Enhanced voltage-controlled magnetic anisotropy via magneto-elasticity in FePt/MgO(001)

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The interplay between magneto-electricity (ME) and magneto-elasticity (MEL) is studied in the context of voltage-controlled magnetic anisotropy (VCMA). Strain plays more than a role of changing lattice constant but that of the internal electric field in the heterostructure. As a prototype, FePt/MgO(001) is visited, where the behavior of two interfaces are drastically different: one exhibits switching the other does not. Whether an external electric field ($E_{ext}$) is present or not, we found VCMA coefficient larger than 1 pJ/V m, as a consequence of the rearrangement of $d$ orbitals with $m = \pm 1$ and $\pm 2$ in response to an external electric field. In addition, magneto-crystalline anisotropy (MA) is analyzed with strain taken into account, where non-linear feature is presented only accountable by invoking second-order MEL.

I. Introduction

The advent of spintronics has witnessed a realization of magnetic random access memory (MRAM), which compliments or replaces conventional memories. This progress has relied on giant magneto-resistance (GMR) and tunnel magneto-resistance (TMR). Moreover, the advancement is further pushed forward with the incorporation of spin-transfer torque (SST) and spin-orbit torque (SOT) for magnetization switching. In all cases, perpendicular magneto-crystalline anisotropy (PMA) is an essential ingredient to guarantee high bit density, lower switching current ($I_{SW}$) and thermal stability, $\Delta = K/\beta T$, where $K$ is anisotropy; $\beta$ is the Boltzmann constant; $T$ is temperature. In spite of notable success in MRAM, high $I_{SW}$ for switching and associated Joule heating are major obstacles to overcome.

Magneto-electric random access memory (MeRAM) has emerged as an alternative or compliments to MRAM, which utilizes voltage-controlled magnetic anisotropy (VCMA), where an external electric field ($E_{ext}$) manipulates switching from one magnetization state to the other. The efficiency of VCMA is characterized by a single parameter, the VCMA coefficient, $\beta = \Delta E_{MA}/\Delta E_{eff}$. The effective electric field, $E_{eff} = E_{ext}/\epsilon_\perp$, where $\epsilon_\perp$ is the out-of-plane component of the dielectric tensor of an insulator, and $E_{MA}$ is the magneto-crystalline anisotropy energy. In the pursuit of VCMA, various heterostructures have been explored, where FePt/MgO is one choice. $L_10$ FePt is ferromagnetic with a high Curie temperature of 750 K and MgO has widely been used substrate. In addition to $E_{ext}$, strain can be another driving force of VCMA, which influences $\beta$ through $\epsilon_\perp$ of the insulator or acts as an effective electric field at ferromagnetic-insulator interface even in the absence of $E_{ext}$. Hence, comparative studies of VCMA with and without strain would be intriguing.

In this work, magneto-electricity (ME) as well as magneto-elasticity (MEL) of FePt/MgO is investigated. The non-linear magneto-crystalline anisotropy as a function of strain ($\eta$) is explained by invoking second-order MEL contribution, which is usually ignored. Fe-interface shows spin-reorientation for $4.5 < \eta < 7\%$ while for Pt case MA is positive regardless of $\eta$. This difference stems from the competition between the positive effective anisotropy and negative first-order magneto-elasticity. Later, extremely large $\beta$ of FePt/MgO is presented as a result of an interplay between $\eta$ and $E_{ext}$. More specifically, the rearrangement of $d$ orbitals at the interface in response to $E_{ext}$ is the key, whose details are analyzed with band- and atom-resolved decompositions of MA.

II. Computational methods

First-principles calculations have been carried out using Vienna ab initio Simulation Package (VASP) package, with projector augmented wave (PAW) basis. Generalized gradient approximation is employed for the exchange-correlation potential. Cutoff of 500 eV for plane wave expansion and a $12 \times 12 \times 1 k$ mesh are used.

