1. Introduction

Two dimensional (2D) systems have been the subject of numerous studies addressing not only the fundamental research but also technological applications focusing the development of electronic devices. Such a 2D scenario in the material science was predicted by Geim and Grigorieva [1], where they present the concept of van der Waals (vdW) heterostructures, and more recently by Novoselov et al [2]. Here, the electronic properties of those vdW heterostructures can be tuned by stacking different sets of layered, semiconductor or metallic, materials.

Since the successful synthesis of single layer MoS\textsubscript{2} transistor [3], transition metal dichalcogenides (TMDCs) have been considered quite promising to be used in 2D vdW heterostructures. For instance, semiconductor/semiconductor vdW heterojunction composed by layered MoSe\textsubscript{2}/WSe\textsubscript{2} [4], and MoS\textsubscript{2}/WS\textsubscript{2} [5]. Here a formidable bandgap engineering can be done through a suitable choice of the stacked 2D materials, as well as the number of the stacked layers. Based on first-principles calculations, Kang et al [6] performed an extensive study of the band offsets of TMDCs. The band offsets were estimated by comparing the ionization potentials and the band gaps of the stacked 2D components, showing that MoSe\textsubscript{2}/WSe\textsubscript{2}, MoS\textsubscript{2}/WS\textsubscript{2} and MoS\textsubscript{2}/WSe\textsubscript{2} heterojunctions present type-II band alignment. Indeed, such a type-II band offset was verified in a recent experimental realization of MoS\textsubscript{2}/WSe\textsubscript{2} p–n heterojunction [7]. Meanwhile, metal/semiconductor 2D vdW heterostructures have been successfully synthesized through deposition of 2D (semi)metal on layered TMDC, for instance, graphene on TMDCs [8, 9], or 2D metallic TMDCs, like H-NbS\textsubscript{2}, on semiconductor TMDCs [10].

In vdW heterostructures, the Schottky barrier ($\Phi_B$) can be estimated by comparing the work function of the metal and the electronic affinity (n-type $\Phi_B$) or the ionization potential (p-type $\Phi_B$) of the semiconductor. Similarly to their 3D
counterpart, the height of the Schottky barrier can be tuned by an external electric field, as observed in field effect transistors (FETs). However, the hole injection in FETs based on (semiconductor) TMDC has been limited by the larger values of the p-type $\Phi_B$. There are some of proposals aiming to provide an efficient hole injection in TMDCs; for instance, by using the oxidized graphene at the source/drain contacts [11, 12], and more recently the inclusion of a BN monolayer at the metal/semiconductor interface [13]. However, the control of the p-type $\Phi_B$, in order to get an efficient hole injection in the metal/TMDCs heterojunctions, is still a challenge. Fortunately, nowadays we are facing an intense research on the new materials, including 2D crystals, allowing to make a number of material combinations focusing on a given electronic property; for instance the p-type Schottky barrier in metal/semiconductor-TMDCs.

Very recently metallic 2D boron sheets lying on the Ag(1 1 1) surface have been successfully synthesized, where one is characterized by vertically buckled boron atoms, hereafter named S0 (figures 1(a1) and (a2)) [14]. While the others, upon the presence of boron vacancies, are flat (S1 and S2 in figures 1(b1), (b2) and (c1), (c2)) [15]. Here one can guess that those 2D boron sheets may act as the metal contact in 2D vdW heterostructures. In a recent theoretical study [16], supported by the experimental findings [14], the authors verified that the oxidation of S0 is quite likely, giving rise to boron vacancies, which somewhat mimic the planar geometries of S1 and S2, as verified by Feng et al [15]. Beside the inertness with respect to the oxidation process, it has been reported that the boron sheets S1 and S2 are energetically more stable than the buckled geometry of borophene, S0.

In this work, based on the first-principles calculations, we investigate the energetic stability and the electronic properties of 2D metal/semiconductor heterojunctions. We have considered the recently synthesized boron sheets S0–S2 [14, 15] as the 2D metallic layer; and monolayers (MLs) of TMDCs MoSe$_2$ and WSe$_2$ as the semiconductor system. Our total energy results show that the energetic stability of those metal/semiconductor interfaces is mostly dictated by the vdW interactions. Further electronic band structure calculations reveal the formation of interface (metallic) states in S0/TMDC, pinning the Fermi level within the energy gap of the TMDC. On the other hand, S1/ and S2/TMDC heterojunctions present a tunable p-type Schottky barrier; where we show that the former system presents a p-type ohmic contact upon an external electric field smaller than 4 V nm$^{-1}$.

