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First-Principles Studies on the Band Gap of WO_3

Maryum Iqbal [a], Muhammad Bilal Khursheed [a], Malik Sajjad Mehmood [a]

[a] *Department of Physical Sciences, University of engineering and technology, Taxila 47050, Pakistan*

A B S T R A C T

Density functional theory (DFT)- based first-principles study is used to investigate and compare the effect of doping Ge on the lattice constant and band gap of WO3. The cubic crystal structure was examined, which belongs to the pn-3n and pm-3m space groups. For the band structure calculations, the Perdew-Burke-Ernzerhof (PBE) functional was used. Ultrasoft pseudopotentials were used for the calculation, as these pseudopotentials provide better accuracy compared to other pseudopotentials.

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

Introduction

Tungsten trioxide (WO_3) exhibits interesting optoelectronic properties, which have long captivated the attention of researchers in condensed matter physics, materials science, and related fields, underscoring its potential for transformative applications. WO_3 is a transition metal oxide, due to its electronic structure, and exhibits tunable electronic properties, making it a suitable material for applications such as photoelectrochemical cells and gas sensors. The high photocatalytic activity underscores its significance as a solution to challenges in energy-related applications. WO_3 is known for its wide bandgap. Due to the value of its band gap, WO_3 can absorb light in the visible and ultraviolet regions, making it a potential candidate for photovoltaic applications. Due to its electrochromic properties, WO_3 can change colors under applied electric fields, which makes it useful for energy-efficient bright lights and display technologies [1]. As we know, WO_3 is highly reactive with gases such as NO_2 and NH_3. Due to its remarkable reactivity, it can be used in chemical sensors [2]. The performance of WO_3 is highly dependent on its crystal structure, defect chemistry, and electronic properties, and the understanding of these properties is limited. Experimental investigations provide accurate data; however, experimental studies cannot isolate the microscopic mechanisms occurring at the atomic level. For the understanding of the underlying phenomenon, computational techniques are essential. This is the point at which DFT provides the link between experimental data and theoretical knowledge. Density functional theory has revolutionized computational material science by enabling the modeling of electronic properties of materials within a quantum mechanical framework. Using electron density as the variable quantity in the Schrödinger wave equation, DFT allows researchers to estimate the electronic and optical properties of materials [3, 4].

Research methodology

Quantum espresso [5] is used to calculate the band gap. The convergence test for the planewave cutoff energy and k-points was performed. The cutoff energy turned out to be 50 Ry, and the convergence of k-points was observed at 8×8×8. The convergence values of total energy of the system was selected to be $1x10^{-6}$ Ry.

Result and discussion

The geometric optimization of WO_3 was conducted for two cubic space groups, pm-3m and pn-3n. In the pm-3m configuration, tungsten (W) atoms are situated at the corners of the unit cell at fractional coordinates (0, 0, 0), whereas oxygen (O) atoms are located at the midpoints of each edge with coordinates O_1 (0.5, 0, 0), O_2 (0, 0.5, 0), and O_3 (0, 0, 0.5). For the pn-3n space group, tungsten atoms are positioned both at the corners (0, 0, 0) and at the center (0.5, 0.5, 0.5) of the unit cell, while oxygen atoms are distributed along the edges and faces, with coordinates O_1 (0.5, 0, 0), O_2 (0, 0.5, 0), O_3 (0, 0, 0.5), and face-centered positions O_4 (0.5, 0. 0.5), O_5 (0, 0.5, 0.5), and O_6 (0.5, 0.5, 0). Prior to the calculations, an optimization of the k- point mesh and cutoff energy was performed, with values set to 8 × 8 × 8 and 50 Ry respectively, and the charge density cutoff was established at 400 Ry (eight times the energy cutoff). The optimized lattice parameters, obtained via variable- cell calculations using Quantum ESPRESSO, were 3.84 Å for the pm-3m structure and 4.21 Å for the pn-3n structure. The increase in the lattice constant for the pn-3n configuration aligns with the expectation, owing to the larger number of atoms (eight compared to four in pm-3m), which necessitates additional space. Band structure analyses indicated a band gap of 0.63 eV for the pm-3m configuration, denoting its nature as a low band gap semiconductor. Conversely, the pn-3n structure exhibited a zero-band gap, classifying

it as metallic, attributable to the presence of free electrons. The band structure of pm-3m further revealed that the valence band maximum (VBM) is located at the R point, while the conduction band minimum (CBM) is at the Γ point, indicating an indirect band gap. In contrast, the metallic behavior observed in the pn-3n structure results from the increased atomic population, which introduces additional energy states within the forbidden gap, effectively reducing the band gap to zero. These findings elucidate the relationship between atomic arrangement and electronic properties in WO_3 crystal structures.

