The electronic properties of ferropericlase under pressure calculated by first principles

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Abstract. In this paper, we used the first principles (CASTEP) method to calculate the electronic properties ferropericlase (Mg0.9375Fe0.0625O) under 0 and 80 GPA. The calculated band gaps show that ferropericlase is a metal under 0 GPA, while it is a narrow-band semiconductor at 80 GPA. The ferropericlase at 0 GPA has some magnetic moment, while it has no moment at 80 GPA. The relations between band and Mg 2p, 2s Fe 3d and O 2s, 2p versus DOS have been discussed. We also find the ferropericlase exhibits metal behavior at some energies. Our calculations not only provide a reference to identify the ferropericlase in geological specimen but stimulate experiments in future.

Introduction

Ferropericlase is an important mineral in the mantle [1-4]. Ferropericlase is under high pressure in the mantle [5, 6]. The electronic properties of ferropericlase should be studied to identify the behavior of ferropericlase in the mantle. The properties can also be used to identify ferropericlase in geological specimen. Based on the reasons, more and more experts devote to studying ferropericlase under pressure [7-9]. Some experts used the high-pressure equipments [10, 11], which have high running costs. On the other hand, stimulations by computer provide a cheap and fast method to study the properties of ferropericlase.

Among these stimulate method, the first principles method is an effective method to study the properties of materials under pressure [12-14]. In this paper, we intend to study the electronic properties of ferropericlase under pressure.

Computational details

Our calculations have been performed in a program (CASTEP) in Materials Studio software [15]. We first built an $Mg_{0.9375}Fe_{0.0625}O$ supercell (Fig. 1). The obtained iron content is 6.25%, which is a typical value of ferropericlase. The used pressures are 0 and 80 GPa, which is a typical pressure in the mantle. After test, we used 400 eV as the cutoff energy. The *k* points for first Brillouin zone used in our calculations is 3×3×6. The valence electrons used in our calculations are $2p^6 3s^2$, $2d^6 4s^2$ and $2s^2 2p^4$ for Mg, Fe and O, respectively. Ultrasoft pseudopotential was used in our calculations. Our calculations were performed in a reciprocal space. The tolerance of the SCF is $5e^{-7}$ eV/atom. We first optimized the structure and then calculated the electronic properties.

Results and discussions

Structure and bands. The optimized lattice constants of $Mg_{0.9375}Fe_{0.0625}O$ under 0 GPA is $a=b=4.31$ and $c=4.27$ Å, while the constants under 80 GPA is $a=b=3.88$ and $c=3.88$ Å. We can see that the pressure decreases the lattice constants. The decreased ratios of *a* (*b*) and *c* are 10.0% and 9.1%. The constants in MgO are equal to each other. After Fe doping, the constant is not equal. The rate of the decreasing is not equal to each other. Pressure induces the constants equal to each other. The lattice constants *a*, *b* and *c* are not equal under 0 GPa, while these constants equal to each other under 80 GPa.

Cell angles (α, β and γ) are all 90°. The pressure can change the lattice constants but cannot change the cell angels.

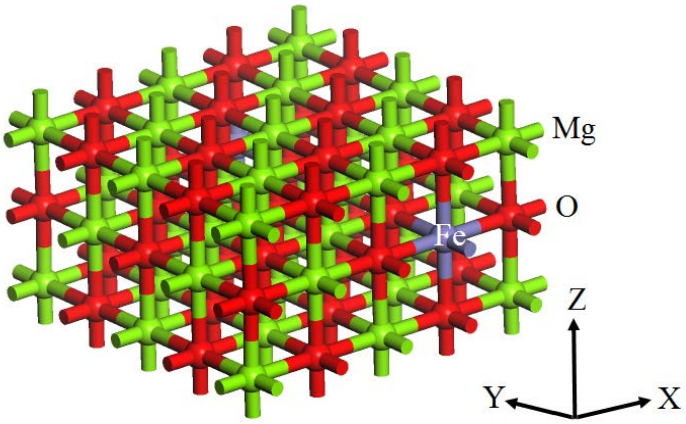

Fig. 1. The scheme crystal of $Mg_{0.9375}Fe_{0.0625}O$.

