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Magnetic ground state of face-centered-cubic structure of iron

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Abstract

First principles calculations reveal that the antiferromagnetic double layer (AFMD) along the magnetization direction of ⟨0 0 1⟩ is the magnetic ground state of face-centered-cubic (FCC) structure of iron (Fe) due to its lowest total energy among all the studied magnetic states. This magnetic ground state of AFMD-⟨0 0 1⟩ is fundamentally due to a stronger chemical bonding in terms of electronic structure, and could be confirmed by its mechanical properties for the first time. Calculations also show that lattice constant has an important effect to determine the magnetic state of FCC Fe, and a transition of magnetic state between AFMD-⟨0 0 1⟩ and ferromagnetic happens at the critical lattice constant of 3.666 Å. The derived results are in good agreement with experimental and theoretical observations, and could clarify the controversy regarding magnetic ground state of FCC Fe in the literature.

Keywords: magnetic ground state, face-centered-cubic structure, iron, first principles calculation

(Some figures may appear in colour only in the online journal)

1. Introduction

It is well known that the face-centered cubic (FCC) structure of iron (Fe) can only exist within a high temperature range of 1184–1665 K, while could be stabilized at low temperature as precipitants in alloys or thin films deposited in FCC substrates such as copper [1–4]. The magnetic ground state of FCC Fe, however, has become controversial for decades in the literature [1–25]. Specifically, the reported magnetic ground states of FCC Fe from experiments and calculations are ferromagnetic (FM) [4–10], antiferromagnetic (AFM) [3, 6, 11], antiferromagnetic double layer (AFMD) [7–9, 12–14], paramagnetic [11], ferrimagnetic [2], AFM + AFMD [15], FM + AFM [16, 17], and ferrimagnetic + AFM + FM [2]. In addition, the magnetic ground state of FCC Fe has been also found to change between FM and AFM [6, 18], FM and AFMD [7, 9], or nonmagnetic (NM) and AFM [18] with the change of lattice constant or the thickness of the layer. It is, therefore, of vital importance to theoretically clarify the magnetic ground state of FCC Fe.

By means of highly accurate first principles calculation based on density functional theory, the present study is aimed to derive the lattice constants, magnetic moment, mechanical properties, and electronic structure of FCC Fe. Accordingly, the possible NM, FM, AFM, and AFMD states are considered, and their total energy are compared as a function of lattice constant to reveal the magnetic ground state of FCC Fe as well as the potential transition between these magnetic states. In addition, the elastic constants and elastic moduli of these possible magnetic states are also derived and compared with experimental results for the first time to confirm the magnetic ground state of FCC Fe. The derived results are in good agreement with available experimental and calculated observations in the literature, and could clarify the above-mentioned controversy regarding magnetic ground state of FCC Fe in the literature.