![Fig. 1. (a) Bulk FePt $L_10$ structure. 5 MLs of FePt on 8 MLs MgO (001) with (b) Fe- and (c) Pt-interface, respectively. Blue, green, cyan and red spheres represent Fe, Pt, O and Mg atoms, respectively. Surface, sub-surface, center, interface, and sub-interface layers are denoted by S, S-1, C, I, and I-1](image-url)

Fig. 1 shows the structure of bulk FePt and FePt/MgO film. Bulk FePt has $L_10$ structure [Fig. 1(a)] while the film consists of 5 monolayers (MLs) of FePt on 8 MLs MgO(001) [Fig. 1(b) and (c)]. In film, two different interfaces are taken into account by placing (i) Fe atoms on top of O atoms [Fig. 1(b)]
and (ii) Pt atoms on top of O atoms [Fig. 1(c)], which are referred to Fe- and Pt-interface, respectively. The vacuum region of 12 Å is taken between adjacent cells. Both interfaces are systematically studied, where S, S-1, C, I, and I refer to the surface, sub-surface, center, interface, and sub-interface layer, respectively. The optimized lattice constant of FePt and MgO are 3.864 and 4.212 Å, respectively, resulting in a large tensile strain (η) ~ 8.2% on the FePt layer, assuming the MgO substrate is unstrained. In order to study strain dependent MA of the system, η, defined as (a - aFePt)/aFePt, is varied from 0% (unstrained FePt lattice constant) to 8% (nearly unstrained MgO lattice constant), where aFePt is the equilibrium lattice constant of bulk FePt. Interlayer distances are relaxed for each strain with force criteria. Under tensile strain, both interfaces exhibit parabolic curve as shown in Fig. 2. However, one interface shows switching behavior but the other does not. For Fe-interface $E_{MA} < 0$ for 4.5 < η < 7%, whereas for Pt-interface $E_{MA}$ decreases with strain. The overall feature is expressed as

$$E_{MA} = E_{MA}^0 + b_1 t \sum_{k=1}^{3} \eta_k a_k^2 + \frac{1}{2} B_1 t \sum_{k=1}^{3} \eta_k^2 a_k^2, \quad (1)$$

where $E_{MA}^0$ is the zero strain anisotropy energy per area; $a_k$ and $\eta_k (k = 1, 2, 3)$ are the direction cosines of magnetization and the strain tensor, respectively; $t$ is the film thickness; $b_1$ and $B_1$ are the first- and second-order MEL coefficients, respectively.

MEL energy is expanded up to second-order of η, whose coefficient $B_1$ is usually small and ignored. However, it is explicitly taken into account here, whose consequence is discussed later. The zero-strain anisotropy energy is approximated as $K_1 t (1 - \alpha_2^2)$ for uniaxial symmetry. It is decomposed into bulk and interface contributions, $K_1 = K_1^b + K_1^i/t \approx K_1^i/t$ for thin film limit. In tetragonal structure, $\eta_1 = \eta_2 = \eta$ and the perpendicular strain $\eta_3$ is determined from magneto-elastic equation of state [See Supplementary Information]. Substituting the calculated strain value in Eq. (1) gives

$$E_{MA} = K_{eff} + (1 + \omega) b_1 t \eta + (1 - \omega) \frac{B_1}{2} t \eta^2, \quad (2)$$

where

$$K_{eff} = K_1^i + \frac{b_1^2}{c_{11}} \left( 1 + \frac{B_1}{2c_{11}} \right) t, \quad (3)$$

and

$$\omega = c_{11}^2 / (c_{11} + B_1)^2. \quad (4)$$

where $c_{11}$ is the elastic stiffness constant at constant magnetization. The derivation of Eq. (2) is also given in Supplementary Information.

