Long range of indirect exchange interaction on the edges of MoS$_2$ flakes

O Ávalos-Ovando$^1$©, D Mastrogiuseppe$^2$© and S E Ulloa$^1$©

$^1$ Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701–2979, United States of America
$^2$ Instituto de Física Rosario (CONICET), 2000 Rosario, Argentina

E-mail: oa237913@ohio.edu

Received 15 November 2017, revised 6 December 2017
Accepted for publication 15 December 2017
Published 4 January 2018

Abstract
We study the Ruderman–Kittel–Kasuya–Yosida interaction between two magnetic impurities connected to the edges of zigzag-terminated MoS$_2$ flakes. When the impurities lie on the edges of the flake, the effective exchange interaction exhibits sizable noncollinear Dzyaloshinskii–Moriya character that competes with a strong Ising coupling. We analyze the characteristic decay exponent for doping levels inside the band gap of the infinite layer, corresponding to edge states of the flake at the Fermi level. The characteristic exponents show sub-two-dimensional behavior for these band fillings, with decays much slower than quadratic. The Ising interaction has effectively one-dimensional long range, while the noncollinear component that grows for short impurity separation becomes comparable in magnitude. The resulting tunable exchange interaction on these systems opens the way for the study of interesting phases of impurity arrays with long-range stable helical order.

Keywords: MoS$_2$, RKKY interaction, magnetic impurity, transition metal dichalcogenide, tight-binding, Dzyaloshinskii–Moriya interaction

(Some figures may appear in colour only in the online journal)
long range interactions between such magnetic impurities hybridized near crystalline borders.

Magnetic species in a metallic sample can interact effectively via the conduction electrons by the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction [24–26]. In conventional metals, the interaction can be written as $\propto |2k_F|^d \cos (2k_F \rho)$ [27, 28], the superposition of an oscillatory component and a decaying envelope $(2kr)^d$, $d < 0$, where $r$ is the distance between impurities, $k_F$ is the Fermi momentum and $|d|$ is the dimensionality of the host electron system. The first component describes how the interaction changes between ferromagnetic (FM) and antiferromagnetic (AFM) alignment of the magnetic moments (with characteristic scale given by half the Fermi wavelength). However, the spin and orbital content of the conduction states involved can result in unusual interaction features. For instance, in graphene, the interaction is dominated by the Fermi wavelength. However, the spin and orbital content of the conduction states involved can result in unusual interaction features. For instance, in graphene, the interaction is found to decay as $r^{-3}$ at the Dirac point, while in doped or spin-polarized graphene it decays as $r^{-2}$ [29], as in conventional 2D materials. As we will see, TMD edges result in unusual decay with $|d| < 2$, which we call sub-2D behavior.

Many TMDs are semiconducting materials, but can be doped with electrons and/or holes. This allows one to reach energy sectors in which the SOC has strong influence in the band structure. It is well known that SOC can introduce anisotropic interactions between magnetic moments [30], which can give rise to helical spin assembly structures. In TMDs the band splitting due to SOC is much larger near the valence band maximum (VBM) than close to the conduction band minimum (CBM), so that the p-doped case is more attractive for studying the RKKY interaction between localized magnetic impurities, and find possible ways of tuning the interaction for further use. The RKKY interaction on p-doped TMD 2D-bulk monolayers has been studied in previous works, considering only the bands near the Brillouin zone corners $K$ and $K'$ [31, 32], and with the inclusion of the important valence band at the $\Gamma$ point, whose maximum lies close in energy to those at the $K, K'$ valleys [33].

Although analyzing the case of infinite layers is essential, the process of exfoliation often produces nanoscale samples with different shapes—often triangular—and boundaries [34–36]. Finite samples often have richer properties than the bulk counterparts, with characteristics that depend on the shape and termination. For instance, MoS$_2$ zigzag nanoribbons exhibit unusual ferromagnetic properties [37–39], probably due to the presence of edge states [40]. Intrinsic magnetism also arises in triangular MoS$_2$ films, depending on the type of edge termination [36, 41]. TMD zigzag edges have also been proposed to host Majorana fermions when in proximity to superconductors [42, 43], and MoS$_2$ triangular flake edges to host collective plasmon-like excitations with strong optical response [44].

