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Electronic structure and magnetic anisotropy of a constrained Fe chain in an electric field

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Abstract

The electronic structure and magnetic anisotropy were studied for a constrained iron chain in an electric field by means of the first-principles approach. The electron induced by the electric field was found to occupy mainly the extended s-like orbitals which is well hybridized with the $d_{3z^2-r^2}$ localized orbital. The magnetic anisotropy was observed to decrease with the number of induced electrons and to depend on the magnetization direction. The magnetization perpendicular both to the chain and the electric field modifies the electron dispersion relation to be asymmetrical, which implies an expectation of variable transport property with both the external electric and magnetic fields.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The electronic technology to control magnetization by using an electric field or an electric current has been studied to develop a high-density recording media for the next generation. Chiba *et al* have succeeded in changing the magnetic anisotropy energy (MAE) of a ferromagnetic semiconductor (In, Mn)As by using the electric field [1]. It was confirmed that it is also possible to change the coercivity of FePd and FePt thin films by an electric field [2]. The last material has been found to keep a stability of the magnetic property in the nanosized structure [3] and has been a candidate for high-density recording media. Such magnetic systems have been interesting in building spintronics devices [4].

In surface science, Gambardella *et al* fabricated a Co nanowire on a Pt(111) surface by using a self-assembly epitaxial technique and characterized magnetic properties of the system [5]. The similar system, thin Fe layer on Pt surfaces, has also been studied by Repetto *et al* [6]. In the previous work, we have investigated magnetic anisotropy of the iron chain on Pt(111) and (664) surfaces by using the first-principles approach [7, 8]. In the next theoretical approach, it is interesting to investigate magnetic properties of nanostructures in an electric field. Magnetic properties in such a magnetic system may be controlled through the change of electronic

state by the electric field. As a first step to evaluate the changes of magnetic properties by an electric field, we investigated magnetic anisotropy and electronic structure of a constrained iron chain in the present work. The electrons induced by the electric field are distributed in the s-component of Fe orbitals. Due to orbital hybridization, this gives a redistribution of electron occupation in the Fe 3d orbital extended along the chain, resulting in a decrease of MAE when increasing the number of electrons. For neutral iron chains, some groups have already published details of the electronic structure and the magnetic anisotropy [9–11].

2. System and method

We investigated the electronic structure and magnetic anisotropy of the iron chain in an electric field. We employed the local spin density approximation (LSDA) [12, 13] in the Kohn–Sham (KS) theory [14]. We used the pseudopotential plane-wave method [15, 16] with the fully relativistic version [17] in which the wavefunction has the two-component spinor form [18]. This method self-consistently contains the spin–orbit interaction (SOI) [19, 20], which is the main origin of magnetic anisotropy. We can apply the electric field on the iron chain by using the effective screening medium (ESM)

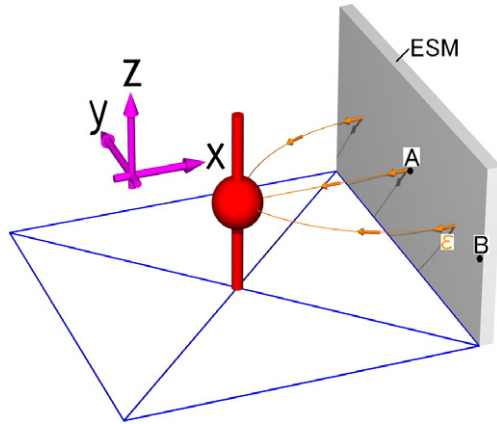


Figure 1. Schematic diagram and coordination of axes for the iron chain in the electric field. The effective screening medium (ESM) indicates the ideal conductor.

method developed by Otani and Sugino [21]. To set up such an electric field, one needs the system to charge up by a variable number of electrons in the system with a separately placed ideal conductor (this is the ESM). The schematic configuration of the calculated system is drawn in figure 1. In this work, we investigated systems with a number of induced electrons which varies from -0.2 to 0.2 per atom. The tetragonal cell parameters in solving the KS equation were set to $a = b = 20$ au and $c = 5.23$ au. The iron atom is centered in the cell and the ideal conductor is placed at the edge of the cell. The iron-iron distance is set to the same length in the iron chain on the Pt(111) surface. The energy cutoffs of 30 and 300 Ryd were taken for wavefunctions and densities, respectively [16]. We estimated MAEs by the total energy difference with the calculations of the $1 \times 1 \times 32$ \mathbf{k} point mesh.

