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# Assessing Effect of Structural Modification in MgO on the Band Gap Properties by DFT

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**A B S T R A C T**

In this study, first-principles calculations are employed to investigate and compare the electronic properties of pristine MgO. Using plane-wave pseudopotential methods, we analyze the band structure. The cubic investigated crystal structure belongs to the 221-space group. The Perdew-Burke-Ernzerhof (PBE) functional is used for structure optimization and band structure calculations. Ultrasoft pseudopotentials were used for the calculations.

Keywords: First principle, DFT, lattice constant, band structure

## Introduction

Metal oxides are important for the conservation of the environment, protecting the environment from pollutants, these metal oxides play a key role in detecting pollutants. Metal oxides are found to have variety of different crystal structures. Metal oxides can have different compositions and morphology. These characteristics of metal oxides determine their optical, electronic and chemical properties [1].

The electronic properties of metal oxides, band structure, partial density of states (PDOS) and total density of states (TDOS) are tunable, which means that we can control these properties of metal oxides by controlling the dimension of the unit cell. This tunability of metal oxides opens the possibilities of multifunctional application based on metal oxides. In applications like heterogeneous photocatalysts, the capability to change the band gap and increase the surface area of reaction is very important. Synthesis of metal oxides through different methods like chemical or physical methods have highlighted the variation in the crystal structure [2].

Pharmaceuticals and paint producing companies along with textile factories are the main source of toxic pollutants in water as well as soil. These toxic pollutants are often non-degradable. To remove these toxic non-degradable pollutants from the water and pollutants the required photocatalytic properties are known to be possessed by metals and metal oxide. A photocatalyst increases the rate of degradation of toxic pollutants through the process of oxidation and reduction. The toxic pollutants are of two types organic and inorganic pollutants. Dyes, antibiotics and pesticides are the examples of organic pollutants, while heavy metals, radioactive compounds, and sulfur-based compounds are the examples of inorganic pollutants. To maintain the cleanliness of the environment, the accurate measurement of the pollutants levels in the water must be done vigilantly [3]. Metal oxides are known for their role in eco-friendly and bearable energy sources like hydrogen fuel. Metal oxides are the key component of photoelectrochemical water splitting. Metal oxides favor both types of reactions due to their band gaps, position of band edges in valence band and conduction band, stability and low synthesis expenses.

## Research methodology

Quantum espresso [4] is used to calculate lattice constant and band gap. The convergence values for energy and forces are $1x10^{-6}$ Ry and $1x10^{-3}$ Ry/Bohr. The convergence value of cutoff energy is 50 Ry and the cutoff for charge density is selected as 400 Ry i.e. 8 times the cutoff energy. The converged value for k-points grid is 10×10×10.

## Result and discussion

Geometric optimization of MgO was done for space group related to the cubic crystal structure. This space groups is pm-3m. In pm-3m space group, Mg is at corner of the unit cell at (0,0,0) coordinates and O is placed at center at (0.5, 0.5, 0.5). The optimized lattice constant for the pm-3m space group is found out to be 2.66 Å. After successfully optimizing the geometry of MgO, than I have calculated the band structure. The band structure also helps us to characterize the material as semiconductor, conductor or metal. So, the band gap calculated for the pm-3m space group is 2.26 eV. If the VBM and CBM lie on the same wave vector point than material is known as direct band gap material, and if the VBM and CBM are on the same wave vector point than material is known as indirect band gap material. We can see that in the pm-3m space group the VBM point lies on the M wave vector point while

CBM lies on G wave vector point, which makes the pm-3m space group of MgO the indirect band gap material. Now based on the band gap nature and value the pm-3m space group can be characterized as indirect band gap semiconductor.

## Conclusion

The lattice constant calculated of pm-3m in cubic structure is 2.66 Å. The indirect band gap between VBM and CBM of pm-3m space group is 2.26 eV for pristine crystal structure.

## Figure

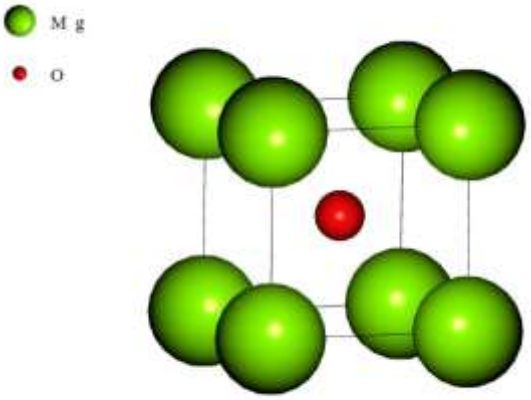


**Figure 1: Cubic structure of MgO, Mg is at (0, 0, 0) and O (0.5, 0.5, 0.5).**

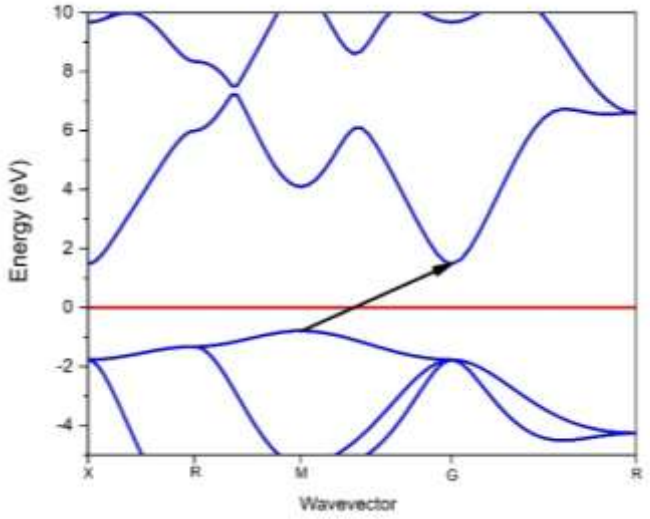


**Figure 2: Band structure of MgO.**

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