Using an effective three-orbital tight-binding model [45] for MoS$_2$, we present here a systematic study of the interaction decay between magnetic impurities along the edges of flakes, where carriers in such localized states mediate the interaction. We analyze the features of the exchange, including the appearance of a nonlinear component due to the strong SOC, and focus on the decay exponent of the interactions as the chemical potential sweeps the midgap states, reached experimentally by gating or doping [35, 46]. We find that the exponent signals general sub-2D behavior, with the Ising component dominating over the in-plane components, especially at larger separations. Moreover, the non-collinear Dzyaloshinskii–Moriya (DM) component increases gradually with separation, before reaching a strength the competes with the Ising interaction. Although we had found 2D behavior for the interaction between impurities in the interior of flakes before [47], and some evidence of long range interaction for hybridization near the edges [48], we present here the full systematics. We find that indeed whenever the Fermi level is midgap, the sub-2D behavior dominates the effective exchange interaction, with unusual long-range characteristics. These results suggest that whenever magnetic impurities lie at/near the edges of TMD flakes, the long-ranged interaction with strong noncollinear character may give rise to interesting helically ordered impurity assemblies with stable phases. As the Fermi level and impurity separation may be tunable via doping and manipulation, respectively, these systems may provide interesting new playground to explore the behavior of 1D magnetic ensembles. Although such helical structures have been recently shown controllable in metallic systems [49–51], our predictions on TMDs would have interesting advantages, since several TMDs have similar band gaps, large SOC strengths, and well-defined crystallite edges, suggesting the exploration of long-range interaction would be supported by stable and accessible structures, less susceptible to quantum or thermal fluctuations.

2. Model and approach

We consider triangular zigzag-terminated MoS$_2$ nanoflakes [35], with two magnetic impurities hybridized to different lattice sites, as shown in figure 1. A suitable approximation is to describe the system by a lattice of only Mo atoms (see figure 1) since at low energies (near the optical gap) three Mo d-orbitals ($d_x^2$, $d_y^2$, and $d_z^2$) contribute the most to the states, with almost no p-orbital weight from the chalcogens. The Hamiltonian is given by $H = H_{3OBT} + H_I$, where $H_{3OBT}$ describes the triangular TMD lattice and $H_I$ is the Hamiltonian for the magnetic impurities interacting with the charge carriers in the host. The MoS$_2$ tight-binding Hamiltonian can be written as $H_{3OBT} = H_0 + H_I + H_{SOC}$, with

$$H_0 = \sum_{i} \sum_{s=\uparrow,\downarrow} \sum_{\alpha,\alpha'} \varepsilon_{\alpha\alpha'} d_{\alpha,i}^\dagger d_{\alpha',i},$$

where $d_{\alpha,i}$ ($d_{\alpha,i}^\dagger$) annihilates (creates) a spin-$s$ electron in orbital $\alpha \in \{d_x^2, d_y^2, d_z^2\}$ on site $i = i_1 a_1 + i_2 a_2$;

$$a_1 = a(1,0), \quad a_2 = a(1/2, \sqrt{3}/2),$$

are lattice vectors of the triangular Mo lattice, with $a = 3.19$ Å. The nearest-neighbor hopping Hamiltonian is given by

$$H_I = \sum_{i} \sum_{s=\uparrow,\downarrow} \sum_{\alpha,\alpha'} \langle a_1 | i_{\alpha\alpha'} d_{\alpha,i}^\dagger d_{\alpha',i+\hat{a}_1} + H.c. \rangle,$$

2
are hopping parameters in three different directions, $j = 1, 2, 3$, with $a_i = a_{i+} - a_i$. There are 27 hopping parameters, nine for each direction. For direction $a_1$, they are taken from [45] (table II), while for directions $a_2$ and $a_3$, they are calculated from symmetry transformations (see e.g. equations (4)–(6) in [52]). The SOC is approximated by considering the onsite Mo contributions as $H_{SOC} = \lambda_S z S_z$, where $L_z$ is the $z$ component of the orbital angular momentum, $S_z$ is the spin Pauli matrix, and $\lambda$ is the SOC strength. This results in different orbital mixing within the same site, $\varepsilon d_{i\alpha} d_{j\beta} \uparrow = \varepsilon d_{i\alpha} d_{j\beta} \downarrow = i\lambda$ and $\varepsilon d_{i\alpha} d_{j\beta} \uparrow = \varepsilon d_{j\beta} \downarrow = 0$. We use $2\lambda = 150$ meV, in good agreement with DFT calculations [5, 45] and experimental values [53, 138 meV [54] and 145 meV [55]]. With this Hamiltonian and the right choice of boundaries, one can construct a flake like the triangle we consider in [45].