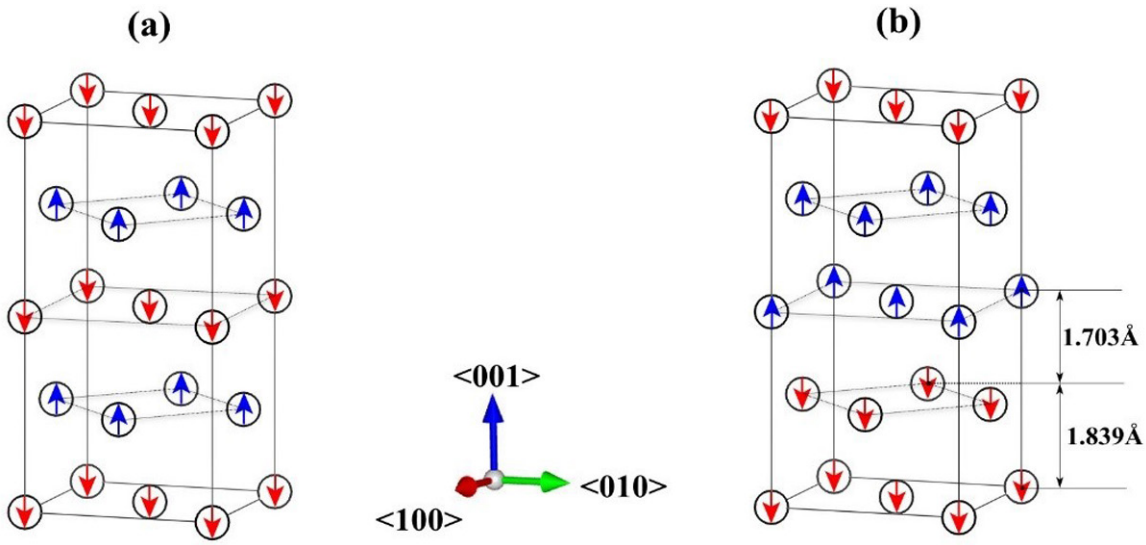

Figure 1. Magnetization arrangement along the ⟨0 0 1⟩ direction in (a) antiferromagnetic (AFM) and (b) AFMD states of FCC Fe.

2. Theory and methods

The present calculation is based on the first-principle calculation through the well-established Vienna *ab initio* simulation package (VASP) with the projector-augmented wave method (PAW) [26–28]. For the exchange and correlation items, generalized gradient approximation (GGA) [29, 30], local density approximation (LDA) [31], LDA + U [32, 33], and GGA + *U* [32, 33] are considered and compared with each other. In the GGA + *U* and LDA + *U* calculations, *U* and *J* are spherically averaged matrix elements of the onsite Coulomb interactions, and the optimized *U* and *J* values are 3 and 1 eV, respectively [32, 33]. The cutoff energies are 600 eV for plane-wave basis, the modified tetrahedron method is selected for *k*-space integration, and the periodic boundary conditions are chosen for three directions.

Accordingly, a unit cell of 8 atoms is chosen for the FCC structure of Fe. The considered magnetic states are NM, ferromagnetic with low spin (FM-LS), ferromagnetic with high spin (FM-HS), AFM, and AFMD. For both AFM and AFMD, the possible magnetization directions of ⟨0 0 1⟩, ⟨1 1 0⟩, and ⟨1 1 1⟩ are calculated, respectively, while the easily- magnetized direction of ⟨0 0 1⟩ is selected for FM. As typical examples, figure 1 shows the magnetization arrangement along the ⟨0 0 1⟩ direction in the AFM and AFMD states of FCC Fe from the PAW + GGA method. It is of interest to see from figure 1(b) that the layer distance of FCC Fe in the AFMD state becomes uneven after relaxation.

The lattice constant of each magnetic state of FCC Fe is optimized through the relationship of total energy and lattice spacing, i.e. the lattice constant is varied from 3.3 Å to 4.3 Å with a spacing of 0.001 Å, and at each lattice constant, the total energy of FCC Fe is obtained after the optimization of ions, electrons, and magnetic moments, while the FCC structure and the lattice constant are kept. The total energy is converged to 10^{-6} and 10^{-5} eV/cell in static and relaxation calculations, respectively, and the magnetic accuracy value here is 0.0001 μB/atom. After the tests, a gamma centered *k* grid is adopted, i.e. $9 \times 9 \times 9$ and $19 \times 19 \times 11$ for relaxation and static calculations, respectively. The elastic constants of each magnetic state of FCC Fe are calculated from the energy variation by applying small strains to the equilibrium lattice configuration [34], and the elastic moduli are derived by the Voigt–Reuss–Hill's approximations [35–38].

3. Results and discussion

After a series of calculations, the total energies of FCC Fe under the magnetic states of NM, FM, AFM, and AFMD are derived as a function of lattice constants from the PAW + GGA, PAW + LDA, PAW + GGA + U, and PAW + LDA + U methods, respectively. As typical examples, figure 2 shows the obtained total energies of FCC Fe various magnetic states from the PAW + GGA + U and PAW + LDA + U methods. It should be pointed out that for each AFM or AFMD state, the possible magnetization directions of ⟨0 0 1⟩, ⟨1 1 0⟩, and ⟨1 1 1⟩ are calculated, and the magnetization direction with the lowest total energy is therefore shown in figure 2.