Conclusion

The geometric and electronic properties of WO_3 were systematically studied for two cubic space groups, pm-3m and pn-3n. Structural optimization revealed an increase in lattice constant with the addition of more atoms in the pn-3n configuration. Band structure analysis showed that pm-3m WO_3 behaves as an indirect band gap semiconductor with a gap of 0.63 eV, while pn-3n exhibits metallic behavior with a zero band gap. These findings demonstrate that the electronic nature of WO_3 can be effectively tuned by altering its crystal symmetry and atomic arrangement, offering valuable insights for its potential use in semiconductor and electronic device applications.

Figure

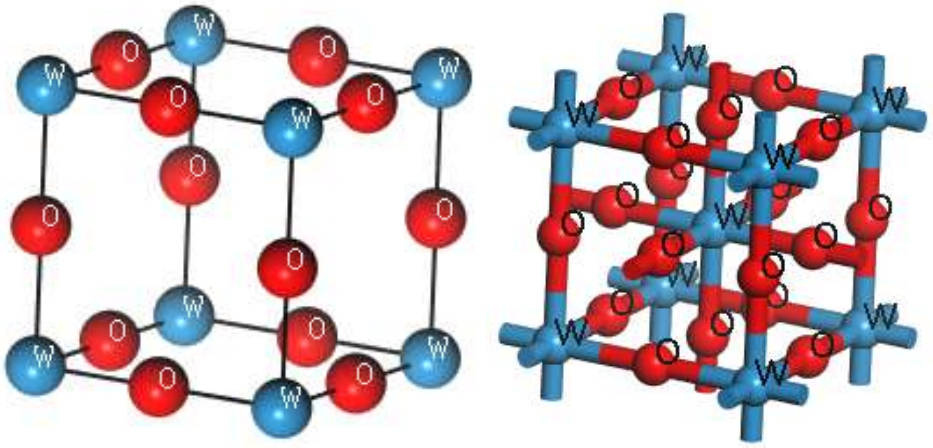

Figure 1: Cubic structure of (left) pm-3m WO_3 (right) pn-3n.

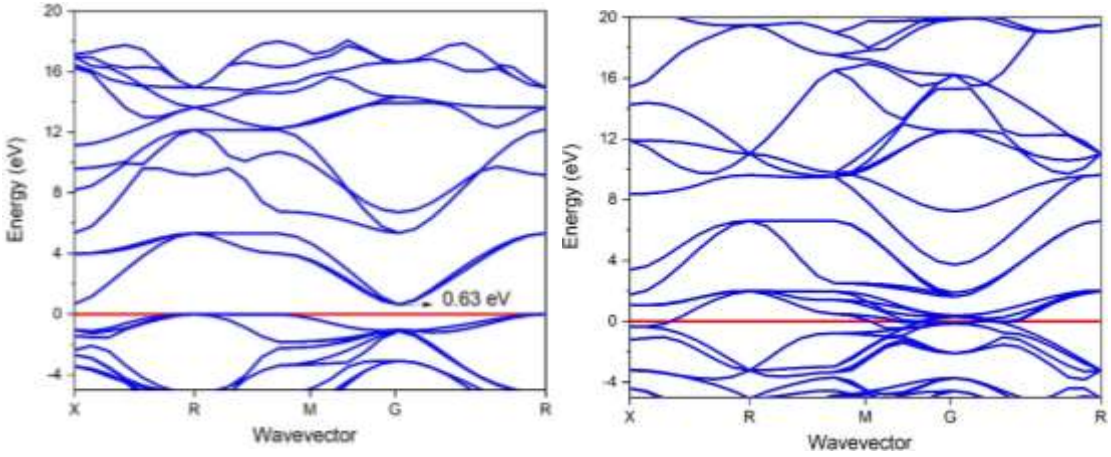

Figure 2: Band structure of WO_3 (left) pm-3m space group (right) pn-3n space group.

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