In the infinite 2D MoS$_2$ monolayer, the first Brillouin zone has two inequivalent $K$ and $K'$ points, with a sizable spin-splitting around the VBM due to SOC (see figure 2(a)). There is a direct band gap (~1.6 eV) between the VBM and CBM at these two points, with definite spin-valley relation due to the absence of inversion symmetry in the unit cell. On the other hand, for finite systems the electronic spectrum (see figure 2(b)) shows both bulk- and edge-like states. The latter, coming from both the valence and conduction bands, appear into the 2D bulk gap, signaling the presence of 1D-like extended states localized near the borders of the sample [40, 56, 57].

The Hamiltonian for the magnetic impurities connected to specific sites of the TMD lattice is given by $H_i = J_{\alpha} \sum_{j=1,2} S_i^\alpha \cdot S_j (l_j)$, where $J_{\alpha}$ is the exchange coupling between the localized magnetic moment (either $i = 1$, 2) and the conduction electrons at lattice site $l$, and orbital $\alpha$ ($d_{z^2}, d_{xy}$ or $d_{x^2-y^2}$). $S_i^\alpha$ is the spin operator for the local magnetic moment $i$, and $S_0 (l)$ is the electron spin operator at site $l$, for orbital $\alpha$. When $J$ is small, the electronic degrees of freedom can be integrated out (using second order perturbation theory, for example) in the bulk 2D crystal, yielding an effective exchange interaction of the form

$$H_{RKKY} = J_{XX} (S_1^x S_2^x + S_1^y S_2^y) + J_{ZZ} S_1^z S_2^z + J_{DM} (S_1^z \times S_2^z),$$

where the $J$'s are proportional to the static spin susceptibility tensor of the electron gas [24–26]. The total effective interaction is a competition between in-plane $J_{XX}$ (= $J_{YY}$), Ising $J_{ZZ}$, and Dzyaloshinskii–Moriya $J_{DM}$ terms. In TMDs the Ising and DM terms are generated by the SOC; their competition has been recently discussed for bulk samples [31, 33] and flakes [47, 48]. To calculate the effective $J$'s in our finite sample,
we take the difference of triplet and singlet configurations of impurities in the electronic ground state [58, 59] as

$$J_{\beta\beta'} = \frac{E(\uparrow\beta, \uparrow\beta') - E(\uparrow\beta, \downarrow\beta')}{2S^2}$$

with $S = 1/2$ in our case. $\beta, \beta'$ represent the spin projection $(x, y, z)$ for magnetic impurities. For instance, $J_{d^z d^z}$ (XY = DM throughout the text) is the interaction strength between impurities when the spin of the first points along the $x$ direction and is hybridized to a $d_z$ orbital in the lattice, while the spin of the second points along $y$ and is hybridized to a $d_{z^2}$ orbital. This non-perturbative approach has been proved to be valid even for large values of local $J_n$ and is capable of generating results for any separation between impurities [59]. The ground state energy of the system, including both impurities, is calculated from the eigenvalue spectrum of the full Hamiltonian up to the Fermi energy $\epsilon_F$, as $E(S_1, S_2) = \sum_{i,\alpha} \epsilon_{i,\alpha} - \sum_{i,\alpha} \epsilon_{i,\alpha}$, where the $\epsilon_{i,\alpha}$ are obtained by exact numerical diagonalization of the full Hamiltonian, given here by a matrix of $6N_{\text{sites}} \times 6N_{\text{sites}}$.