Table I lists magneto-elastic and effective anisotropy coefficients, extracted by fitting ab initio results. The second-order term, $B_1$, responsible for the non-linearity is significantly large with 1.29 and 0.79 × 10^6 erg/cm^3 for Fe- and Pt-interface, respectively. The difference in magnitudes of $B_1$ for both interfaces arises due to different local environment of two interfaces. Fe atoms experience larger magneto-elasticity in the presence of MgO substrate than Pt interface. The difference of two interfaces is further discussed now.

**Table I.** First-order ($b_1$) and second-order ($B_1$) bulk magneto-elastic coefficients in (×10^6 erg/cm^3), and effective anisotropy ($K_{eff}$) coefficient in (erg/cm^2) for Fe- and Pt-interface, respectively.

| Interface | $b_1$ | $B_1$ | $K_{eff}$ |
|-----------|-------|-------|-----------|
| Fe        | -3.16 | 1.29  | 12.44     |
| Pt        | -2.43 | 0.79  | 21.57     |

The calculated $B_1$ is of the opposite sign to that of $b_1$ for both interfaces. Further, it has been asserted that in the presence of strain, $b_1(\eta) = b_1 + B_1 \eta^{19,20}$. In our study, the ratio $|B_1/b_1|$ is large for Fe-interface as compared to Pt-interface, leading to a change in sign of $b_1$ for large strain values. For the Fe-interface, a competition between $K_{eff}$ and $b_1 \cdot t$ produces

![Fig. 2. $E_{MA}$ as a function of η for (a) Fe- and (b) Pt-interface. Circles denote calculations and solid line represents fitting curve according to Eq. 2. Atomic layer decomposed $E_{MA}$ for (c) Fe- and (d) Pt-interface, respectively. Blue, red, and black bars represent η = 4, 6 and 8%, respectively.](image)
spin reorientation, for $4.5 < \eta < 7\%$. On the other hand, for the Pt-interface, $K_{eff, \text{Pt}} > b_1 \cdot t$ results in PMA for $\eta$ up to $8\%$.

Due to spin reorientation transition, we focus on $\eta = 4$, 6, and $8\%$. Fig. 2(c-d) provides atomic layer resolved $E_{MA}$-PMA mainly arises from Pt layers. Especially, the dominant PMA contribution comes from Pt(S-1) for Fe-interface and from Pt(I) for Pt-interface. Pt contribution to PMA is consistent with hard X-ray photoemission experiment$^{22}$. On the contrary, Fe atoms mostly contribute to $E_{MA} < 0$, except Fe(I) and Fe(S) layers. Under strain, the overall behavior of $E_{MA}$ remains the same for most of the atoms with changes in magnitude only. PMA from Fe(S), Pt(I-1) and Pt(C) at $\eta = 4\%$ becomes in-plane as $\eta$ approaches to $8\%$.

Now switching to VCMA, Fig. 3 shows change in MA as a function of $E_{eff}$ for $\eta = 4$, 6, and $8\%$. VCMA coefficient is defined as $\beta = \frac{\Delta E_{MA}}{\Delta \eta}$ in the linear regime of $E_{eff}$ as mentioned earlier. We choose $\varepsilon_{\uparrow}/\varepsilon_0$=20.0, 12.0, 9.8 for MgO when $\eta = 4$, 6, and $8\%$, respectively, taken from Ref. $^{22}$. Large VCMA coefficients are found for both interfaces. For Pt-interface, $\beta = 1.24$, -1.35, and -1.36 pJ/(V m) under $\eta = 4$, 6, and $8\%$, respectively. On the other hand, Fe-interface exhibits qualitatively different VCMA with strain. The V-shape curve is apparent for $\eta = 4$ and $6\%$ with $\beta = 1.70$ (-0.44) and 0.79 (-1.53) when $E_{eff} > 0$ ($E_{eff} < 0$), respectively. At $\eta = 8\%$, the VCMA curve changes to A-shape with $\beta = -1.77$ (1.68) under $E_{eff} > 0$ ($E_{eff} < 0$).