One can observe clearly from figure 2 that the magnetic ground state of FCC Fe from both PAW + GGA + U and PAW + LDA + U methods is FM, which should be inconsistent with the obtained AFMD or AFM ground state from other calculations and main experiments in the literature [3, 7–9, 12–14]. The calculated lattice constants of the AFMD-⟨0 0 1⟩ state of FCC Fe from the PAW + GGA + U and PAW + LDA + U methods are 3.732 and 3.372 Å, respectively, which would be much bigger and smaller than the corresponding experimental value of 3.577 Å [14], respectively. The above points suggest that the PAW + GGA + U and PAW + LDA + U methods should be unable to reflect the magnetic states of FCC Fe. In addition, the PAW + LDA method is also not suitable to describe FCC Fe, as the initial setting of NM, FM, AFM, and AFMD states all leads to the NM state without any magnetic moments (figures not shown).

On the contrary, the following paragraphs will demonstrate that the PAW + GGA method is appropriate to reveal

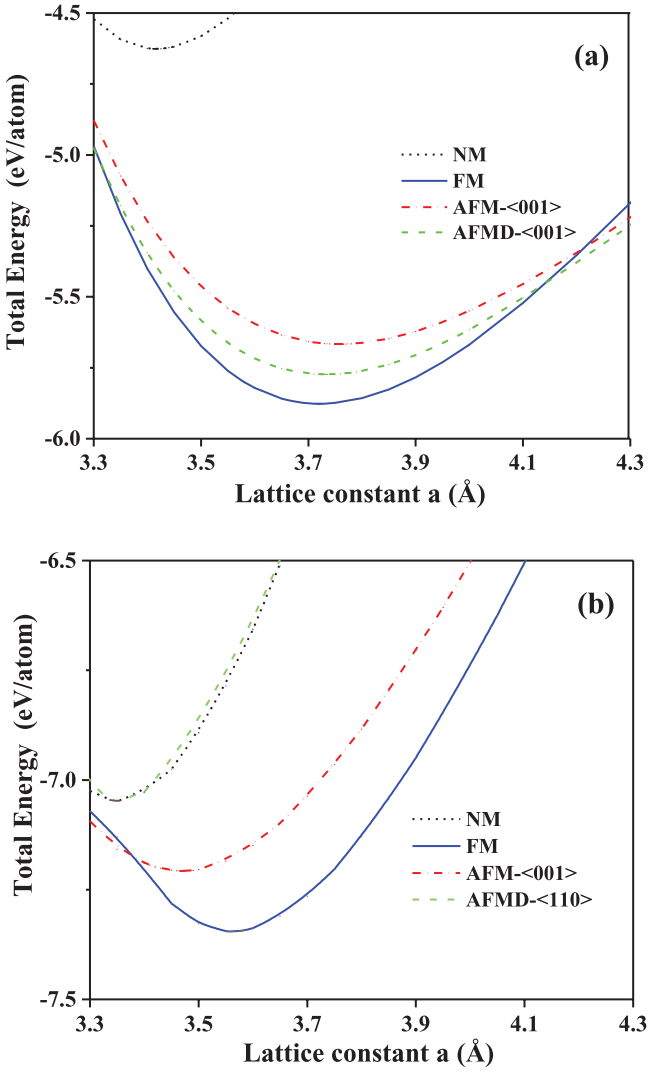

Figure 2. Total energies of FCC Fe as a function of lattice constant under the magnetic states of NM, ferromagnetic (FM), antiferromagnetic (AFM), and AFMD from the (a) PAW + GGA + U and (b) PAW + LDA + U methods. The expressions of ⟨0 0 1⟩, ⟨1 1 0⟩, and ⟨1 1 1⟩ after AFM and AFMD signify the possible magnetization directions, respectively.