3. Results

We present here results for triangular flakes of 50 rows, with a total of 1275 Mo atoms ($\approx 160$ Å on edge), within the range of sizes of real flakes that go from just a few sites [36] to several micrometers on edge [35]. This flake, large enough to yield experimentally relevant results, is shown schematically in figure 1. We study the RKKY interaction for doping levels lying inside the optical gap (see figure 2(b)). In this case, nearly 100 energy states have been brought from the bulk bands into the gap, with dominating $d_{z^2}$ character. As such, midgap levels correspond to $p$-doping levels from 1.82 to 9.08 $\times 10^{12}$ holes cm$^{-2}$. Such MoS$_2$ $p$-doping can be achieved by substituting Mo with Nb [60, 61], and are also predicted for different dopants [15, 22, 62], including P implantation [63].

Two magnetic impurities are hybridized to an edge of the flake, keeping one fixed and moving the second one along the zigzag edge, as shown schematically in figure 1. We fix the first impurity at the tenth row from the flake tip (yellow impurity 1 in figure 1), and move the second one from the 11th row onwards (brown impurity 2 in figure 1). The location of the impurities here is arbitrary but the results exhibit the main qualitative behavior, characterized by the impurity separation. We set $J_n = 0.3$ eV, and consider both impurities to be hybridized to Mo $d_{z^2}$ orbitals, since they are dominant on the edge states [48, 56]. This value of $J_n$ is a choice in accordance with predictions that range from a few meV to a couple hundred meV [18, 19, 21, 64], even at the edges [23].

In general, microscopic calculations could provide input for specific material-impurity pairs.

As mentioned, all midgap levels have wave functions entirely localized at/near the edges of the flake. Notice that energy levels fall into groups of six nearly-degenerate states, with wave function modulations along the edge, due to finite size effects. For instance, the first six midgap states closest to the VBM (see inset of figure 2(b)) show one antinode located in the middle of the flake edge, while the last six midgap states have 15 antinodes with a three-site period along the flake edge. The interaction $J_{p^z p^z}$ between magnetic impurities hybridized to these modulated wave functions on the edges, is largely dependent on the energy doping [48], since different states close to a given Fermi level carry different information on spin/spatial structure. This gives rise to complex oscillation patterns on the interaction between impurities. Effective RKKY interactions between impurities hybridized to other orbitals, $d_{xy}$ and $d_{x^2-y^2}$, are also possible on the edges, but are found to have smaller strength than for $d_{z^2}$ hybridization, given their correspondingly smaller contribution to the states. However, those interactions show the same separation dependence and relative strength of different exchange terms.

In what follows, the positive (negative) values of these $J_{d^z d^z}$ correspond to AFM (FM) alignment between impurities (we will omit the superindex labels from now on). Figure 3 shows two RKKY interaction profiles, for Fermi levels fixed at two different $p$-doped levels in the optical gap, with 82 and 22 holes, respectively. These two Fermi levels are indicated in the inset of figure 2(b). The results show typical oscillating RKKY behavior for all midgap energy levels. The three components (Ising, XX, and DM) oscillate between AFM and FM behavior, and have different oscillation pattern for different doping levels, as one would expect (see below). These oscillations are closely related to the $d_{z^2}$-orbital distribution along the flake edge of the wave function near the Fermi level, which shows similar spatial pattern of antinodes, as the characteristic Fermi wavelength dominates the resulting $J$. More importantly, the DM interaction is quite sizable, giving rise to a strong noncollinear interaction.

The Ising $J_{ZZ}$ and in-plane interactions $J_{XX} (= J_{YY})$ both decay with impurity separation, with $J_{XX}$ decaying faster than $J_{ZZ}$. The DM component $J_{DM}$ is seen to increase with distance, and reach larger amplitudes at the antinodes located after $r/a \approx 10$. The weaker $J_{DM}$ at short separation can be understood in terms of the finite size of the spin precession length induced by SOC, so that for close separations the host carrier scattering has not undergone significant spin rotation to generate a DM coupling. Clearly, the onset for DM interaction would depend on the strength of the SOC in the underlying band structure.