MA and VCMA, orbital resolved bands at $\eta = 8\%$ are plotted in Fig. 4 along high symmetry lines in two-dimensional Brillouin zone (BZ) under $E_{eff} = +76.5$, 0, and -76.5 mV/Å. The $\eta = 8\%$ case are discussed in detail as it shows largest VCMA coefficient. For Fe- and Pt-interfaces, only the majority spin channel of Fe $d$ bands and majority spin channel of Pt $d$ bands are presented, respectively, as other spin channels do not contribute significantly to PMA. The $d_{yz}$ orbitals for both interfaces can contribute negatively to PMA and are shown in Supplementary Information. Both spin channels for Fe and Pt $d$ bands at $\eta = 8\%$, 6%, and 4% are also provided in Fig. S1 and Fig. S2 in Supplementary Information, respectively.

In the framework of perturbation theory$^{23}$, positive (negative) $E_{MA}$ comes from spin-orbit coupling (SOC) between the unoccupied and occupied majority or minority spin states with the same (different) magnetic quantum number through $\ell_z(\ell_z)$. This approach has been widely applied in various systems$^{24-29}$.

First, we discuss without $E_{cut}$, namely, strain-induced MA. For Fe-interface, $E_{MA} > 0$ arises from $\langle d_{xy} | \ell_z | d_{yz} \downarrow \rangle$ and $\langle d_{xz} \downarrow | \ell_z | d_{yz} \downarrow \rangle$ along $\Gamma X M$ [Fig. 4(b)]. Similarly, for Pt-interface $E_{MA} > 0$ mainly comes from $\langle d_{z^2-\ell_x} \uparrow | \ell_z | d_{sy} \uparrow \rangle$ along $\Gamma T$ [Fig. 4(e)]. As tensile strain decreases, $d$ bands experi-

FIG. 3. VCMA of FePt/MgO heterostructure at different strain values for Fe- (left-panel) and Pt-interface (right-panel), respectively. Upper, middle, and lower row represent strain ($\eta$) of 4, 6, and $8\%$, respectively. VCMA coefficient are denoted inside each plot.

FIG. 4. Orbital resolved interfacial (a-c) Fe $d$ bands for minority spin, (d-f) Pt $d$ bands for majority spin along $\Gamma X M \Gamma$ at $\eta = 8\%$ under $E_{eff} = +76.5$, 0, -76.5 mV/Å. Blue, cyan, pink, and yellow for $d_{xz}, d_{z^2-\ell_y}, d_{yz}$, and $d_{xy}$. The $d_{z^2}$ bands can contribute negatively to PMA and are not plotted here.
ence overall downward shift for Fe-interface. However, for Pt-interface, $d_{xy}$ and $d_{z^2-r^2}$ moves upward and downward, respectively, with decreasing strain, which is shown in Fig. ?? and Fig. ?? in Supplementary Information. Strain driven band rearrangement leads to substantial change in $E_{MA}$ as $E_{MA} \propto \Delta = 1/(e_u - e_o)$, where $e_u$ ($e_o$) denotes energies of unoccupied (occupied) bands. In particular, at $\eta = 6\%$ for Fe-interface, $E_{MA} < 0$ comes from $\langle d_{xy} \downarrow | \epsilon \downarrow d_{z^2-r^2} \downarrow \rangle$ around $\nabla \Sigma M$. Also, at $\eta = 8\%$, $E_{MA} > 0$ is through $\langle d_{xy} \downarrow | \epsilon \uparrow d_{z^2-r^2} \downarrow \rangle$ around $\nabla X$.

Moving to VCMA, bands shift at $\eta = 8\%$ under $E_{eff} = \pm 76.5\ mV/\AA$ are shown in top and bottom panels of Fig. 4. To understand in a simple picture, a schematic diagram is illustrated in Fig. 5. $\Delta^\alpha = 1/(e_u - e_o)$ ($\alpha = +,0, -$) denotes the inverse of the energy difference between unoccupied and occupied bands when $E_{eff}$ is positive, zero, and negative, respectively.