For the bulk system, to treat a variable number of electrons, one can apply a compensated jellium (CJ) model in which the uniform density is added to realize a electrically neutral system. In the present work, it is interesting to see the difference between the CJ approximation and the ESM model.

3. Result

Total energies of the constrained Fe chain were calculated for the x (anti-parallel to the electric field at the ESM), y , and z (along the chain) magnetization directions with respect to strengths of the electric field. The resulting MAEs are shown with respect to the number of induced electrons in figure 2, compared with the results for the CJ model. The MAE at the neutral is 3.23 meV/Fe and the magnetic easy axis is along the chain. This value is comparable to those of the previous work for the absolutely free-standing and elongated Fe chains [9–11]. The easy axis direction never changes in all cases in the present investigation. The electric field averaged over the surface of the ESM is estimated with respect to the number of electrons in figure 2(b). This electric field is insensitive to the magnetization of the system for a given number of induced electrons but the position dependence in the surface of the ESM was observed; the value at point A in figure 1 monotonically decreases with moving to point B and the electric field of B is about 0.7 times smaller than that of A. Along the z axis, the electric field on the ESM is also insensitive.

In figure 2(a), the MAE monotonically decreases with the increase in the number of induced electrons from neutral. On the other hand, it gradually increases as the number of electrons decreases. The MAE of $E_x - E_y$, where E_α is the total energy for the magnetization of the α axis, monotonically increases as the number of electrons increases, as shown in figure 2(b). This non-vanishing property of the MAE is caused by the symmetry breaking imposed by the electric field. When the number of induced electrons is 0.2, the value of $E_x - E_z$ in the electric field decreases by 24% from that of the neutral. The CJ model provides an intermediate between $E_x - E_z$ and $E_y - E_z$ around neutral but, when the number of electrons increases, the MAE did not decrease rapidly unlike the cases of the electric field.

The contribution to MAE from each \mathbf{k} point is considered to be of two types [22]. When there are orbital degenerate levels at the Fermi level, the SOI lifts them off, depending on the magnetization direction. This level splitting can be described by $\xi m \cos \theta$, where ξ is the spin-orbit coupling

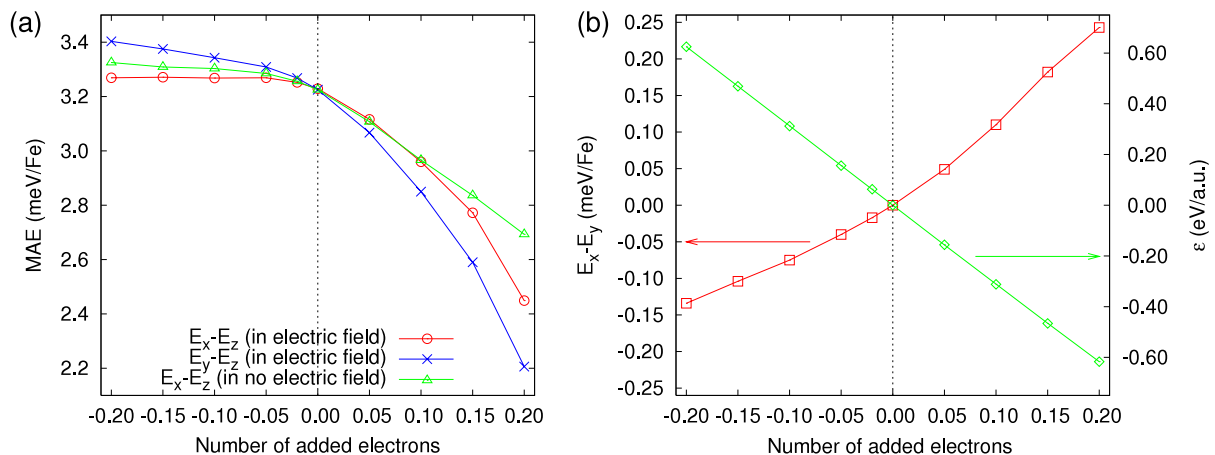


Figure 2. Magnetic anisotropy energies (MAEs) in the electric field as a function of the number of induced electrons; $E_x - E_z$ (red circles), $E_y - E_z$ (blue crosses), $E_x - E_y$ (red squares), compared with $E_x - E_z$ of the compensated jellium (CJ) model (green triangles). The green diamonds in (b) show the observed relation between the electric field and the number of induced electrons.