The strong DM interaction would be expected to yield a helical ground state for an assembly of multiple impurities. This tendency is exemplified in the lower panels of figure 3, where we schematically show the (classical) ground-state configuration of two impurities from different viewpoints (front, top and side). The first impurity is shown as a yellow arrow, while the second is shown in brown. The first impurity is fixed at an arbitrary orientation ($\theta_1 = \pi/4$ and $\phi_1 = \pi/2$), and the orientation of the second impurity that minimizes the energy at every $r/a$, is shown in the lower panels. Taking as input the parameters of the RKKY interaction strength shown in the upper panels of figure 3, the lowest energy configuration for the second magnetic moment is given by $\tan(\phi_2 - \phi_1) = J_{DM}/J_{XX}$, and $\tan \theta_2 = J_{ZZ} \sqrt{J_{DM}^2 + J_{XX}^2} \tan \theta_1$. The orientation of the second impurity is seen to twist gradually as $r/a$ increases.
with respect to the first impurity, a clear manifestation of the effect of the increasing DM interaction. If DM were not present, either in an Ising \(+XX\) model or a Heisenberg model, the relative orientation of the impurities will remain in just one plane.

We will now analyze the RKKY interaction for other midgap doping levels. Considering the same trajectory along the flake edge and \(dz^2\)-orbital hybridization as before, figure 4 shows two-dimensional maps of the Ising (panel (a)) and the DM (panel (b)) components of the RKKY indirect exchange, as a function of doping level, represented by the number of holes in the sample (horizontal axis), and as a function of the impurity separation \(r/a\) (vertical axis). The two doping levels shown in figure 3 (82 and 22 holes) are indicated at the top of the panels by magenta and cyan arrows, respectively. We can observe that at all doping levels the interaction is oscillatory between FM (in orange) or AFM (in violet), changing sign along the trajectory, with oscillation frequency that increases with higher Fermi energy (to the right on figure 4), associated with the shorter Fermi wavelength. Notice also that as the Fermi level moves up towards the edge of the conduction band, the overall magnitude of the interaction decreases, although oscillations are still visible. The drop in the effective exchange components is expected as the states higher in energy have a decreasing component of the \(dz^2\) orbital, have an overall lower density of states, and are increasingly more bulk-like—which moves the state into the bulk of the crystal and away from the edges. Regions of weak interaction, for doping such as between 24 and 30 (or 54 and 60), are the result of the first impurity being hybridized near a node of the \(dz^2\) orbital component at that Fermi level, suppressing the overall value of all \(J_s\). The in-plane \(J_{XX}\) interaction terms (not shown) show the same qualitatively behavior as \(J_{ZZ}\), but are seen to decay much more rapidly with separation, as illustrated by the cases shown in figure 3. Indeed, for small separations \((r/a \lesssim 20)\) the general trend is \(J_{ZZ} \approx J_{YY}\), and weak \(J_{DM}\), signaling a Heisenberg-like interaction; but for larger separations \((r/a \gtrsim 20)\), we see \(|J_{XX}| \ll |J_{ZZ}|\), while \(J_{DM}\) has become comparable to the Ising component. Hence, control of the doping levels throughout the optical gap provides a real tool for tuning the indirect exchange between impurities, being able to select non-collinear or isotropic, weak or strong, and AFM or FM behavior.

We now study the different spatial decay exponents for all the midgap doping levels. In order to extract the decay exponent for each term of the effective interaction, \(J_{\beta\beta'} \simeq r^d\), we plot the antinodes of each interaction curve versus impurity separation. Examples of such plots, in a log-log scale, are shown in figure 5. The effect of the increasing DM interaction is clearly seen, especially in side views, where the second impurity tends to twist towards the \(xy\) plane as \(r/a\) increases.
shown in the insets to each panel in figure 3, with a simple linear fit at large separations indicated by the dotted black lines. Notice that both $J_{ZZ}$ and $J_{XX}$ have negative slopes in the insets, as expected, while $J_{DM}$ has a positive slope (reflecting the fact that this term increases initially with separation, as discussed above). Figure 5 shows the evolution of the envelope $d$-exponent as a function of the midgap energy levels for each effective interaction term, $J_{ββ'} ∼ r^d$. For the Ising and XX interactions, $d$ has an ever more negative if slightly oscillating value for higher Fermi energy. $J_{ZZ}$ has an exponent $d$ predominantly between $−1/2$ and $−1$, showing that a rather long-range Ising interaction is present for all midgap states. In contrast, $J_{XX}$ is seen to quickly reach $d ≃ −2$, so that $J_{ZZ}$ clearly dominates at larger distances for all midgap dopings. The DM $d$ value oscillates around zero, as that interaction appears to not have yet reached the fully asymptotic regime for all midgap states. It is also clear that the DM interaction is of the same general magnitude as the Ising component, giving rise to strong non-collinear relative alignment of impurities.

