

# First principles study of the electronic properties of MgO under pressure

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**Abstract.** We have studied the electronic properties of MgO by first principles (CASTEP program). The calculated band gap of MgO shows MgO is an insulator. Pressure increases the band gap from 4.253 to 7.585 eV. The band above the Fermi level shifts to higher energy, while the band below the Fermi level shifts to lower energy. The shift comes from effect of pressure. The density of states (DOS) have been calculated and the relations between band and DOS have been discussed. The DOS also have shift and the shifts is according to the shifts in band. The electronic properties have also been calculated. We also find the pressure shifts the electronic properties to higher energy. The electronic shift come from the increased band gap. Our result provides a reference for future experiments.

## Introduction

MgO is an important mineral in the mantle [1-3]. MgO can be widely used in industry. For example, MgO also is an excellent insulator [4] and carrier of catalyst [5]. MgO can also be used as expansive cement and concrete [6]. As an important mineral, the properties of MgO under pressure is important to identify some geological process. With the development of high-pressure equipment, experts devote to studying the properties of materials under pressure [7-9]. The high-pressure equipment is relative expensive for operation and maintenance. Few laboratories in our world have these equipment. These hinder the studies about the properties of materials under pressure.

On the other hand, First principles is a powerful tool to study the properties of materials under pressure [10-12]. With the develop of first principles [13] and high performance computer, First principles method is becoming more and more feasible to study material properties under pressure. So, more and more experts use computers and first principles to study material electronic properties under pressure. In this paper, we intend to study the electronic properties of MgO under pressure.

## Computational details

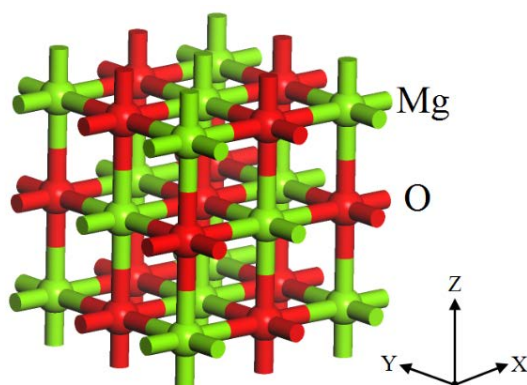


Fig. 1 The scheme crystal structure of MgO.

Our calculations were performed by the Cambridge Sequential Total Energy Package (CASTEP) program, which is based on the Density-functional theory (DFT). The crystal of MgO showed in Fig. 1. It belongs to FM-3M space group, which was used in our calculations. The used valence electrons are  $3s^2$  and  $2p^4$ . The ultrasoft pseudopotential was used in our calculations. Our calculations were carried out in a reciprocal space. After test, the used  $k$ -points and cut-off energy  $6 \times 6 \times 6$  and 400 eV. The SCF tolerance is  $1 \times 10^{-5}$  eV/atom. We chose typical pressures (0 and 80 GPa) and used them in our calculations. We first optimized the crystal structure and then calculated the electronic properties.

## Results and discussions

**Structure and band.** In this section, we first discuss the structure and then discuss the band. At 0 GPa, the optimized lattice parameters are  $a=b=c=4.295$  Å and  $\alpha=\beta=\gamma=90^\circ$ . On the other hand, the optimized lattice parameters are  $a=b=c=3.884$  Å and  $\alpha=\beta=\gamma=90^\circ$  at 80 GPa. From the different parameters under different pressure, the crystal angle is unchanged. The lattice constants decrease with increasing pressure and the ratio of decrease is as high as 10%. The compression will induce a changes in the electronic properties. Our results are in line with the other results. The reliable constants can guarantee our calculations are reliable.

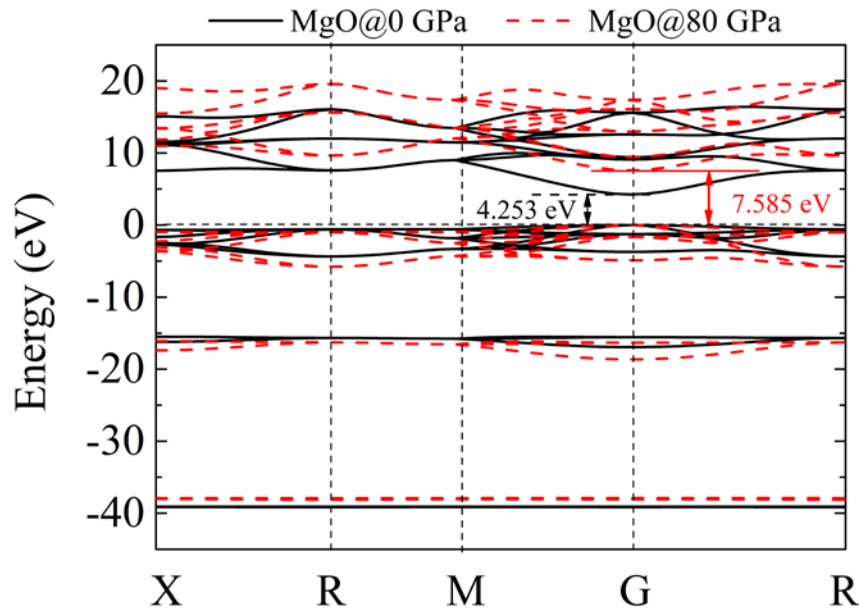


Fig. 2. The calculated band of MgO at 0 and 80 GPa.