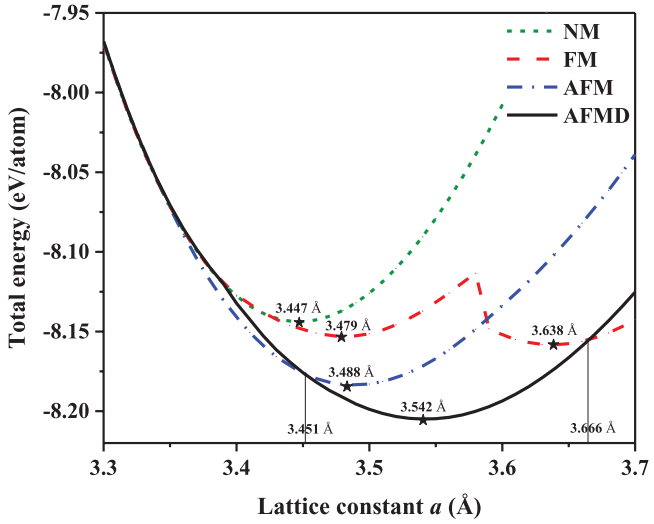

Figure 3. Total energy of Fe atom with the FCC structure as a function of lattice constant in the magnetic states of NM, FM-LS, FM-HS, antiferromagnetic (AFM) along the ⟨0 0 1⟩ direction, and AFMD along the ⟨0 0 1⟩ direction.

the magnetic ground state of FCC Fe, and the PAW + GGA method is therefore chosen in the present study to show the calculated results of FCC Fe in the following texts, tables, and figures. Accordingly, table 1 summarizes the optimized lattice constants (a), total magnetic moments per unit cell (M_T), magnetic moment per atom (M), and total energy (E) of FCC Fe under the magnetic states of NM, FM, AFM, and AFMD from the present PAW-GGA method. Moreover, the corresponding experimental and calculated values of FCC Fe in the literature [1, 3–5, 7, 10, 11, 13, 14] are also listed in table 1 for the sake of comparison.

Several characteristics could be deduced from table 1. Firstly, the total energies of the AFM-⟨0 0 1⟩ and AFM-⟨1 1 0⟩ states are very close to each other and are lower than that of AFM-⟨1 1 1⟩, suggesting that the ⟨0 0 1⟩ and ⟨1 1 0⟩ directions of magnetization could coexist in the AFM state of FCC Fe, which matches well with the similar statement from experiments [3]. Moreover, the AFMD-⟨0 0 1⟩ state is energetically more favorable with the lowest total energy among the three AFMD states and could be more easily obtained in actual situation, which is in excellent agreement with similar experimental observation in the literature [14].

Secondly, the ascending sequence of the total energies of these magnetic states of FCC Fe is as follows: AFMD-⟨0 0 1⟩ → AFM → FM → NM. That is to say, the AFMD-⟨0 0 1⟩ state has the lowest total energy of −8.2049 eV/atom among all the studied magnetic states, and is therefore regarded as the magnetic ground state of FCC Fe. Interestingly, the ground state of AFMD-⟨0 0 1⟩ revealed from the present PAW-GGA method agrees well with the discovered AFMD-⟨0 0 1⟩ state from experimental measurements of neutron scattering [14] and with the predicted AFMD-⟨0 0 1⟩ ground state from the methods of linear muffin tin orbital (LMTO) [7, 8] and full-potential linearized augmented plane wave (FLAPW) [13].

Thirdly, the lattice constants of various magnetic states of FCC Fe from the present PAW-GGA method are consistent with the experimental and calculated results in the literature [1, 13]. For instance, the present lattice constant of the FM state of FCC Fe is 3.638 Å, which matches well with the corresponding experimental value of about 3.615 Å [4, 10]. The calculated lattice constant of the ground state of AFMD-⟨0 0 1⟩ from the present study at 0K is 3.542 Å, which is in good agreement with the experimental values of 3.577 Å at 70 K [14], 3.588 Å at room temperature [3], and about 3.615 Å at 295 K [11].

Fourthly, the present magnetic moment (2.575 μB/atom) of the FM-HS state is compatible with the experimental value of 1.9 ± 0.6 μB/atom [10] and the calculated value of 2.6 μB/atom from the FLAPW method [13]. The calculated magnetic moments per atom in the AFMD-⟨0 0 1⟩ and AFM-⟨0 0 1⟩ states from the present study are 1.936 and 1.275 μB/atom, respectively, which are in good agreement with the predicted

Table 1. Optimized lattice constants a (Å), total magnetic moments per unit cell M_T (μB), magnetic moment per atom M (μB/atom), and total energy E (eV/atom) of FCC structure of Fe under several possible magnetic states from the present PAW-GGA method. The corresponding experimental and calculated values of FCC Fe in the literature are also listed for comparison. The possible magnetic states are nonmagnetic (NM), FM-LS, FM-HS, AFM, and AFMD. The theoretical methods are PAW with GGA, full-potential linearized augmented plane wave (FLAPW), linear muffin tin orbital (LMTO), and augmented-spherical-wave (ASW). ⟨0 0 1⟩, ⟨1 1 0⟩, and ⟨1 1 1⟩ after AFM and AFMD are the directions of magnetization.