Summing all SOC matrices, $\Delta^0 > \Delta^+ > \Delta^-$ justifies the $\Lambda$-shaped VCMA for Fe-interface. Under zero-field, occupied $d_{z^2-r^2}$ ($d_{xz}$) bands couples with unoccupied $d_{xy}$ ($d_{yz}$) bands at $\nabla \Sigma M$, giving $E_{MA} > 0$. With $E_{eff} = \pm 76.5\ mV/\AA$, unoccupied bands $d_{xy}$ and $d_{yz}$ becomes occupied, resulting in $E_{MA} = 0$. Moreover, when $E_{eff} > 0$, $d_{xy}$ and $d_{xz}$ occupied bands along with $d_{z^2-r^2}$ and $d_{yz}$ unoccupied bands move towards $E_F$ at $\nabla X$ and $\nabla M$, providing large PMA. While when $E_{eff} < 0$, these bands moves away from $E_F$, as a result contributing small PMA. On the other hand, for Pt-interface, $\Delta^- > \Delta^0 > \Delta^+$ explains linear VCMA. When $E_{eff} < 0$, the unoccupied $d_{xy}$ band and occupied $d_{z^2-r^2}$ band at $\nabla X$, shift towards $E_F$ with respect to zero-field, resulting in enhanced PMA. However, when $E_{eff} > 0$, both these bands move away from $E_F$ as compared to zero-field, hence PMA is reduced.

FIG. 5. Schematic diagram of bands shift under $E_{eff}$, $\Delta^\alpha = 1/(e_u - e_o)$ represents the strength of SOC, where $e_i$ ($e_o$) are energies of unoccupied (occupied) band; $\alpha = +,0, -$ denotes when $E_{eff} > 0$, $E_{eff} = 0$, and $E_{eff} < 0$, respectively. Vertical arrows indicates possible coupling responsible for PMA.

IV. Conclusions

In summary, we investigated strain dependent voltage-controlled magnetic anisotropy for both Fe- and Pt-interfaces of FePt/MgO(001) film using $ab\ initio$ electronic structure calculations. We predicted a huge VCMA coefficient $\sim 1.77\ pJ/(V\cdot m)$ due to the internal electric field as a result of strain. Moreover, magneto-crystalline anisotropy as a function of strain is also discussed. The strain-dependent non-linear magneto-crystalline anisotropy is explained by invoking second-order magneto-elastic (MEL) term in MA energy. Fe-interface shows spin-reorientation for $4.5 < \eta < 7\%$ as a consequence of the competition between the positive $K_{eff}$ and negative $b_1 \cdot t$. Magneto-crystalline anisotropy turns out to be extremely sensitive to strain and interface. Our finding provides a direction for experiments to achieve enhanced VCMA coefficient along with large PMA for ultra-low power non-volatile memory devices.

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Supplementary Material:

Qurat-ul-ain\textsuperscript{1}, D. Odkhuu\textsuperscript{2}, S. H. Rhim\textsuperscript{1} \& S. C. Hong\textsuperscript{1}\

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Derivation of magneto-crystalline anisotropy energy density

The magneto-crystalline anisotropy energy \( E_{MA} \) is written as

\[
E_{MA} = K_1 t(1 - \alpha_3^2) + b_1 t \sum_{k=1}^{3} \eta_k \alpha_k^2 + \frac{1}{2} B_1 t \sum_{k=1}^{3} \eta_k^2 \alpha_k^2,
\]