2. Method

The calculations were performed using the density functional theory (DFT) as implemented in the VASP code [17, 18]. The exchange-correlation potential was described within the generalized gradient approximation (PBE-GGA) [19], and the electron–ion interactions were treated by using the the projected augmented wave approach [20, 21]. The Kohn-Sham wave functions were expanded in a plane-wave basis set with an energy cutoff of 400 eV. The atomic positions were fully relaxed by including the van der Waals (vdW) interactions based on (i) the method developed by Tkatchenko and Scheffler (TS) [22], and (ii) the optimized version of the geometry unrestricted vdW-DF functional [23], optB88-vdW [24]. We have considered a force convergence tolerance of 20 meV Å$^{-1}$. In order to verify the validity of our results, the electronic structure of the pristine systems, viz.: single layer MoSe$_2$, WSe$_2$, and the boron sheets S0–S2 were calculated using HSE06 hybrid functional [25]. The metal/semiconductor interfaces were described within the slab method, where we have introduced a vacuum region of $\sim$15 Å, perpendicular to the metal/semiconductor interface, in order to prevent spurious interactions between a given interface and its (periodic) image. The Brillouin zone sampling was performed by using a set of $12 \times 12 \times 1$ k-points within the Monkhorst-Pack scheme [26].

3. Results

In figure 1 we present the structural models and the electronic band structures of pristine free-standing boron sheets S0–S2. In agreement with the recent experimental findings, boron atoms in S0 (figures 1(a1) and (a2)) present a vertical buckling of 0.91 Å, giving rise to boron stripes along the $\hat{a}$ direction. Meanwhile, upon the formation of boron vacancies, the structural models S1 and S2 become planar, figures 1(b1), (b2) and (c1), (c2). The electronic band structure of S0, figure 1(a3), presents a set of metallic bands for wave vectors parallel to the $\hat{a}$ direction, that is along the boron stripes; whereas there are no metallic bands for wave vectors along the $\Gamma Y$ and $SX$ directions. Such a band structure anisotropy is reduced in S1 and S2, figures 1(b3) and (c3). The energy bands of boron sheets S1 and S2 are characterized by the formation of dispersionless metallic bands along the YS, and higher density of states (DOS) near the Fermi level ($E_F$), when compared with the DOS of S0. In a previous work, we find that the anisotropy of the energy bands in borophene promotes a peculiar directional dependence of its electronic transport properties [27]. Here we will examine how those energy bands change upon the formation of 2D metal/semiconductor heterostructures, and their role on the Schottky barrier.

In figure 2 we present the structural models of metal/semiconductor systems (semiconductor = TMDCs MoSe$_2$ and WSe$_2$ monolayers), for metal = S0 (a), S1 (b), and S2 (c). In order to minimize the lattice mismatch between the boron sheets and the TMDC monolayers, the former were described by orthorhombic supercells with (2 $\times$ 2) surface periodicity along the $\hat{a}$ and $\hat{b}$ directions. In this case, the boron sheets are strained by up to $\pm 2.2\%$ with respect to their equilibrium lattice constant. For the MoSe$_2$ (WSe$_2$) MLs we have considered orthorhombic unit cells with the following surface periodicities, (1 $\times$ 1), (3 $\times$ 1), and (5 $\times$ 1) for S0/MoSe$_2$, S0/WSe$_2$, S1/MoSe$_2$, and S2/MoSe$_2$, S2/WSe$_2$, respectively. In this case, the MoSe$_2$ (WSe$_2$) monolayers are strained by up to $\pm 0.9\%$, when compared with their equilibrium lattice constant.
The energetic stability of 2D heterostructures was inferred through the calculation of the metal/TMDC binding energy ($E_b$), defined as