Magnetic states	Methods	a (Å)	M_T (μB)	M (μB/atom)	E (eV/atom)
NM	PAW + GGA	3.447	0	0	−8.1439
	FLAPW + GGA [13]	3.45	0	0	
FM-LS	PAW + GGA	3.479	8.2960	1.0370	−8.1576
	FLAPW + GGA [13]	3.48	0	1.0	
	PAW + GGA [1]	3.5	8.32	1.04	
FM-HS	PAW + GGA	3.638	20.6000	2.5750	−8.1583
	PAW + GGA [1]	3.632	20.3200	2.5400	
	LMTO [7]	3.68			
	FLAPW + GGA [13]	3.64	0	2.6	
	Exp. [10]	~3.615		1.9 ± 0.6	
	Exp.[4]	~3.615			
AFM-⟨0 0 1⟩	PAW + GGA	3.488	0	1.2750	−8.1838
AFM-⟨1 1 0⟩	PAW + GGA	3.489	0	1.2820	−8.1839
AFM-⟨1 1 1⟩	PAW + GGA	3.463	0	0.7960	−8.1456
AFM	ASW [5]	3.45	0	0.45	
AFM	FLAPW + GGA [13]	3.49	0	1.33	
AFMD-⟨0 0 1⟩	PAW + GGA	3.542	0	1.9360	−8.2049
AFMD-⟨1 1 0⟩	PAW + GGA	3.447	0	0	−8.1439
AFMD-⟨1 1 1⟩	PAW + GGA	4.74	0	2.3450	−7.4317
AFMD-⟨0 0 1⟩	LMTO [7]	3.61			
AFMD	FLAPW + GGA [13]	3.54	0	1.90	
AFM	Exp. [3]	3.588		0.7	
AFMD-⟨0 0 1⟩	Exp.[14]	3.577			
AFM	Exp.[11]	~3.615			

values of 1.90 and 1.33 μB/atom [13]. Nevertheless, the present magnetic moments of the AFMD-⟨0 0 1⟩ and AFM-⟨0 0 1⟩ states are much bigger than the experimental value of 0.7 μB/atom [3]. Such a difference of magnetic moments between experimental and theoretical studies would be mainly due to the different conditions of FCC Fe, i.e. the deposited FCC Fe in experiments would have some stress as it should follow the lattice constant of the substrate of Cu, while FCC Fe is fully relaxed during calculations; the experimental FCC Fe is film with only several layers, whereas the calculated FCC Fe is bulk [3,13].

We now turn to compare the mechanical properties of FCC Fe under the above possible magnetic states. The elastic constants of each magnetic state of FCC Fe are calculated from the energy variation by applying small strains to the equilibrium lattice configuration [34], and the elastic moduli are derived by the Voigt–Reuss–Hill's approximations [35–38]. Consequently, table 2 summarizes the obtained elastic constants (C_{ij}), elastic moduli (B, G, E), Poisson's ratio (v), and G/B value [39] of FCC Fe at 0K under the magnetic states of NM, FM-LS, FM-HS, AFM-⟨0 0 1⟩, and AFMD-⟨0 0 1⟩. The experimental mechanical properties of FCC Fe at 1428 K [40] are also listed in table 2 for comparison.