(1)

where the first-term is the zero strain anisotropy energy and the latter two are the magneto-elastic energy terms[1]. As mentioned in the main text, \( K_1 \) is the anisotropy constant, \( \alpha_k (k = 1, 2, 3) \) are the direction cosines of magnetization with respect to the principal axis, \( b_1 \) and \( B_1 \) are the first- and second-order magneto-elastic coefficients, respectively[2], and \( \eta_k (k = 1 - 6) \) is the strain tensor in Voigt’s notation. For a thin film grown epitaxially along the [001] crystallographic directions, shear strains, i.e., \( \eta_4 = \eta_5 = \eta_6 = 0 \) and \( \eta_1 = \eta_2 = \eta \) due to tetragonal symmetry. The lattice strain \( \eta_k \) in Eq. 1 can be calculated via boundary conditions of the problem using the magneto-elastic equation of state, given as:

\[
\sigma_k = \frac{\partial}{\partial \eta_k} \left( b_1 t \sum_{k=1}^{3} \eta_k \alpha_k^2 + \frac{1}{2} B_1 t \sum_{k=1}^{3} \eta_k^2 \alpha_k^2 + \frac{1}{2} c_{11} \sum_{k=1}^{3} \eta_k^2 + c_{12} \sum_{j,k=1 \atop j \neq k}^{3} \eta_j \eta_k \right),
\]

(2)

where \( \sigma_k \) is the mechanical stress. \( c_{11} \) and \( c_{12} \) are the elastic stiffnesses at constant magnetization. From the condition \( \sigma_3 = 0 \), which follows from the relaxation of the interlayer distance perpendicular to the film plane. One further obtains:

\[
\eta_3 = -\frac{2 \eta c_{12} + b_1 \alpha_3^2}{c_{11} + B_1 \alpha_3^2},
\]

(3)

From the Poisson’s ratio expression \( \nu = c_{12}/(c_{11} + c_{12}) \), we obtain \( c_{12}/c_{11} = \nu/(1 - \nu) \). Where \( \nu \approx \frac{1}{3} \) for transition metals[1], which gives \( c_{12} = c_{11}/2 \). The zero strain anisotropy energy can be further decomposed into bulk and interface contributions, \( K_1 = K_1^I + K_1^V/t \approx K_1^I/t \) for thin film limit. By substituting \( \eta_3 \) in Eq. 1 and calculating the energy required to rotate magnetization from in-plane (\( \alpha_1 = 1 \)) to out-of-plane (\( \alpha_3 = 1 \)), we get:

\[
E_{MA} = K_{eff} + (1 + \omega) b_1 t \eta + (1 - \omega) \frac{B_1}{2} t \eta^2,
\]

(4)

where

\[
K_{eff} = K_1^I + \omega \frac{b_1^2}{c_{11}} \left( 1 + \frac{B_1}{2c_{11}} \right) t,
\]

(5)

and

\[
\omega = c_{11}^2 / (c_{11} + B_1)^2.
\]

(6)
Orbital resolved band structure

Orbital resolved bands at $\eta = 4\%, 6\%$, and $8\%$ are plotted along high symmetry direction in 2-D Brillouin zone as shown in Fig. S1 for Fe-interface and Fig. S2 for Pt-interface. For Fe-interface, majority spins are almost occupied. Most of the perpendicular magneto-crystalline anisotropy (PMA) arises from minority spin channel. For Pt-interface, minority spins are the major contributor to PMA. With increasing compressive strain, Fe and Pt $d$ bands overall shift towards lower energy.

Spin-orbit coupling between $d$ bands

In Table. S1 we provide a list of positive spin-orbit coupling (SOC) between $d$ bands for both Fe- and Pt-interfaces. The strength of the SOC is $\Delta^\alpha = \frac{1}{e_u - e_o}$. Here, $e_u$ and $e_o$ are the energies of unoccupied and occupied bands; $\alpha = +, 0, -$ denotes when $E_{eff} > 0$, $E_{eff} = 0$, and $E_{eff} < 0$, respectively. For Fe-interface, $d_{xy}$ and $d_{x^2-y^2}$ bands couples at $\overline{X}$ providing large PMA at $E_{eff} = 0$. Under $E_{eff} > 0$, this coupling increased up to two times due to band shift towards $E_F$. Alternatively, due to band shift away from $E_F$ under $E_{eff} < 0$, this coupling reduces. Moreover, $d_{xz}$ and $d_{yz}$ bands also yield large PMA at $\overline{M}$. For Pt-interface, electric field effects the SOC strength linearly, i.e. $\Delta^- > \Delta^0 > \Delta^+$. $d_{xy}$ and $d_{x^2-y^2}$ bands at $\overline{X}$ shift towards $E_F$ under $E_{eff} < 0$, providing large PMA. However, these bands move away from $E_F$ under $E_{eff} > 0$, reducing PMA contribution.