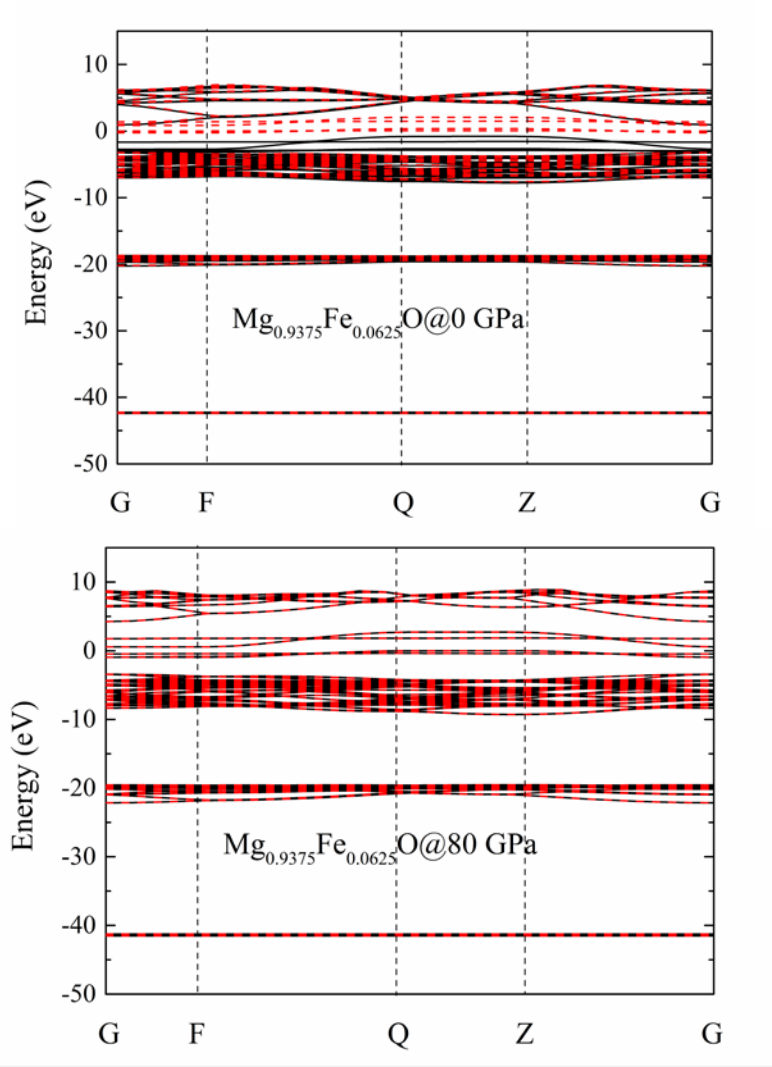

Fig. 2. Bands of Mg0.975Fe0.625O under 0 GPa (left) and 80 GPa (right).

Density of states. Fig. 3. The density of states (DOS) of Mg0.975Fe0.625O under 0 GPA (left) and 80 GPA (right).The density of states (DOS) relate closely to study the band. In this section, we calculated the DOS and discuss the relation between DOS and band. The calculated DOS shows of Fig. 3. The left of Fig. 3 ($Mg_{0.975}Fe_{0.625}O$ under 0 GPa) shows there is a net magnetic moment around the Fermi level, which means $Mg_{0.975}Fe_{0.625}O$ under 0 GPa is a magnetic material. The DOS above

the Fermi level come from Mg 2*p* state. The DOS around -5.4 eV mainly come from O 2*p* state, while the DOS around -19.0 come from the O 2*s* state. In the deep energy around -42.3 eV, the DOS come from the Mg 2*s* state.