It can be discerned from table 2 that the G/B values of NM, FM-LS, and AFM-⟨0 0 1⟩ states are all bigger than the critical point of 0.57 [41], suggesting that FCC Fe under the NM, FM-LS, and AFM-⟨0 0 1⟩ states should be intrinsically brittle, which seems contradictory to the ductile nature of FCC Fe from experimental observations [40]. Moreover, the FM-HS state of FCC Fe seems mechanically unstable at 0 K as its C_{11} is much smaller than C_{12} [42]. On the other hand, the Poisson's ratio (v) and the G/B value of the AFMD-⟨0 0 1⟩ state from the present study are in good agreement with the corresponding experimental results [40]. Such nice agreements confirm, for the first time, that AFMD-⟨0 0 1⟩ should be the magnetic ground state of FCC Fe. It should be pointed out that the present elastic constants and elastic moduli of the AFMD-⟨0 0 1⟩ state at 0K are bigger than the experimental values at 1428 K [40], and these differences would be mainly attributed to the effect of temperature [43].

To further find out the possible transition between these magnetic states, the calculated total energies of FCC Fe under the NM, FM-LS, FM-HS, AFM-⟨0 0 1⟩, and AFMD-⟨0 0 1⟩ states from the PAW + GGA method are displayed in figure 3. It can be seen obviously from this figure that the lattice constant (a) has an important effect to determine the magnetic state of FCC Fe. When the lattice constant is less than 3.35 Å, the FM, AFM, and AFMD states are found to possess zero atomic magnetic moments, and have the same total energies as the NM state, implying that only NM state could exist in FCC Fe when a <3.35 Å. As the lattice constant exceeds 3.35 Å, however, magnetism begins to play an

Table 2. Calculated elastic constants (C_{ij}), elastic moduli (B, G, E), Poisson's ratio (v), and G/B value of FCC Fe at 0K under magnetic states of under magnetic states of NM, FM-LS, FM-HS, antiferromagnetic along the ⟨001⟩ direction (AFM-⟨001⟩), and antiferromagnetic double layer along the ⟨001⟩ direction (AFMD-⟨001⟩). The experimental values of FCC Fe at 1428 K [32] are also listed for comparison.

Magnetic states	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	G (GPa)	E (GPa)	v	G/B
NM	449.83	206.36	242.59	285.19	181.81	449.83	0.237	0.638
FM-LS	304.23	140.41	221.34	195.02	148.62	355.55	0.196	0.762
FM-HS	42.95	174.4	23.73	130.58	20.03	57.15	0.427	0.153
AFM-⟨001⟩	482.5	135.19	150.01	250.96	159.06	393.95	0.238	0.634
AFMD-⟨001⟩	296.61	165.47	98.76	205.3	80.73	214.12	0.326	0.393
Exp. [40] (1428 K)	154 ± 14	122 ± 13	77 ± 8	133 ± 13	42 ± 3	114 ± 8	0.357 ± 0.003	0.312 ± 0.063

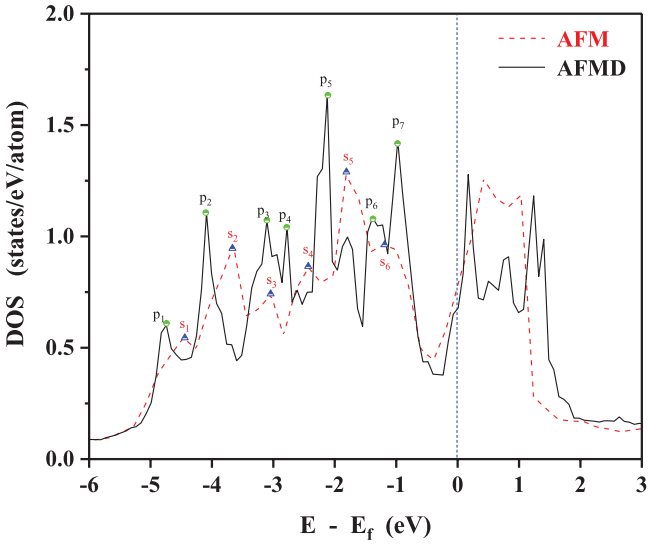

Figure 4. Total DOSs of FCC Fe under the magnetic states of AFMD and antiferromagnetic (AFM) along the ⟨001⟩ direction.

important role and the FM, AFM, and AFMD states could possibly appear in FCC Fe. It is of interest to see that there are two intersections between the curves of AFMD and AFM/FM at the critical lattice constants of 3.666 and 3.451Å. Specifically, when the lattice constant is less than 3.451Å, the AFMD and AFM states have very close total energies and could be thus considered as the coexistent magnetic state of FCC Fe, which agrees well with another theoretical prediction from the LAPW method [15].