The unusual long range interaction between impurities reported here ($d ≥ −1$) can be seen to arise mainly from the confinement of the edge/midgap states, which results in their effective 1D behavior, extended along the crystallite edge. This reduction in dimensionality is further aided by the finite size of the flake. This is evident in the overall modulation of the states deeper in the gap, with an effective wavelength along the edge limited by the size of the flake. It is remarkable that this modulation enhances the effective range of the indirect exchange interaction even for states closer to the conduction band (figure 5), although eventually $d ≃ −1$ for the Ising term. Notice that the envelope is further affected by the presence of antinodes in the edge states close to the Fermi level, as seen in figure 4. Although we had seen evidence of unusually long-range interaction on edges of triangular MoS$_2$ flakes before [48], this was studied only for two midgap states, and we thought the effect fragile. However, as we now see, the long range is rather robust to shifts in the Fermi level and for rather large flakes. This should facilitate its experimental study without the need for fine tuning, and allow for simple gating STM studies, as reported recently [46].

We should also comment on the transferability of these results to other TMDs. We have performed explicit calculations for WS$_2$, and found qualitatively similar results (not shown). That is, we find slow decay of the envelope function—as well as oscillations—with the same general features as discussed for MoS$_2$. As the structure features of these two materials are rather similar, it is not surprising that the indirect exchange results agree even quantitatively for Ising and XX
terms. However, the stronger SOC coupling results in relatively larger DM terms. Other materials would exhibit the same qualitative behavior.

Finally, we note that the bulk/edge correspondence of the interaction has been previously reported in other 2D materials, such as graphene [59, 65] and silicene [66]. For impurities on graphene nanoribbon edges, both zigzag [59] and armchair [65], the decay has been found to be slower than $r^{-2}$ but only for small impurity separations, while for larger separations there is an exponential decay; for impurities interacting in the bulk of the nanoribbon the $r^{-2}$ decay is naturally recovered. Silicene shows a topological insulator phase, and when impurities sit on zigzag edges, the interaction decays as $r^{-4}$ and is much stronger than in the bulk [66]. No unusually long range is reported for graphene or silicene, however. An interesting and different reduction of dimensionality in RKKY was also reported across graphene PN junctions [67].

4. Conclusions
We have studied the indirect interaction between magnetic impurities on the edges of a zigzag-terminated MoS$_2$ and WS$_2$ flakes. We focused on the role that edge states play on the interaction between impurities. We find that the 1D character of these states changes the dimensionality of the effective exchange interaction. This gives rise, especially, to long ranged Ising interactions that could be tuned via the deposition of magnetic impurities on the edge, and the selection of midgap states through doping. All midgap states localized on the edges are shown to exhibit sub-2D decay behavior. However, the in-plane component (XX) exhibits 2D behavior, especially at high doping. The non-collinear Dyaloshinskii–Moriya interaction is seen to gradually rise with separation, reaching an amplitude comparable to the Ising interaction after a separation of nearly ten lattice constants. All this behavior would suggest probing the tunable interaction between impurities near the edges of such TMD flakes, which would further result in stable helical structures for many-impurity assemblies which could be examined by local probes, such as spin-polarized STM [49–51]. Given the electronic and structural similarity of several TMDs, stable and well defined phases in these systems may open the door to interesting spintronic applications in these versatile material systems. We hope our predictions will motivate experiments with STM probes in the near future.

Acknowledgments
We acknowledge support from NSF grant DMR 1508325. O Á-O acknowledges a research fellowship from the Condensed Matter and Surface Science program at Ohio University.

