The Electronic Properties of Defected MgO

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Abstract

The effect of impurity on the electronic properties of MgO is investigated using full potential linearized augmented plane wave plus local orbitals method based on Density Functional Theory. Electronic band structures and density of states of MgO in the presence of Ca, Li, and Na impurities were calculated. It is found that increasing the amount of Ca impurity decreases the band gap of energy and increases the width of the upper part of the valence band. Some of the considered impurities (Li and Na) change the electronic properties of MgO extensively.

Keywords: Magnesium Oxide, Density Functional Theory, Impurity, Linearized Augmented Plane Wave.

Introduction

Alkaline earth oxides have been widely used in catalysis, electrochemistry, optical fibers, and sensors. Magnesium oxide with its simple rock salt structure is one of the most significant metal oxides for theoretical and experimental studies. Alkaline metals can be easily doped in alkaline earth oxides and this doping has been found quite useful in industry. For example, when MgO is used as an insulator in nuclear reactors, lithium doping can reduce the radiation damage to the MgO crystal. In recent years, the metal oxides with impurities are studied extensively. In contrast to the extensive studies, obtaining more information about the electronic properties of doped MgO is useful.

In this paper, we discussed the electronic properties of Ca, Li, and Na-doped MgO. For each type of impurity, the electronic band structure and the density of state (DOS) were calculated.

Computational method

The calculations were performed with the WIEN2K package, which is a full potential linearized augmented plane wave plus local orbitals (FP-LAPW-LO) method based on Density Functional Theory (DFT). The generalized gradient approximation of Perdew-Burke-ernzerhof 96 was used to describe the treatment of the exchange-correlation energy.

Results and discussion

First, we have studied the electronic properties of magnesium oxide. The analysis of band structure and DOS indicates that MgO is a semiconductor. The size of the band gap is 4.8 eV at F point, which is in acceptable agreement with other calculations.

To simulate impurity in MgO, we have constructed a super unit cell by doubling the original simple cubic cell of MgO, this corresponds to the stoichimetry of Mg_8O_8. In this supercell, first one of the Mg atoms is replaced by one impurity and the electronic properties of doped MgO were investigated, then the amount of impurity was increased by replacing other Mg atoms with impurity. Our results indicate that increasing the number of Ca impurity decreases the band gap of energy and enhances the band width of upper valence band. The electronic band structures of $Mg_{1-x}Ca_xO$ for $x \leq 0.5$ are shown in Fig 1.

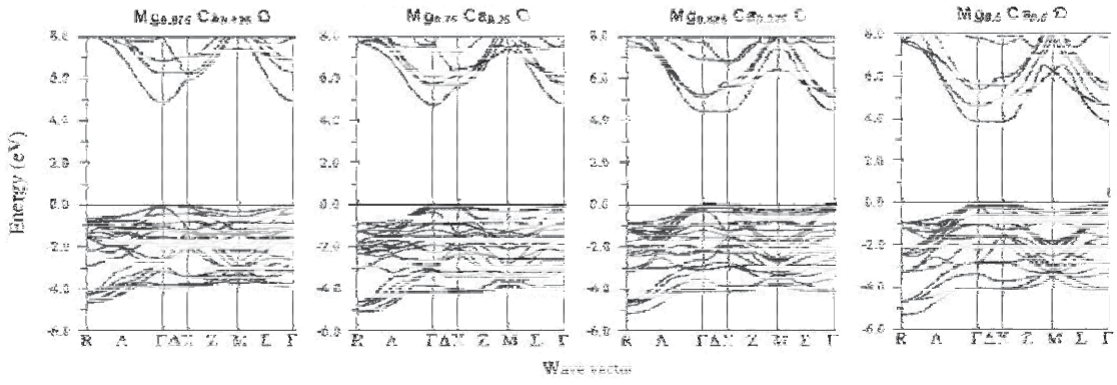

Figure 1. Electronic band structure for $Mg_{1-x}Ca_xO$

The electronic structures of Li or Na impurity in MgO were studied by using the above procedure. Li and Na have one valence electron less than Mg. If one of the Mg atoms is replaced with a Li or Na, one electron is removed. Hence doping of these

atoms strongly enhance the hole carriers and electrical conductivity of MgO. These impurities are called acceptors. When an electron moves from the valence band to these empty states, a hole leaves in the valence band. Thus acceptor levels raise the concentration of the holes by accepting electrons from the valence band. MgO doped with acceptors like Li and Na are known as p-type semiconductors.

In summery, we have investigated electronic properties of MgO in the presence of impurity. The Ca impurity increases the conductivity of MgO but we did not find significant effect on the electronic properties. Some of the considered impurities (Li and Na) change the electronic properties of MgO extensively.

References

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