graphene spectrum is quite large, on the order of 200 meV for almost all cases, see Fig. 5. Certainly, the interplay of short-ranged

proximity-exchange and the layer degree of freedom is also recognizable, given that the bilayer graphene conduction and valence bands show rather different spin splitting strengths [37]. However, we also find one rather special case, in which the spin-down channel shows a gapped spectrum, while the spin-up channel is nearly gapless, see Fig. 5. Hence, this local stacking configuration would support 100% polarized islands within otherwise insulating stackings inside moiré structures. Eventually, one can think of spin-polarized network channels within the bilayer graphene.

V. LOCAL VARIATIONS OF TUNNELING SPIN POLARIZATION

In Ref. [38], it was demonstrated that Co/hBN interfaces show a Brillouin zone spin filtering mechanism due to the specific complex band structure of hBN. Additionally, in Refs. [39,40] it was demonstrated that graphene acts as an ideal spin filter supporting minority carriers of hcp-Co. The reason is that near the Fermi level, graphene Dirac states are present only near K, where also only minority carriers of Co are present.

In our case, since each different stacking registry provides vastly different results in terms of low-energy Dirac dispersion, DOS, and magnetic moments, we are additionally interested in the local tunneling spin polarization (TSP). We believe that in experimental setups, spatially localized regions of enhanced spin injection emerge due to optimal wave function overlap across the vdW interface, and spin filtering effects [38–40]. Another factor is certainly the band alignment of the different configurations, leading to inhomogeneity in spin injection.

We consider the definition of the TSP in Sec. III. For six representative structures, $S_{1,2}$, $S_{2,2}$, $S_{3,2}$, $S_{4,1}$, $S_{4,2}$, and $S_{4,3}$ we calculate the TSP. This selection is motivated by the appearance of these atomic registries in the medium and large heterostructures we consider. The calculation setup for the TSP is shown in Fig. 2.

The results for the TSP are summarized in Fig. 6 and in the SM [17]. We show the individual spin-resolved transmissions, $T_{\uparrow/\downarrow}$, and the TSP, P_T for the six stacking configurations. We additionally average over these stacking configurations to get an estimate for the total values to be expected in the medium and large supercell.

Looking at the results for $S_{1,2}$ which is the lowest-energy configuration, see Fig. 6, we find that T_{\uparrow} essentially follows the spin-up DOS of the Co lead [17]. Since the spin up DOS of hcp-Co is small and nearly constant for $E - E_F$ above -0.5 eV, also T_{\uparrow} is small and constant for these energies. At lower energies, the large spin-up DOS of Co provides many incoming modes at many different k vectors, see the movie on the spin- and k -resolved DOS of the Co lead (spin_and_k_resolved_DOS_hcp_Co.mp4), that can potentially tunnel through the Co/hBN/graphene/hBN/Co scattering region. From the transmission it is evident that these modes are supported by the scattering region. In contrast, T_{\downarrow} is dominated by distinct peaks at certain energies.

In the Supplemental Material [17], we show movies (trans_movie_config.mp4) of the spin- and k -resolved