$$E_b = E[\text{metal}] + E[\text{TMDC}] - E[\text{metal/TMDC}],$$

where $E[\text{metal}]$ and $E[\text{TMDC}]$ represent the total energies of the separated systems, boron sheets and the TMDCs; and $E[\text{metal/TMDC}]$ is the total energy of the final system, metal/TMDC 2D heterojunction. Initially we have considered four different S0/TMDC interface configurations, where we found $E_b$ between 34 and 44 meV Å$^{-2}$ for S0/MoSe$_2$, and $E_b = 29–41$ meV Å$^{-2}$ for S0/WSe$_2$. At the equilibrium geometry, the borophene sheet S0 and MoSe$_2$ (WSe$_2$) ML presents a vertical distance ($d$) between 2.79 (2.90) and 3.17 Å (3.55 Å). Those findings of $E_b$ and $d$ are somewhat comparable with the ones obtained for bilayer-graphene on the Cu(111) surface [28], and allow us to infer that the energetic stability of borophene/TMDC systems is mostly dictated by vdW forces.

---

**Figure 1.** Structural models and the electronic band structure of the pristine borophene (a), and the boron sheets S1 (b), and S2 (c). In (a3)–(c3) the Fermi level is set to zero.

**Figure 2.** Structural models of S0/TMDC top view (a1) and side view (a2), S1/TMDC top view (b1) and side view (b2), S2/TMDC top view (c1) and side view (c2).
interactions. Indeed, by turning off the vdW contribution, we obtained $E_b$ of 0.13 meV $\AA^{-2}$ and $d = 3.97 \AA$. The binding energy reduces for the planar boron sheets S1 and S2, namely we obtained $E_b = 33$ and 31 meV $\AA^{-2}$ for S1/MoSe2 and S2/MoSe2, respectively, and $d > 3 \AA$. In order to provide further support to the energetic stability of the metal/TMDC interfaces, we have performed additional calculations by using the optB88-vdW [24] approach to describe the vdW interaction. The energetic stability of S0/TMDC has been confirmed, however, we find lower values of binding energies accompanied with larger values of equilibrium vertical distances. For instance, in S0/MoSe2 $E_b$ reduces to 26 meV $\AA^{-2}$, and $d$ increases to 3.03 $\AA$. Our results of binding energies and equilibrium geometries, for the energetically most stable configurations, are summarized in table 1.

Upon the formation of metal/TMDC heterostructures, there is a net charge transfer ($\Delta \rho$) at the metal/TMDC interface region. We may have a spacial picture of $\Delta \rho$ by comparing the total charge densities of the final system ($\rho[\text{metal/TMDC}]$) with the ones of the (initial) separated components, metallic boron sheet ($\rho[\text{metal}]$) and semiconductor MoSe2 and WSe2 ($\rho[\text{TMDC}]$),

$$\Delta \rho = \rho[\text{metal/TMDC}] - \rho[\text{metal}] - \rho[\text{TMDC}],$$

Figure 3. Total charge transfers, $\Delta \rho$, at the S0/MoSe2 (a), and S0/WSe2 (b) interface. Green regions indicate a net charge gain ($\Delta \rho > 0$), and blue regions indicate a net charge loss ($\Delta \rho < 0$) with respect to the isolated components (isosurfaces of $5 \times 10^{-4} e \AA^{-3}$).

In figures 3(a) and (b) we present our result of $\Delta \rho$ for S0/MoSe2 and S0/WSe2, where we verify that the interface region near the Se layer presents a charge density loss ($\Delta \rho < 0$), whereas near the borophene layer we find (mostly) $\Delta \rho > 0$. Based on the Bader charge density analysis [29], we find that the total charge density of the MoSe2 and WSe2 MLs reduces by 0.75 and $1.12 \times 10^{13} e \text{ cm}^{-2}$. By considering the vertical distance of 3.03 $\AA$ within the optB88-vdW approach (table 1), we find that the total charge densities of the MoSe2 and WSe2 MLs reduce by 0.52 and $0.93 \times 10^{13} e \text{ cm}^{-2}$. That is, indeed, there is a net charge transfer from the MoSe2 and WSe2 MLs to the boron sheet S0.

In figures 4(a) and (b) we present the projected electronic band structure of the S0/MoSe2 (a) and S0/WSe2 (b), projected on S0 (a1)–(b1), and projected on the MoSe2 (a2) and WSe2 (b2) MLs. The size of (blue and red) circles are proportional to the projected density of states. The Fermi level is set to zero.