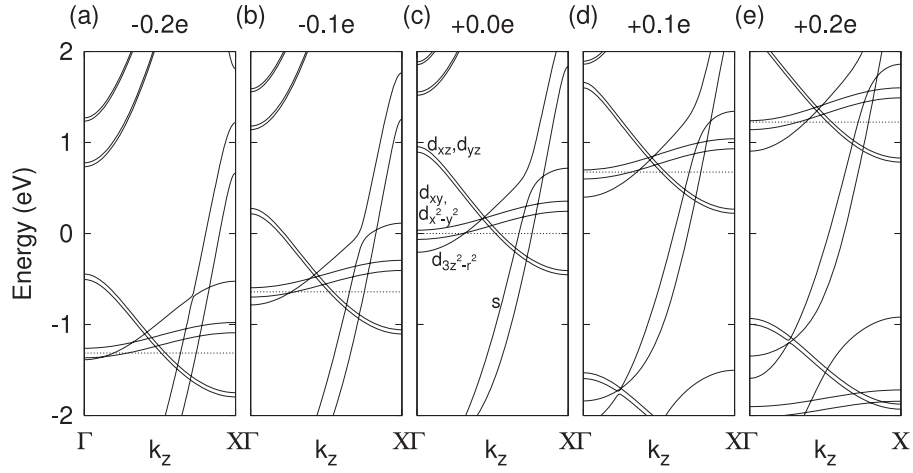


Figure 3. Band dispersions along the chain in the electric field for the magnetization easy axis (magnetization along the chain); the number of induced electrons (a) -0.2 , (b) -0.1 , (c) 0 , (d) 0.1 , (e) 0.2 . The energies are taken with respect to the Fermi level of the neutral system.

coefficient, m is the orbital magnetic quantum number for the quantization axis and θ is the angle formed by the magnetization direction and the quantization axis. The total energy change of such a level splitting is the first contribution. The second contribution is the second perturbative one, which is given by the following;

$$E_x - E_z \propto \sum_{o,u} \frac{|\langle o | \ell_z | u \rangle|^2 - |\langle o | \ell_x | u \rangle|^2}{\epsilon_u - \epsilon_o}, \quad (1)$$

where o and u specify occupied and unoccupied states and the ℓ_x and ℓ_z are angular momentum operators. The pair of occupied and unoccupied states around the Fermi level is important. The coupling by ℓ_x connects between the atomic orbitals of the different magnetic quantum number ($\Delta m = \pm 1$, for example, $d_{3z^2-r^2}$ ($m = 0$) and d_{xz}, d_{yz} ($m = \pm 1$)). Such contributions decrease the MAE in equation (1). The operator of ℓ_z , which does not change the magnetic quantum number, participates in an increase of the MAE. In our previous work [11], we found that the contribution from the d_{xy} and $d_{x^2-y^2}$ bands is very important for magnetic anisotropy of the iron chain in the neutral. The contribution from the lifting degeneracy of these bands at the Fermi level increases the MAE of $E_x - E_z$. It cannot explain the decrease of the MAE with respect to the number of induced electrons (figure 2(a)), only from the contribution of such a lifting of degeneracy.

To access the origins of the change in the MAEs, we consider changes of band dispersions along the chain. Figure 3 shows the band dispersions for the magnetization easy axis direction (along the chain) for the selected numbers of induced electrons. The figure shows that the Fermi level (E_F) increases as the number of induced electrons and the band dispersions also move with E_F . It is interesting to see that the s and $d_{3z^2-r^2}$ bands around E_F move upwards more slowly than the other d bands. As a result the s and $d_{3z^2-r^2}$ bands move downward with respect to E_F and the other d bands almost keep position against E_F . These result in the different electron occupation between $d_{3z^2-r^2}$ and $d_{xy}-d_{x^2-y^2}$ bands, as confirmed in figure 4. Such different behaviors for the induced electrons may cause a