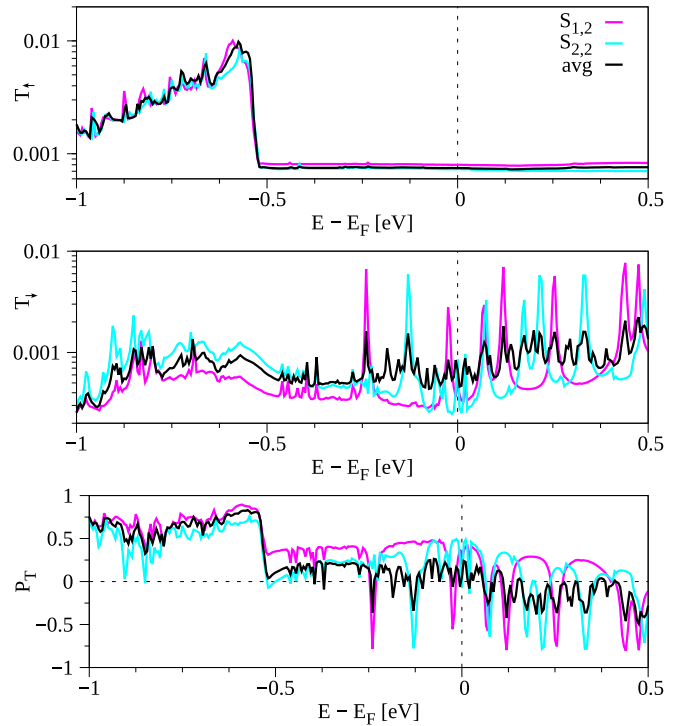


FIG. 6. The spin-resolved transmissions, $T_{\uparrow/\downarrow}$, and the tunneling spin polarization, P_T . We present results for two exemplary stacking configurations, as well as for the average when considering the six configurations from Fig. 4(a). Results for all configurations are summarized in the SM.

transmissions as function of energy for the different stacking configurations. The total transmission for each spin-channel is given above the subfigures, which is a weighted sum of k -resolved transmissions within the Brillouin zone. The value of spin polarization, P_T , is also given for each energy. From there, it is evident that the peaks in T_{\downarrow} are tunneling events near the Brillouin zone corners. In other words, the Brillouin zone spin filter mechanism for Co minority carriers produces resonance peaks.

For clarification, in Fig. 7, we compare the spin- and k -resolved transmissions, $T_{\uparrow/\downarrow}$, for $S_{1,2}$ and $S_{2,2}$ scattering regions for $E - E_F = -0.13$ eV. We note that the overall T_{\uparrow} for both scattering regions is rather similar, while there are pronounced differences in T_{\downarrow} , at this energy. Compared to $S_{1,2}$, $S_{2,2}$ exhibits localized maxima in T_{\downarrow} near the Brillouin zone corners, which are responsible for the strong resonance in P_T , see Fig. 6.

Overall, while T_{\uparrow} is rather similar for the different stacking configurations, T_{\downarrow} sensitively depends on the atomic alignment, supporting the resonance modes at different energies. Even though the resonances are suppressed in the configuration average, their local nature points to localized regions of strong spin tunneling.

To bridge theory and experiment, we suggest that Spin-Polarized Scanning Tunneling Spectroscopy (SP-STs) is the most viable probe for these localized resonances. Given the predicted exchange splitting of up to 100 meV, SP-STs can resolve the spin-polarized LDOS at specific registries.