Figure 4. Electronic band structures of the S0/MoSe2 (a) and S0/WSe2 (b), projected on S0 (a1)–(b1), and projected on the MoSe2 (a2) and WSe2 (b2) MLs. The size of (blue and red) circles are proportional to the projected density of states. The Fermi level is set to zero.

| Metal/semic. | $E_b$ (meV $\AA^{-2}$) | $d$ (Å) | $E_b$ (meV $\AA^{-2}$) | $d$ (Å) |
|-------------|----------------|------|----------------|------|
| S0/MoSe2    | 44             | 2.79 | 26             | 3.03 |
| S0/WSe2     | 41             | 2.90 | 26             | 3.03 |
| S1/MoSe2    | 33             | 3.33 | 24             | 3.32 |
| S1/WSe2     | 31             | 3.23 | 24             | 3.35 |
| S2/MoSe2    | 31             | 3.36 | 23             | 3.37 |
| S2/WSe2     | 30             | 3.39 | 23             | 3.37 |

Table 1. Results of binding energy ($E_b$) and equilibrium vertical distance ($d$) of S0/TMDC, S1/TMDC, and S2/TMDC considering two different vdW approaches, TS [22], and optB88 [24].
the TMDCs, indicated by red circles in figures 4(a2) and (b2), show that the MoSe2 and WSe2 MLs also contribute to the formation of $c_1$. Thus, it is indicated that the metallic interface states come from the hybridization between the electronic states of S0 and the TMDCs. Similar results were obtained by using optB88-vdW, however, the hybridization of $c_1$ is somewhat reduced due to the larger interlayer distance $d = 3.03 \text{Å}$.

Indeed, by increasing the vertical separation between S0 and the TMDC, we find that for $d$ about 4 Å the electronic contributions from the MoSe2 and WSe2 MLs to $c_1$ become negligible. $c_1$ becomes fully occupied and localized on the borophene layer. That is, the metallic interface states in S0/TMDC are suppressed by increasing the vertical distance, $d \gtrsim 4 \text{Å}$.

Our results of $E^*$ for S1 and S2 lying on the MoSe2 and WSe2 MLs are lower when compared with S0/MoSe2 and S0/WSe2; in addition, the interlayer separation increases to $d \approx 3.3 \text{Å}$, table 1. Those findings indicate that the electronic interaction between the boron sheets (S1 and S2) and the semiconductor MoSe2 and WSe2 MLs are weaker compared to the S0/TMDC systems. Indeed, this is what we find in figure 5, where we can see that the energy bands of the separated components are mostly preserved. Based on the Schottky-Mott approach, we find that the MoSe2 and WSe2 MLs on S1 present a p-type Schottky barrier. Here $\Phi_B$ is given by the energy difference between the VBM of the semiconductor ML and the Fermi level ($E_F$) of the metal/semiconductor heterostructure, $\Phi_B = E_F - E_{\text{VBM}}$. We find a p-type Schottky barrier of 0.15 eV in S1/MoSe2, while it reduces to $\Phi_B = 0.11 \text{ eV}$ in S1/WSe2. It is worth noting that, although the structural and energetic similarities with the S1/TMDC, the S2/MoSe2, and
S2/WSe2 interfaces present larger values of Schottky barrier, viz.: 0.44 and 0.31 eV. In S0/MoSe2 and S0/WSe2 we may infer $\Phi_B$ of 0.72 and 0.56 eV, respectively, considering the highest occupied states of $v1$ shown in figures 4(a2) and (b2). However, it is worth noting that (in this case) $\Phi_B$ is not well defined within the Schottky–Mott approach, due to the formation of hybridized energy band $c1$.

The control of the Schottky barrier through an external field, somewhat mimicking the gate electrical field, has been explored in other 2D metal/semiconductor systems [30, 31]. Here, based on the same approach, we examine the dependence between $\Phi_B$ and an external electric field perpendicular to the metal/TMDC interface ($E_\perp$). We find that $\Phi_B$ increases for $E_\perp$ pointing from the TMDC ML towards the boron sheet (i.e. positive values of $E_\perp$). While for negative values of $E_\perp$, the Schottky barrier reduces, becoming negative for $E_\perp$ less than $\approx -2$ V nm$^{-1}$ in S1/MoSe2 and S1/WSe2, giving rise to p-type ohmic contacts. Those results of $\Phi_B$ as a function of $E_\perp$ are summarized in figure 6. It is worth noting that, by increasing the strength of $E_\perp$, the other S2/MoSe2 and S2/WSe2 systems will also present p-type ohmic contacts. On the other hand, in contrast with the [31], we did not find any significative change of $\Phi_B$ as a function of $E_\perp$ in S0/TMDC; which can be attributed to the presence of metallic interface
states pinning the Fermi level in S0/TMDC, figure 4. Here, the dependence of $\Phi_B$ with the $E_\perp$, in S0/MoSe$_2$ and S0/WSe$_2$, was examined by considering both TS and optB88-vD approaches.