ORCID iDs
O Ávalos-Ovando (https://orcid.org/0000-0003-3572-7675)
D Mastrogiuseppe (https://orcid.org/0000-0003-4606-2883)
S E Ulloa (https://orcid.org/0000-0002-3091-4984)

References
[1] Novoselov K S, Jiang D, Schedin F, Booth T J, Khotkevich V V, Morozov S V and Geim A K 2005 Proc. Natl Acad. Sci. USA 102 10451–53
[2] Geim A K and Grigorieva I V 2013 Nature 499 419–25
[3] Zhu Z Y, Cheng Y C and Schwingenschl"ogl U 2011 Phys. Rev. B 84 153402
[4] Cheiwchanwamnigan J and Lambrecht W R L 2012 Phys. Rev. B 85 205302
[5] Xiao D, Liu G B, Feng W, Xu X and Yao W 2012 Phys. Rev. Lett. 108 196802
[6] Mak K F, Lee C, Hone J, Shan J and Heinz T F 2010 Phys. Rev. Lett. 105 136805
[7] Radisavljevic B, Radenovic A, Brivio J, Giacometti V and Kis A 2011 Nat. Nanotechnol. 6 147–50
[8] Han W 2016 APL Mater. 4 032401
[9] Zhang K et al 2015 Nano Lett. 15 6586–91
[10] Wang J, Sun F, Yang S, Li Y, Zhao C, Xu M, Zhang Y and Zeng H 2016 Appl. Phys. Lett. 109 092401
[11] Huang C, Jin Y, Wang W, Tang L, Song C and Xiu F 2017 J. Semicond. 38 035004
[12] Tan H et al 2017 Small 13 1701389
[13] Liu G et al 2017 Nat. Chem. 9 810–6
[14] Nethravathi C, Prabhu J, Lakshmini B and Rajamathi M 2017 ACS Omega 2 5891–7
[15] Mishra R, Zhou W, Pennycook S J, Pantelides S T and Idoiro J C 2013 Phys. Rev. B 88 144409
[16] Andriotis A N and Menon M 2014 Phys. Rev. B 90 125304
[17] Lu S C and Leburton J P 2014 Nanoscale Res. Lett. 9 676
[18] Cong W T, Tang Z, Zhao X G and Chu J H 2015 Sci. Rep. 5 9361
[19] Shu H, Luo P, Liang P, Cao D and Chen X 2015 ACS Appl. Mater. Interfaces 7 7534–41
[20] Wang Y, Li S and Yi J 2016 Sci. Rep. 6 24153
[21] Vihakangas J, Lantto P, Vaara J, Huttula M and Cao W 2017 Chem. Commun. 53 5428–31
[22] Cheng Y C, Zhu Z Y, Mi W B, Guo Z B and Schwingenschl"ogl U 2013 Phys. Rev. B 87 100401
[23] Saab M and Raybaud P 2016 J. Phys. Chem. C 120 10691–7
[24] Radhakrishna A P, Smith P D and Konar S 1994 Phys. Rev. B 50 1037–45
[25] Kasuya T 1956 Prog. Theor. Phys. 16 45–57
[26] Yoshida K 1957 Phys. Rev. 106 893–8
[27] Fischer B and Klein M W 1975 Phys. Rev. B 11 2025–9
[28] Litvinov V I and Dugaev V K 1998 Phys. Rev. B 58 3584–5
[29] Parhizgar F, Asgari R, Abedinpour S H and Zareyan M 2013 Phys. Rev. B 87 125402
[30] Imamura H, Bruno P and Utsumi Y 2004 Phys. Rev. B 69 121303
[31] Parhizgar F, Rostami H and Asgari R 2013 Phys. Rev. B 87 125401
[32] Hatami H, Kerreiter T and Z"ulicke U 2014 Phys. Rev. B 90 045412
[33] Mastrogiuseppe D, Sandler N and Ulloa S E 2014 Phys. Rev. B 90 161403
[34] Chiu M H, Li M Y, Zhang W, Hsu W T, Chang W H, Terrones M, Terrones H and Li L J 2014 ACS Nano 8 9649–56
[35] van der Zande A M, Huang P Y, Chenet D A, Berkelbach T C, You Y, Lee G H, Heinz T F, Reichman D R, Muller D A and Hone J C 2013 Nat. Mater. 12 551–61