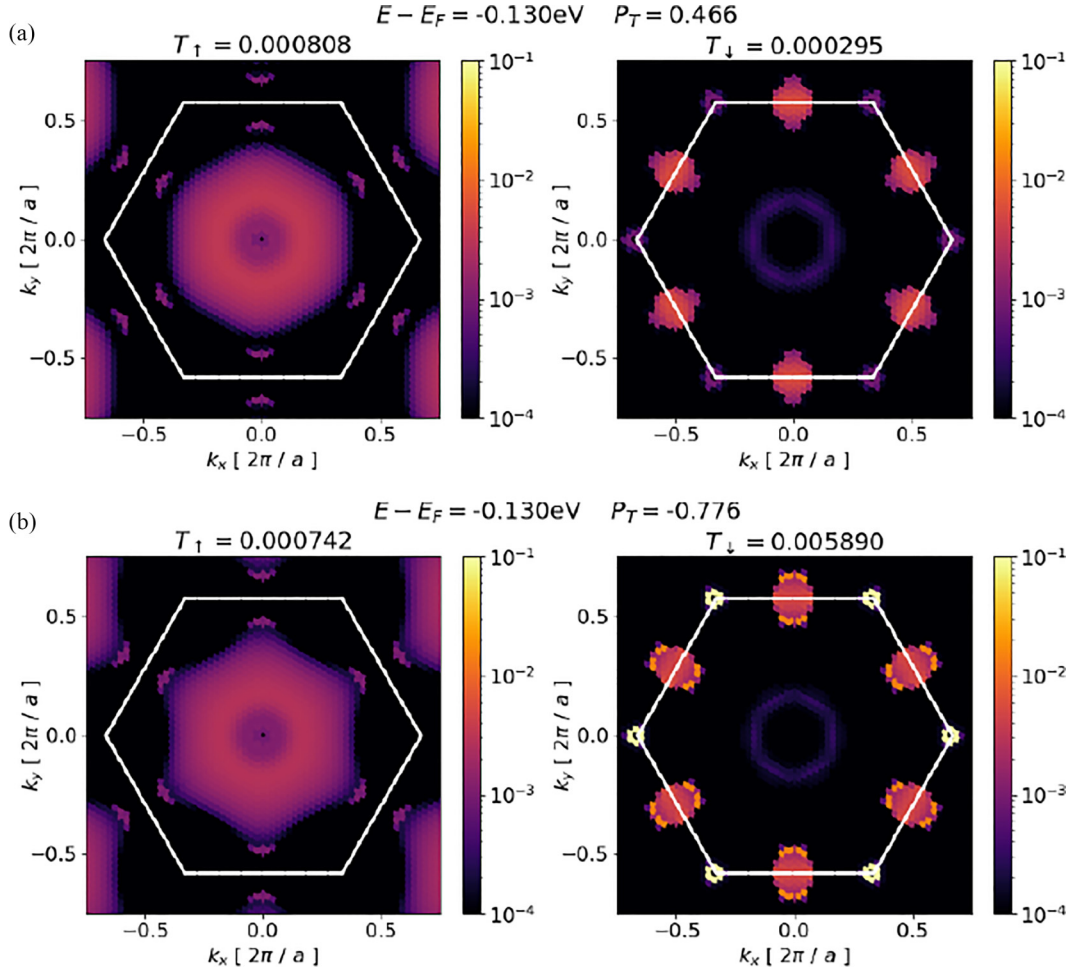


FIG. 7. (a) Spin- and k -resolved transmissions for the $S_{1,2}$ scattering region for $E - E_F = -0.13$ eV. Left (right) panel is for T_\uparrow (T_\downarrow). The color code represents the magnitude of the transmission. The numbers for P_T and $T_{\uparrow/\downarrow}$ above are total values at this particular energy. The white hexagon represents the edges of the Brillouin zone. (b) Same as (a), but for the $S_{2,2}$ scattering region.

VI. TAILORING THE ATOMIC SITE OVERLAP

The coupling between the layers comes primarily from vertically arranged atomic sites and the respective overlap of the z -extended orbitals (p_z of C and N, d_{z^2} of Co). To screen for maximized proximity coupling, mediated by the overlap between these orbitals, we consider the lattices of unstrained graphene, hBN, and a single layer of Co, and calculate the total and atom-resolved site overlap as a function of the two twist angles: one between graphene and hBN, the other between hBN and Co.

We assess the overlap of the z -extended orbitals using a geometric approach. Each layer α (graphene, hBN, and Co) is simulated by a 2D array L_{ij}^α , where 200×200 pixels in a hexagonal arrangement are assigned a value of “1” to symbolize the lattice sites, corresponding to about 25×25 nm of a real space lattice. The lattice sites are then blurred by a Gaussian ($\sigma = 0.3$ Å) to emulate the spatial distribution of the orbitals, see Figs. 8(a) and 8(b). The matrices representing each material are then multiplied element-wise (Hadamard product) to obtain the local overlap. Say, for hBN and Co layers the overlap matrix would be $\Omega_{ij} = L_{ij}^{\text{hBN}} \odot L_{ij}^{\text{Co}}$. As an example, in Fig. 8(c) we show Ω_{ij} for a Co layer and a 10° twisted graphene layer, revealing sixfold symmetric moiré

physics. The calculated Ω is also shown for a line-cut across the sample, representative of the locally varying proximity coupling between the layers.