The p-type ohmic contact in S1/MoSe$_2$ and S1/WSe$_2$ is characterized by net charge transfer from the TMDC layer to S1. Indeed, we find a net charge transfers from the MoSe$_2$ and WSe$_2$ MLs to S1 of 6.9 and 8.9 $\times$ 10$^{12}$ e cm$^{-2}$, respectively. In figures 7(a1), (a2) and (b1), (b2) we present the electronic band structure of S1/MoSe$_2$ and S1/WSe$_2$ upon an external field of $-4$ V nm$^{-1}$. The projected energy bands on the boron sheet S1 (figure 7(a1)) and MoSe$_2$ ML (figure 7(a2)) show that (i) the metallic bands of S1 are preserved, however, near the Fermi level, they present a downshift when compared with the ones at $E_\perp = 0$ (figure 5(a1)); while (ii) the energy bands projected on the MoSe$_2$ is characterized by the formation of partially occupied states near the $\Gamma$-point. Those findings ((i) and (ii)) reveal that, indeed the S1/MoSe$_2$ interface exhibits a p-type ohmic contact which is tunable by an external electric field, $E_\perp$. The same scenario has been verified for the S1/WSe$_2$ interface. In figures 7(a3) and (b3), we present the charge density redistribution at the S1/MoSe$_2$ and S1/WSe$_2$ interfaces, respectively, for $E_\perp = -4$ V nm$^{-1}$, namely $\Delta \rho[E_\perp] = \rho[-4$ V nm$^{-1}] - \rho[0]$. For both S1/TMDC systems, we find $\Delta \rho[E_\perp] < 0$ mostly localized on the Se layer opposite to the interface region; while the boron-sheet S1 presents $\Delta \rho[E_\perp] > 0$, giving rise to a net charge density depletion at the S1/TMDC interface region.

4. Conclusions

Based on the first-principles calculations we have investigated the energetic stability and the electronic properties of 2D metal/TMDC vdW heterojunctions. We find that the recently synthesized planar boron sheets (S1 and S2) are good candidates to form p-type Schottky contacts with the TMDCs (MoSe$_2$ and WSe$_2$), viz.: S1/MoSe$_2$, /WSe$_2$, and S2/MoSe$_2$, and /WSe$_2$. There is a net charge transfer from the TMDCs to the boron sheets. Upon application of external electric field, we verify that the S1/MoSe$_2$ and /WSe$_2$ heterojunctions exhibit a p-type ohmic contact for $E_\perp$ about 4 V nm$^{-1}$ (absolute value). Similar results are expected for S2/MoSe$_2$ and /WSe$_2$, however for larger values of $E_\perp$. In contrast, such a Schottky barrier has not been verified for borophene/TMDCs, S0/MoSe$_2$ and S0/WSe$_2$. Instead we find the formation of metallic interface states, pinning the Fermi level within the bandgap of the TMDCs.

Acknowledgments

We would like to thank the Brazilian funding agencies CNPq, CAPES, FAPEMIG, and FAPESP. Part of calculations were performed using the computational facilities of CENAPAD/SP.

Table A1. Ionization potentials ($E_\text{ip}$ in eV) and the work functions ($W$ in eV) of the pristine systems, TMDCs and boron sheets, calculated using the PBE-GGA and HSE06 functionals.

|        | MoSe$_2$ | WSe$_2$ | S0  | S1  | S2  |
|--------|----------|----------|-----|-----|-----|
| $E_\text{ip}$ | HSE06    | PBE-GGA  |     |     |     |
| PBE-GGA | 5.32     | 5.09     | 5.28| 4.94| 4.78|
| HSE06  | 5.53     | 5.30     | 5.38| 4.95| 4.79|

Appendix

Since the chemical interactions at the metal/semiconductor interface region are negligible, the Schottky–Mott model is quite suitable to estimated the Schottky barrier ($\Phi_B$) in vdW metal/semiconductor heterojunctions. Within such an approach, the p-type Schottky barrier can be written as

$$\Phi_B = E_\text{ip} - W,$$

where $E_\text{ip}$ is the ionization potential of the semiconductor, and $W$ represents the metal work function. That is, the Schottky barrier has been estimated by comparing the intrinsic properties of the isolated components.