[36] Lauritsen J V, Kibsgaard J, Helveg S, Topsøe H, Clausen B S, Lægsgaard E and Besenbacher F 2007 Nano Lett. 7 253–8
[37] Li Y, Zhou Z, Zhang S and Chen Z 2008 J. Am. Chem. Soc. 130 16739–44
[38] Botello-Méndez A R, López-Urías F, Terrones M and Terrones H 2009 Nanotechnology 20 325703
[39] Tongay S, Varnoosfaderani S S, Appleton B R, Wu J and Hebard A F 2012 Appl. Phys. Lett. 101 123105
[40] Bollinger M V, Lauritsen J V, Jacobsen K W, Nørskov J K, Helveg S and Besenbacher F 2001 Phys. Rev. Lett. 87 196803
[41] Zhang J, Soon J M, Loh K P, Yin J, Ding J, Sullivan M B and Wu P 2007 Nano Lett. 7 2370–6
[42] Xu G, Wang J, Yan B and Qi X L 2014 Phys. Rev. B 90 100505
[43] Chu R L, Liu G B, Yao W, Xu X, Xiao D and Zhang C 2014 Phys. Rev. B 89 155317
[44] Rossi T P, Winther K T, Jacobsen K W, Nieminen R M, Puska M J and Thygesen K S 2017 Phys. Rev. B 96 155407
[45] Liu G B, Shan W Y, Yao Y, Yao W and Xiao D 2013 Phys. Rev. B 88 085433
[46] Lu C P, Li G, Mao J, Wang L M and Andrei E Y 2014 Nano Lett. 14 4628–33
[47] Ávalos-Ovando O, Mastrogiuseppe D and Ulloa S E 2016 Phys. Rev. B 94 245429
[48] Ávalos-Ovando O, Mastrogiuseppe D and Ulloa S E 2016 Phys. Rev. B 93 161404
[49] Zhou L, Wiebe J, Lounis S, Vedmedenko E, Meier F, Blügel S, Dederichs P H and Wiesendanger R 2010 Nat. Phys. 6 187–91
[50] Khajetoorians A A, Steinbrecher M, Ternes M, Bouhassoune M, dos Santos Dias M, Lounis S, Wiebe J and Wiesendanger R 2016 Nat. Commun. 7 10620
[51] Steinbrecher M, Rausch R, That K T, Hermanau J, Khajetoorians A A, Pothof F, Wiesendanger R and Wiebe J 2017 arXiv:1710.03515
[52] Pavlović S and Peeters F M 2015 Phys. Rev. B 91 155410
[53] Sun L et al 2013 Phys. Rev. Lett. 111 126801
[54] Alidoust N et al 2014 Nat. Commun. 5 4673
[55] Miwa J A, Ulstrup S, Størensen S G, Dendzik M, Čabo A G, Bianchi M, Lauritsen J V and Hofmann P 2015 Phys. Rev. Lett. 114 046802
[56] Segarra C, Planellés J and Ulloa S E 2016 Phys. Rev. B 93 085312
[57] Gibertini M and Marzari N 2015 Nano Lett. 15 6229–38
[58] Deaven D M, Rokhsar D S and Johnson M 1991 Phys. Rev. B 44 5977
[59] Black-Schaffer A M 2010 Phys. Rev. B 81 205416
[60] Laskar M R et al 2014 Appl. Phys. Lett. 104
[61] Suh J et al 2014 Nano Lett. 14 6976–82
[62] Dolui K, Rungger I, Das Pemmaraju C and Sanvito S 2013 Phys. Rev. B 88 075420
[63] Nipane A, Karmakar D, Kaushik N, Karande S and Lodha S 2016 ACS Nano 10 2128–37
[64] Qi J, Li X, Niu Q and Feng J 2015 Phys. Rev. B 92 121403
[65] Duffy J M, Gorman P D, Power S R and Ferreira M S 2014 J. Phys.: Condens. Matter 26 055007
[66] Zare M, Parhizgar F and Asgari R 2016 Phys. Rev. B 94 045443
[67] Zhang S H, Zhu J J, Yang W and Chang K 2017 2D Mater. 4 035005