In spin-injection geometries, we additionally need to consider the hBN barrier. As argued above, the proximity coupling between graphene and cobalt is then mediated primarily by the N p_z orbitals. To illustrate the effect of monolayer hBN as a *filter* for proximity exchange, we weigh the contribution of the B (N) atom in the hBN lattice positive (negative) to distinguish the proximity coupling via the two atoms. The resulting Ω is shown in Fig. 8(d).

Adding a monolayer hBN changes the local pattern significantly. While the sixfold symmetry of Fig. 8(c) is maintained in the filtered overlap of (d), in the trilayer stack the overlap occurs alternatively across different atomic species. We can identify regions where the proximity is mainly mediated by either N, B, or a mixture. Three respectively colored hexagons highlight these emerging sub-superlattices. This simple approach can be extended to any combination of 2D-lattices comprised of z -extended orbitals, to get an idea of the proximity coupling.

Moreover, we can use the total mean absolute overlap $|\overline{\Omega_{ij}}|$, considering the whole simulated sample, as a measure

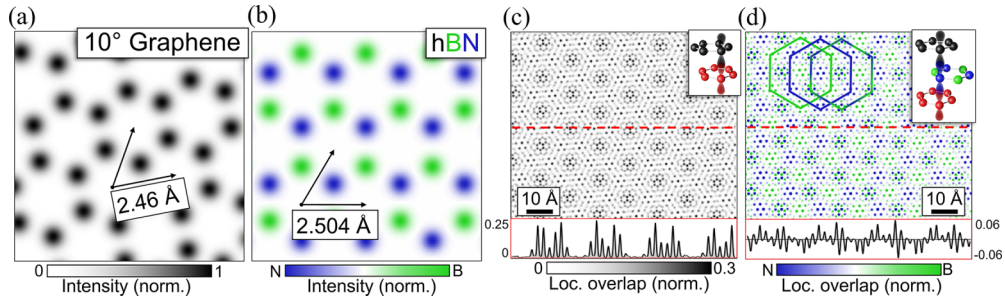


FIG. 8. (a) Top view of 10° rotated graphene, convolved with the Gaussian filter. (b) hBN lattice, where the B (N) atom is color coded green (blue), entering the overlap calculation as positive (negative) values. (c) Local overlap between 10° rotated graphene and 0° Co, showing moiré type patterns. Bottom insert shows a line-cut (red dashed line) of the overlap across the sample. (d) Local overlap between 10° graphene, 0° Co, and 0° hBN. Colored hexagons highlight sixfold patterns for different atomic species (blue for N and green for B). The line-cut shows positive (negative) values indicating predominant vertical coupling through B (N) atoms.

of the proximity interaction. Individually varying both twist angles in the trilayer stack, we can then identify regimes of maximal overlap. We simulate Ω of a graphene/hBN/Co stack—omitting the B atoms of the hBN lattice as they do not mediate the proximity coupling—while twisting the graphene and hBN layers from 0° to 120° . The inset of Fig. 9(a) shows how twist is defined: All simulated materials are constructed with a single coincident lattice site, which acts as the center of rotation. Note that the choice of the center of rotation does not affect our results, as any other center of rotation would correspond to the same rotation combined with a lateral translation. It can be shown that the $|\Omega_{i,j}|$ of unequal lattices is translation invariant.

The results of the simulation are shown in Fig. 9(a). This plot shows the angles at which the total overlap between C and Co (via N) is maximized. We notice that for all twist angles of the hBN layer that are multiples of 60° , we obtain high overlap values. This is to be expected as the lattice constant of hBN and hcp-Co are very similar. High overlap values

are also achieved for graphene twist angles that are multiples of 60° . However, due to the greater lattice disparity between graphene and Co, the overlap is smaller. Along the diagonal, we find the angles where the twist of graphene equals that of hBN. Interestingly, we find that the overlap is reduced, likely due to the lattice mismatch between graphene and hBN, combined with the twist relative to the Co layer. Finally, a few unexpected high-overlap locations appear around the points where the horizontal and vertical strong-overlap lines intersect. Figure 9(b) displays the local overlap for a representative twist angle configuration. Like in Fig. 8, the color indicates the overlap mediated by either N or B. Albeit on a much larger scale, the sixfold patterns described in Fig. 8(d) appear again.