In order to check the validity of our findings, regarding the formation of p-type Schottky barrier in the boron metal/semiconductor heterojunctions studied in the present work, we have performed additional electronic structure calculations of using the HSE06 hybrid functionals.

Our PBE-GGA results of the ionization potential, table A1, are in good agreement with those obtained by Liu et al [10], while $E_\text{ip}$ calculated using the hybrid functionals (HSE06) increases by about 0.20eV. In this case, we find that, within the HSE06 approach, the p-type Schottky barrier (equation (1)) of S1/MoSe$_2$ (S1/WSe$_2$) increases from 0.38 to 0.58eV (0.15–0.35 eV), similarly $\Phi_B$ increases by about 0.2eV in S2/MoSe$_2$ and S2/WSe$_2$.

References

[1] Geim A K and Grigorieva I V 2013 Nature 499 419
[2] Novoselov K, Mishchenko A, Carvalho A and Neto A C 2016 Science 353 99439
[3] Radisavljevic B, Radenovic A, Brivio J, Giacometti I V and Kis A 2011 Nat. Nanotechnol. 6 147
[4] Huang C, Wu S, Sanchez A M, Peters J J, Beanland R, Ross J S, Rivera P, Yao W, Cobden D H and Xu X 2014 Nat. Mater. 13 1096
[5] Gong Y et al 2014 Nat. Mater. 13 1135
[6] Kang J, Tongay S, Zhou J, Li J and Wu J 2013 Appl. Phys. Lett. 102 012111
[7] Lee C H et al 2014 Nat. Nanotechnol. 9 676
[8] Yu L et al 2014 Nano Lett. 14 3055
[9] Shih C, Wang Q H, Son Y, Jin Z, Blankschtein D and Strano M S 2014 ACS Nano 8 5790
[10] Liu Y, Stradins P and Wei S H 2016 Sci. Adv. 2 e1600069
[11] Chuang S et al 2014 Nano Lett. 14 1337
[12] Musso T, Kumar P V, Foster A S and Grossman J C 2014 ACS Nano 8 11432
[13] Farmanbar M and Brooks G 2015 Phys. Rev. B 91 161304
[14] Mannix A J et al 2015 Science 350 1513
[15] Feng B, Zhang J, Zhong Q, Li W, Li S, Li H, Cheng P, Meng S, Chen L and Wu K 2016 Nat. Chem. 8 563
[16] Alvarez-Quiceno J C, Miwa R H, Dalpian G M and Fazzio A 2017 2D Mater. 4 025025
[17] Kresse G and Furthmüller J 1996 Comput. Mater. Sci. 6 15
[18] Kresse G and Furthmüller J 1996 Phys. Rev. B 54 11169
[19] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[20] Blüchl P E 1994 Phys. Rev. B 50 17953
[21] Kresse G and Joubert D 1999 Phys. Rev. B 59 1759
[22] Tckatchenko A and Scheffler M 2009 Phys. Rev. Lett. 102 073005
[23] Dion M, Rydberg H, Schröder E, Langreth D C and Lundqvist B I 2004 Phys. Rev. Lett. 92 246401
[24] Klimeš J, Bowler D R and Michaelides A 2009 J. Phys.: Condens. Matter 22 022201
[25] Heyd J, Scuseria G E and Ernzerhof M 2006 J. Chem. Phys. 124 219906
[26] Monkhorst H J and Pack J D 1976 Phys. Rev. B 13 5188
[27] Padilha J E, Miwa R H and Fazzio A 2016 Phys. Chem. Chem. Phys. 18 25491
[28] Souza E S, Scopel W L and Miwa R 2016 Phys. Rev. B 93 235308
[29] Bader R 1990 Atoms in Molecules: a Quantum Theory (Oxford: Oxford University Press)
[30] Padilha J, Fazzio A and da Silva A J 2015 Phys. Rev. Lett. 114 066803
[31] Liu L, Xiong S and Wu X 2016 Appl. Phys. Lett. 109 061601