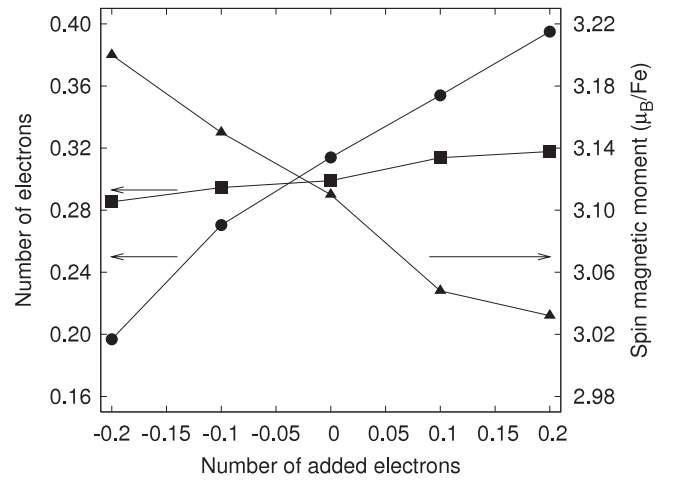


Figure 4. The numbers of occupied electrons in the $d_{3z^2-r^2}$ band (circles) and the $d_{xy}-d_{x^2-y^2}$ bands (squares), respectively, as a function of the number of induced electrons. The comparison with the dependence of the atomic spin magnetic moments (triangles) is also reported.

large change in the MAE. The cross points between the $d_{3z^2-r^2}$ and $d_{xz}-d_{yz}$ bands get closer to the Fermi level as the $d_{3z^2-r^2}$ band is occupied. Owing to the perturbative contribution, this behavior may decrease the MAE of $E_x - E_z$ when the electron number largely increases. For the increased number of electrons (figure 3(e)), the coupling between the occupied $d_{3z^2-r^2}$ and unoccupied $d_{xz}-d_{yz}$ below and above the Fermi level may contribute a decrease in the MAE, while for the decreased number of electrons (figure 3(a)), such coupling does not contribute because of the large energy difference between the states. In the CJ model, the $d_{3z^2-r^2}$ band does not sink as in the electric field, as shown in figure 5(b), and thus the decrease of the MAE is suppressed (green curve with triangles in figure 2(a)).

The spin magnetization decreases as the number of electrons increases, which is just accompanied with the increasing occupation of the $d_{3z^2-r^2}$ band, as shown in

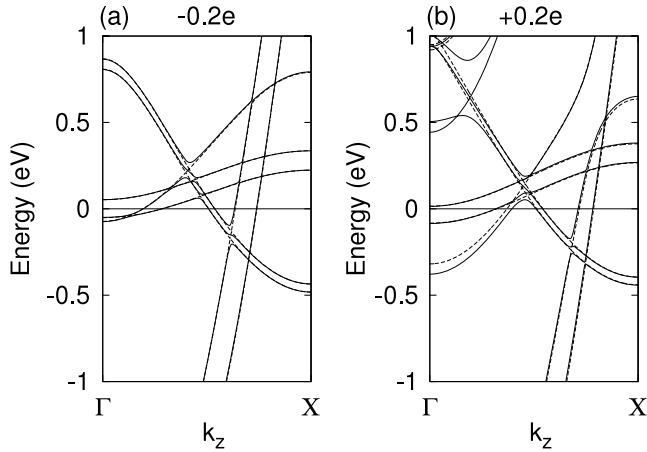


Figure 5. Comparisons of the band dispersions with the compensated jellium (CJ) model. The full curves specify the band dispersions in the electric fields induced by the numbers of electrons, -0.2 (a) and $+0.2$ (b), respectively, and the broken curves by the CJ model.

figure 4. The orbital magnetizations are related with the MAE. This is well known as Bruno’s relation [23]; $E_x - E_z \simeq \xi(m_o(z) - m_o(x))/4\mu_B$, where $m_o(z)$ and $m_o(x)$ are orbital magnetization when the total magnetization is directed along the z and x axes, respectively. This relation has been found to be fulfilled for the neutral Fe chain [9, 11] and this work also confirms the relation for the Fe chain with a given number of electrons (namely a given electric field).