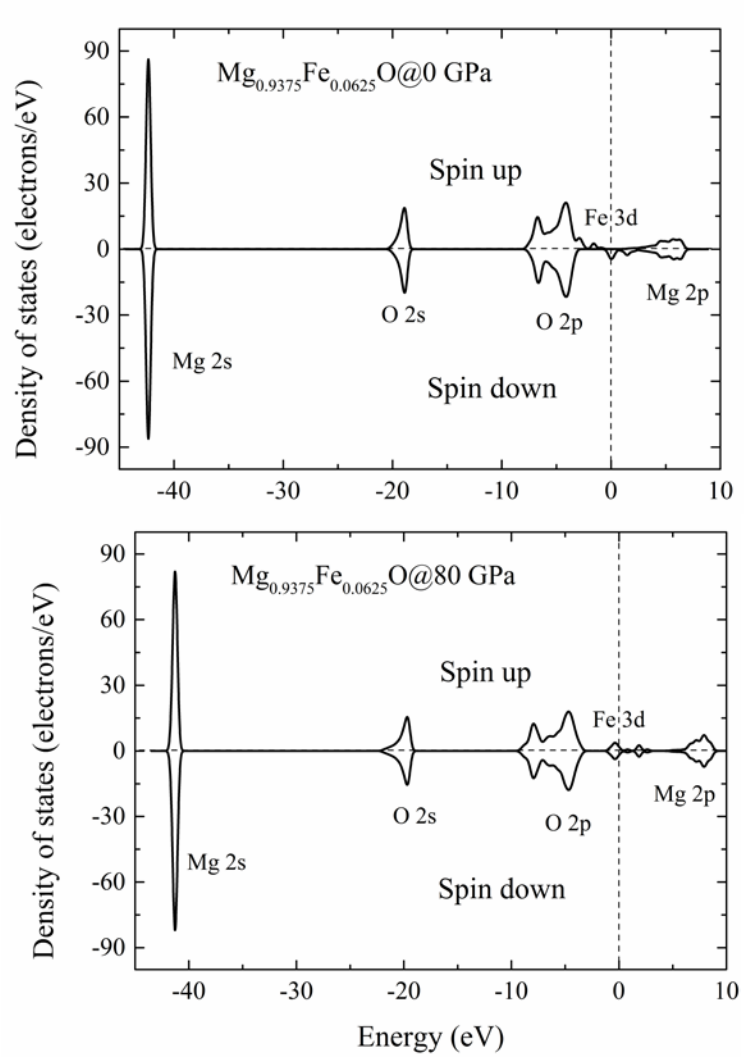

Fig. 3. The density of states (DOS) of $Mg_{0.975}Fe_{0.625}O$ under 0 GPa (left) and 80 GPa (right).

In this paragraph, we will discuss the right of Fig. 3 ($Mg_{0.975}Fe_{0.625}O$ under 80 GPA). The right of Fig. 3 also shows the DOS around the Fermi level come from Fe 3*d* state. The DOS above the Fermi level come from Mg *2p* state. The DOS around -6.0 eV come from the O 2*p* state, while the DOS around -20.1 eV come from the O 2*s* state. In the deep energy, the DOS at -41.3 eV come from Mg 2*s* state. We should notice that the DOS (spin up and down) of Fe 3*d* state around the Fermi level is nearly equal, which means that the $Mg_{0.975}Fe_{0.625}O$ under 80 GPa has no magnetic moment.

Conclusions

In this paper, we study the electronic properties of ferropericlase under pressure. The calculated band gap shows ferropericlase at 0 GPa is a metal, while ferropericlase at 80 GPa is a narrow-band semiconductor (band gap is 0.5 eV). The DOS under pressure has been calculated and the relation between the DOS and band has been discussed. The relations between DOS and Fe 3*d*, O 2*s*, 2*p* and Mg 2*s*, 2*p* have been studied. Our study can be used to identify the ferropericlase specimen and some geological process. We also can stimulate some related experiments.

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