**Density of states.** The band and density of states (DOS) relate closely to the optical properties of MgO. The band also relates closely to the DOS. In this section, we will calculate the DOS and discuss the relation between band and DOS. The relation between DOS and optical properties will be discussed in the next section. The related calculations also performed under 0 and 80 GPa. The results are shown in Fig. 3.

We first discuss the total DOS at 0 and 80 GPa in Fig. 3a. The total DOS in Fig 3a shift to higher energy with pressure increase from 0 to 80 GPa, which is according to the shift of our calculated band. The according energy of the DOS constitute the according band. Except the shifts of the DOS, the correspondence between the band and DOS is similar. We only give the correspondence at 0 GPa and that at 80 GPa is similar. The DOS above the Fermi level mainly come from Mg  $3s$ ,  $3p$  and O  $2p$ , which constitute the conduction band. The total DOS (TDOS) between  $-5.0 \sim 0$  eV come from O  $2p$  state, which constitutes the according valence band. The TDOS around  $-15.6$  eV come from O  $2s$  state, which forms the according valence band. The TDOS at  $-39.1$  eV come from Mg  $2p$  state, which constitutes the deep valence band. The correspondence is important to identify the states.

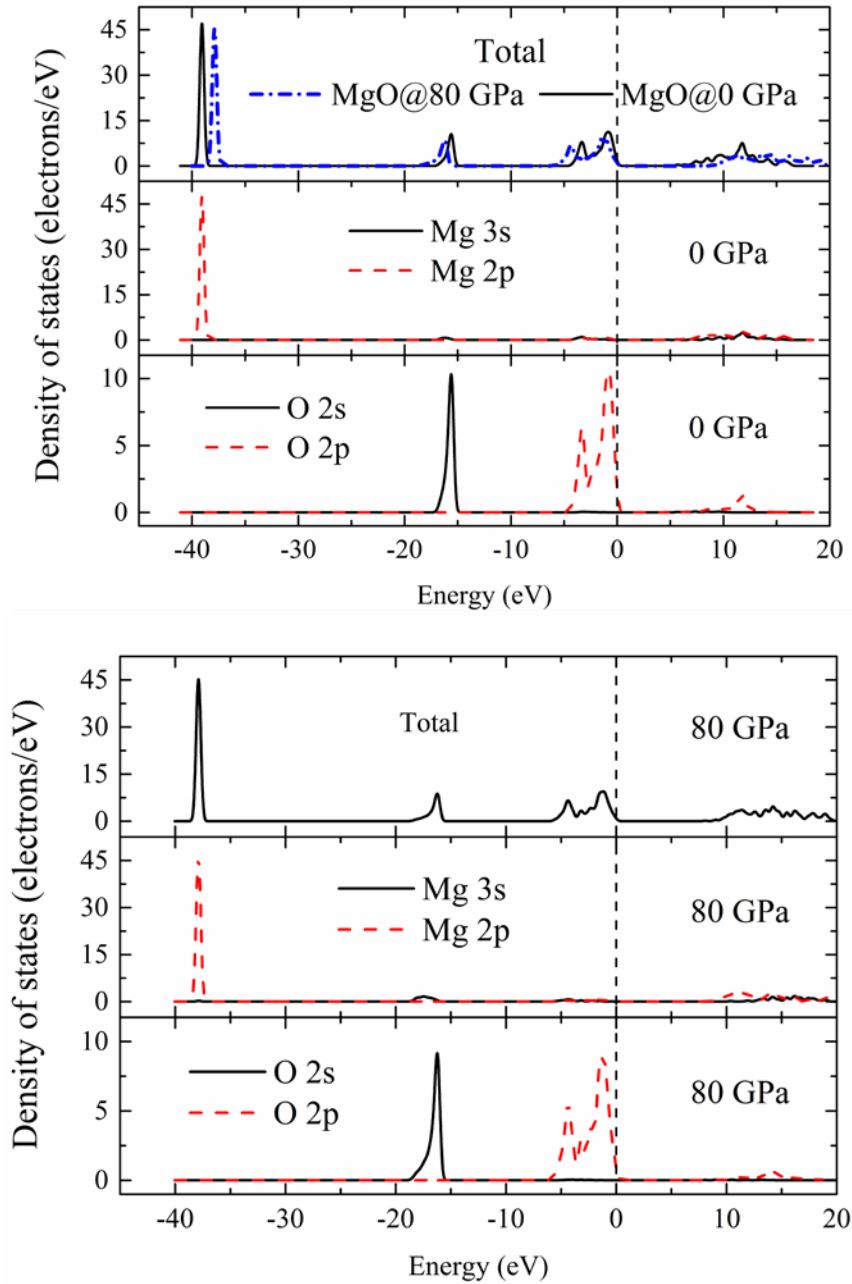


Fig. 3. The density of states (DOS) and partial DOS (PDOS) of MgO at 0 and 80 GPa.

## Conclusions

In this paper, we have calculated the electronic properties of MgO under pressure (0 and 80 GPa). The structure has been optimized and the bands have been discussed. The band gap increases when pressure increases from 0 to 80 GPa. The band gap shows MgO is an insulator. The electronic density of states (DOS) have been calculated and the relation between bands and DOS has been discussed. The electronic properties has also been calculated and discussed, which can be used to identify some geological process. Our studies provide a reference and stimulate the future experiments.

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