In figure 6, we display the contour maps for the electron densities of the induced and reduced electrons in the electric fields. The induced (or reduced) electrons are extended to the wide region between the chain and the ESM. This implies the occupation of s bands with respect to the number of electrons, and, through the band hybridization, the occupation of the

$d_{3z^2-r^2}$ band. The last issue was discussed in figure 4. It is also noted in figure 6 that the density on the atom inversely behaves against the change of the number of electrons. For example, the density on the atom decreases though the number of electrons increases. The electric field slightly removes the electron from the d_{xy} - $d_{x^2-y^2}$ and d_{xz} - d_{yz} orbitals on the atom. This would be ascribed to an atomic localized nature with a large intra-atomic Coulomb interaction of the orbitals.

The electric field along the x axis, introducing the asymmetry in the plane perpendicular to the chain (z axis), additionally induces the SOI in the electrons. This is known as the Rashba effect [24, 25] and the Hamiltonian is written as $H_R = \frac{\hbar e}{4m^2c^2} \vec{\sigma} \cdot (\vec{E} \times \vec{p})$, where $\vec{\sigma}$ and \vec{p} are electron spin and momentum, and \vec{E} is the electric field. Such an effect resolves degeneracies of the spin states in a system with the time-reversal symmetry. In the present spin-polarized system, the remarkable energy change by such an SOI is observed as the asymmetry with respect to the momentum for the magnetization direction parallel to the y axis, as shown in figures 7(d) and (e). These asymmetries seem to appear as the band resonance rather than as the energy change of the Rashba effect itself. When such band resonances occur at the Fermi level, the transport properties of the system should be changed by the electric field.

4. Discussion

In the neutral one-dimensional chain, the intrinsic effective electric field on the electron is imposed by the SOI of the atom. For the magnetization perpendicular to the chain (for example along the y axis), such an effect emerges as the band resonance around $|k_z| \simeq 0.25(2\pi/c)$ in figure 7(b). The intrinsic electric field on electrons is mainly parallel to the x axis for $k_z > 0$ and anti-parallel for $k_z < 0$. Switching on the uniform external

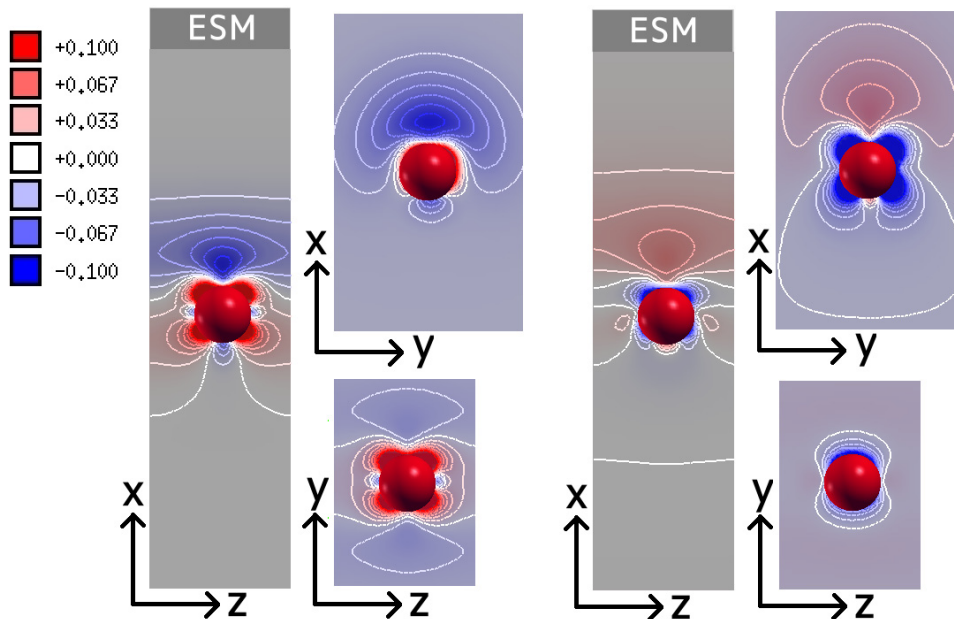


Figure 6. Distributions of the reduced or induced electrons by the electric field for the system with the magnetization easy axis. The contour maps of electron densities (1 au^{-3}) are shown in the xy , xz and yz planes for the induced electrons of -0.2 (left three panels) and 0.2 (right three panels).