When 3.451 Å $\leqslant a \leqslant$ 3.666 Å, the AFMD-⟨001⟩ state in figure 3 should be the magnetic state of FCC Fe due to its lowest total energy. It should be noted that the experimental lattice constant of 3.577 Å of the AFMD-⟨001⟩ state [14] as well as the calculated values of 3.54 and 3.61 Å of the AFMD state from the LMTO and FLAWP methods [7, 13] available in the literature are all within the above predicted range of lattice constant. These nice agreements could provide additional evidence that the present PAW-GGA method should be relevant to reflect the magnetic state of FCC Fe, and the predicted range of 3.451 Å $\leqslant a \leqslant$ 3.666 Å should be realistic for the magnetic state of AFMD-⟨001⟩.

In addition, when the lattice constant is bigger than the critical point of 3.666 Å, FM-HS in figure 3 should become the magnetic state of FCC Fe, which is consistent with the calculated value of 3.68 Å from the LMTO method [7] and the experimental point of about 3.615 Å [4]. That is to say, a transition of magnetic state from AFMD-⟨001⟩ to FM-HS would happen at the critical point of 3.666 Å with the increase of the lattice constant of FCC Fe. This predicted magnetic transition from the present study is in good agreement with similar observations in the literature [7, 9], and would bring about a reasonable explanation to the intrinsic reason why both AFMD/AFM and FM states of FCC Fe have been observed experimentally in the literature [4, 10, 11, 14, 18].

Finally, it is of importance to have a deep understanding of the magnetic ground state of AFMD-⟨001⟩ in terms of electronic structure. As a typical example, figure 4 shows the total densities of states (DOSs) of FCC Fe under the magnetic states of AFMD-⟨001⟩ and AFM-⟨001⟩. For the sake of comparison, the main peaks of the DOSs of FCC Fe under AFMD-⟨001⟩ and AFM-⟨001⟩ states are marked in figure 4 as p_x ($x = 1$–7) and s_x, respectively. One can discern clearly from this figure that compared with each DOS peak of s_x ($x = 1$–6) under the AFM state, the corresponding DOS peak of p_x ($x = 1$–6) below the Fermi level (E_f) under the AFMD state has moved leftward with higher binding energy and peak value, and one more DOS peak (p_7) appears under the AFMD state. In addition, the number of bonding electrons (4.111) under the AFMD state calculated by the integrals of the DOS curves below E_f is bigger than the corresponding value (3.922) under the AFM state, and the DOS value (0.650 states/eV/atom) at E_f under the AFMD state is smaller than the corresponding value of 0.800 states/eV/atom under the AFM state. All the above features indicate that the chemical bonding formed in the AFMD-⟨001⟩ state should be stronger than that in the AFM-⟨001⟩ state. Such a stronger chemical bonding would therefore induce the lower total energy and the magnetic ground state of AFMD-⟨001⟩ shown in table 1 and figure 3 as related before.

4. Conclusions

In summary, first principles calculations have been performed to reveal, for the first time, the magnetic ground state of FCC Fe from a systematic point of views of energetics, mechanical properties, and electronic structure. It is discovered that PAW + GGA is the appropriate theoretical method to describe the magnetic ground state of FCC Fe, while PAW + LDA, PAW + GGA + U and PAW + LDA + U are unsuitable. The magnetic ground state of AFMD-⟨001⟩ of FCC Fe is revealed from the lowest total energy and confirmed by its mechanical

properties for the first time, and is deeply understood in terms of electronic structure. Calculations also reveal that lattice constant (a) plays a decisive role in determining the magnetic state of FCC Fe, i.e. AFMD-$\langle 0\,0\,1\rangle$, FM-HS, and NM become the magnetic state of FCC Fe when 3.451 Å $\leqslant a \leqslant$ 3.666 Å, $a >$ 3.666 Å, and $a <$ 3.35Å, respectively. The predicted results agree well with available experimental measurements, and can clarify the controversy regarding magnetic ground state of FCC Fe in the literature.

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