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FIG. S1. Orbitally resolved Fe $d$ bands for majority and minority spins along $\Gamma$-X-M-$\Gamma$ direction in 2D Brillouin zone at the FM/I interface for $\eta = 8$, 6, and 4%, respectively. The reference energy ($E = 0$ eV) places at $E_F$. Blue, cyan, pink, purple and golden color for $d_{xz}$, $d_{x^2-y^2}$, $d_{yz}$, $d_{z^2}$ and $d_{xy}$. 

Note: The figure shows the band structure for different values of $\eta$ and highlights the orbital contributions for each spin state.
FIG. S2. Orbitally resolved Pt $d$ bands for majority and minority spins, along $\Gamma-X-M-\Gamma$ direction in 2D Brillouin zone at the FM/I interface for $\eta = 8, 6, \text{ and } 4\%$, respectively. The reference energy ($E=0$ eV) places at $E_F$. Blue, cyan, pink, purple and golden color for $d_{xz}$, $d_{x^2-y^2}$, $d_{yz}$, $d_{z^2}$ and $d_{xy}$. 
### Table S1

| Symmetry Point | Coupled Bands | $\Delta^-$ | $\Delta^0$ | $\Delta^+$ |
|----------------|---------------|------------|------------|------------|
| Fe-interface $\bar{X}$ | $d_{xy}, d_{\hat{x}^2-y^2}$ | 2.558 | 6.897 | 12.300 |
| | $d_{xz}, d_{yz}$ | 5.540 | 5.903 | 6.763 |
| | $d_{xy}, d_{\hat{x}^2-y^2}$ | 2.004 | 2.151 | 2.015 |
| | $d_{xz}, d_{yz}$ | 1.998 | 2.010 | 2.109 |
| $\bar{M}$ | $d_{xy}, d_{\hat{x}^2-y^2}$ | 2.782 | 2.782 | 2.961 |
| | $d_{xz}, d_{yz}$ | 1.024 | 1.011 | 1.075 |
| | $d_{xy}, d_{\hat{x}^2-y^2}$ | 1.530 | 1.487 | 1.541 |
| $\frac{1}{2}
\bar{X}\bar{M}$ | $d_{xy}, d_{\hat{x}^2-y^2}$ | 1.783 | 1.700 | 1.792 |
| | $d_{\hat{x}^2-y^2}, d_{xy}$ | 0.000 | 7.100 | 0.000 |
| | $d_{xy}, d_{\hat{x}^2-y^2}$ | 1.447 | 1.335 | 1.475 |
| | $d_{xz}, d_{yz}$ | 1.024 | 1.011 | 1.065 |
| Pt-interface $\bar{X}$ | $d_{xy}, d_{\hat{x}^2-y^2}$ | 0.766 | 0.769 | 0.760 |
| $\bar{M}$ | $d_{\hat{x}^2-y^2}, d_{xy}$ | 0.643 | 0.640 | 0.638 |
| $\frac{1}{2}M\Gamma$ | $d_{\hat{x}^2-y^2}, d_{xy}$ | 0.526 | 0.524 | 0.524 |

$\Delta^\alpha = \frac{1}{e_u - e_o}$ represents the strength of SOC, where $e_u$ ($e_o$) are energies of unoccupied (occupied) band; $\alpha = +, 0, -$ denotes when $E_{eff} > 0$, $E_{eff} = 0$, and $E_{eff} < 0$, respectively.