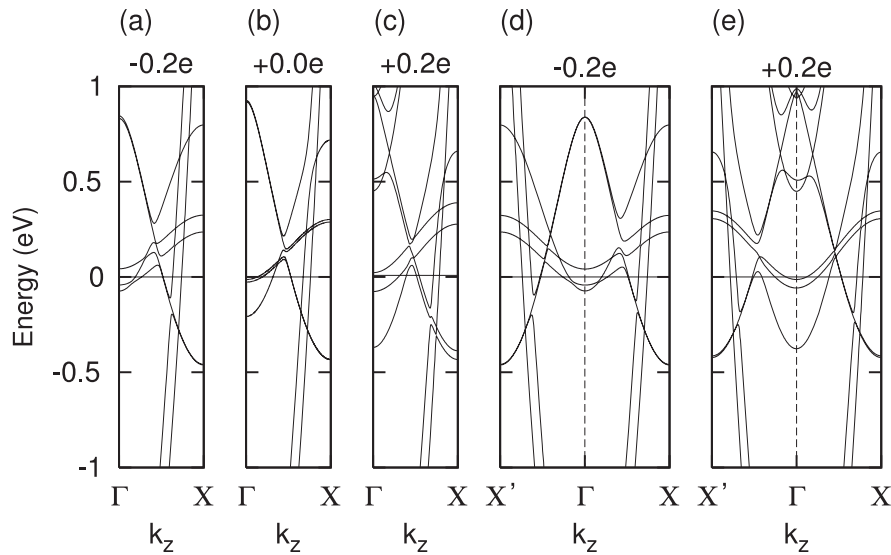


Figure 7. Band dispersions for the magnetizations along the x and y axes in the electric field; (a) x axis with -0.2 induced electrons, (b) x axis with 0 , (c) x axis with 0.2 , (d) y axis with -0.2 and (e) y axis with 0.2 .

electric field along the x direction, the electron with $k_z > 0$ feels a larger electric field and the one with $k_z < 0$ a smaller field. This is observed in figure 7(d) as the remarkable band resonance for $k_z > 0$ and the disappearance for $k_z < 0$. The case of the reversed external field is shown in figure 7(e).

In the present systems, the d_{xy} - $d_{x^2-y^2}$ bands, which degenerate in the neutral system with the magnetization perpendicular to the chain, are sometimes largely split, as shown in figures 3, 5 and 7. For the magnetization along the chain, such splitting is identified to come from the one with $m = \pm 2$. In contrast, for the magnetization perpendicular to the chain, the splittings which are observed for example in figures 7(a), (c) and (d) have another origin. By the symmetry breaking caused by the electric field, the couple of bands are split into the individual d_{xy} and $d_{x^2-y^2}$ components. This should be called an effect of orbital order, assisted by the intra-atomic Coulomb interaction in the 3d orbital. It would be interesting to consider that such modification at the Fermi level, which results in a variable transport property, can also be magnified by the intra-atomic Coulomb interaction of the transition metal.

5. Summary

The constrained iron chain in the electric field has been studied by using the first-principles approach. The magnetization easy axis was found to be along the chain in the investigated range of the electric field. The MAE was found to decrease as the number of induced electrons increases. This behavior could be understood with the synchronized variation in the band dispersions. On the increase of the number of electrons, the s and $d_{3z^2-r^2}$ bands become rapidly occupied, in contrast with the gradual occupation for the d_{xy} and $d_{x^2-y^2}$ bands. The coupling by SOI between the occupied $d_{3z^2-r^2}$ and unoccupied d_{xz} - d_{yz} bands becomes important as the number of electrons increases in order to decrease the MAE. The magnetization rotation

in the direction perpendicular to the chain and the electric field made the band dispersion asymmetrical. This implies an expectation of variable transport properties. It was found that the occurrence of band resonances at the Fermi level in the electric field seems more effective than the energy change itself by the Rashba Hamiltonian. To discuss a more realistic system, the substrate supporting the chain can be included.

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