From these observations follows that the best geometry for maximal exchange proximity effect is obtained by keeping hBN aligned with Co. The alignment of graphene is then not critical. The effective overlap for aligned hBN/Co is three times stronger than for not aligned structures, as seen in Fig. 9. Moreover, we identified other regions that, albeit showing a reduced overlap, present nontrivial superlattice structure, both in periodicity and nature of the coupling mediation through the hBN layer, which can be leveraged for studying the effect of moiré structures (see SM [17]).

VII. SUMMARY AND CONCLUSION

We presented a systematic theoretical investigation of local proximity effects in Co/hBN/graphene heterostructures, focusing on their role in spin injection for 2D spintronic devices. The main findings are (i) Locality of Proximity Exchange: The induced exchange splitting in graphene's Dirac bands varies from 1 to 100 meV depending on the local atomic stacking. Proximity effects are highly localized and sensitive to geometry; (ii) Orbital Hybridization Mechanism: Proximity exchange is driven by hybridization between Co d_{z^2} , hBN p_z , and graphene p_z orbitals. The degree of wave function compatibility governs the strength of the effect; (iii) Variation in Spin Transport Properties: Different stackings lead to diverse induced magnetic moments and tunneling spin polarizations (TSPs), revealing spatial inhomogeneities and local spin-filtering behavior; (iv) Effect of Additional Layers and Twist: Inserting extra hBN or graphene layers and introducing twist angles modulates proximity exchange and TSP, offering

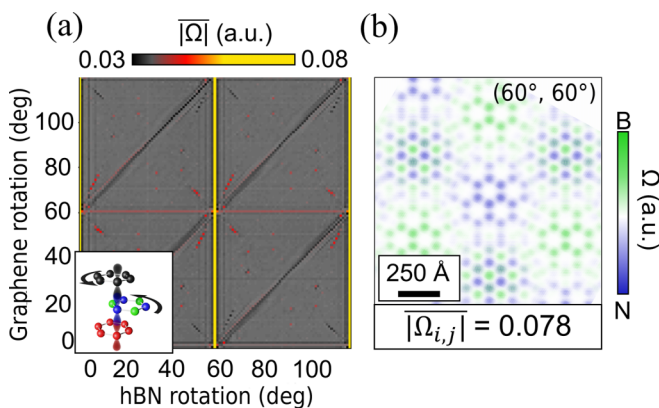


FIG. 9. (a) Angle-resolved mean absolute overlap $|\Omega_{i,j}|$ in a 0° to 120° range for both graphene and hBN rotation. Plotted values are normalized to the value corresponding to three identical lattices with no twist. The inset shows each simulated material aligned with respect to one lattice site acting as a common rotation center. (b) $\Omega_{i,j}$ for the $(60^\circ, 60^\circ)$ twist angle combinations of graphene and hBN, corresponding to the highest mean absolute overlap value. Colors indicate vertical alignment with B (N) atoms.

further control over local spin properties; (v) Implications for Device Design: Our results emphasize that precise control of stacking and interlayer alignment is crucial for optimizing spin injection and interpreting experimental measurements in vdW heterostructures.

ACKNOWLEDGMENTS

K.Z., L.C., and J.F. were supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) SFB 1277 (Project No. 314695032), SPP 2244 (Project No. 443416183), the EU project 2DSPIN-TECH (Project No. 101135853), and FLAGERA project 2DSOTECH. R.S.

and A.V.S. acknowledge the DFG for financial support via the Priority Programmes SPP 2244, as well as the clusters of excellence MCQST (EXS-2111) and e-conversion (EXS-2089) [17].

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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