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Pressure induced electronic and optical properties of rutile SnO_2 by first principle calculations

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A B S T R A C T

Tin dioxide (SnO_2) is the most important semiconductor material due to its large number of technological applications. In this work we carried out the electronic and optical properties under pressure of rutile SnO_2. The ultra-soft pseudopotential method is used by employing the local density approximation functional proposed by Ceperley-Alder and Perdew-Zunger to calculate the exchange correlation potential within the framework of density functional theory. Firstly we optimized the structure to obtain the ground state energy of the system with the increase of cutoff energy (Fig. 1 (b)). The investigated band structure and density of states show that energy bandgap is increasing with the increase of pressure due to the movement of valence bands from higher to low energy levels and the conduction bands from lower to higher energy levels respectively (Fig. 1 (a)). The effect of pressure on lattice constants demonstrates the increase in lattice constants. Optical properties, comprising refractive index, dielectric function, absorption and energy loss spectrum are investigated. The obtained results are in good agreement with the previous reported theoretical and experimental results.

1. Introduction

In current era, technologically most important metal oxides are SnO_2 and TiO_2. Mostly electrical conductors are dense and most of optical transparent materials are insulator but in the case of SnO_2 both the optical transparency and electrical conductivity are present together [1]. In Li-ion batteries, dye-sensitized solar cells and choosy gas sensors, SnO_2 is one of the metal oxides those are used to enhance the performance of these applications [2–4]. The performances of bulk SnO_2 for example, lattice dynamics, electronic properties, phase transitions and optical properties continued to pay attention for both experimental and theoretical studies. For anti-microbial system, self-cleaning and organic oxidation, the material should have photo-catalytic and electro-catalytic characteristics [5,6]. Experimentally by x-ray diffraction Shieh et al., Haines and Leger and Huang et al. calculated structural parameters of tin dioxide [7–9]. The two photon spectroscopy technique was use to measure the electronic bandgap energy of SnO_2 by Frohlich et al., in 1978 [10] and Schweitzer et al., in 1999 [11]. 1n 1972, Jacquemin et al. first time investigated the electronic and optical properties by employing the Hohn-Korringa-Rostoker

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method [12]. Although, many research groups have studied similar properties one after another, such as of SnO_2 such as Chun-Mei Liu et al. [13], Mayer et al. [14], Errico [15], Rehman et al. [16], Li et al. [17] and Liu et al. [18].

SnO_2 have seven polymorphs among which rutile-type is the most stable and occur in large number naturally at ambient temperature and pressure. It has tetragonal structure and it belongs to $P4_2/mnm$ space group [1]. Inspite of that large numbers of theoretical and experimental studies have been done; tin dioxide still needed more studies to explain its electronic and optical properties. So, in this study we have considered the theoretical approach based on Density Functional Theory (DFT) to investigate the pressure induced electronic and optical properties of rutile-SnO_2, including band structure, density of states and dielectric constant. In this paper we have organized our work as follows: Section 2 explains the computational methods. Results and discussion are presented in section 3 and section 4 describes the conclusion.

2. Computational method

In computational materials science DFT is the most popular tool to investigate theoretically the electronic, mechanical, magnetic and optical properties of different materials [19]. Although DFT based methods are very popular in theoretical studies but it also has inherent limitations and defects. Theorists already have been improved and trying to improve the quality of theoretical models by considering missing terms [20–23]. We have employed Cambridge Serial Total Energy Package (CASTEP) code [24] to investigate the pressure induced electronic and optical properties of SnO_2. The effects of electron–electron exchange correlation are depicted by CA-PZ functional in Local Density Approximation (LDA) [25,26] within DFT. The well efficient basis sets the ultrasoft pseudo-potentials are accomplished for electron–ion interactions. In the irreducible Brillion zone the Monkhorst-Pack grid $5 \times 5 \times 8$ K points were considered. The cutoff energy 500 eV is used after finding the minimum ground state energy of the system (as shown in Fig. 1 (b)) to expand the electronic wave function which corresponds to a condition of convergence of energy 0.1×10^{-5} eV/atom.

3. Results and discussion

Firstly, we optimized the geometry by choosing cutoff energies with the difference of 20eV to find out the minimum ground state energy of the $2 \times 2 \times 2$ supper cell of rutile SnO_2. From Fig. 1 (b) one can see that the total energy and energy bandgap of the system remains unchanged or change is in very small fraction around 500 eV at pressure 0 GPa. The third Birch-Murnaghan equation of state is used to calculate the energy-volume data [27].

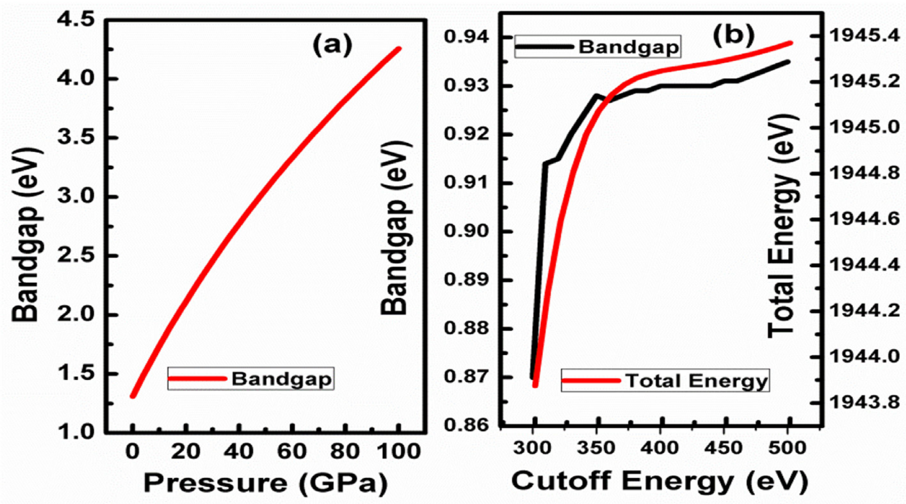

Fig. 1. (a) bandgap vs pressure and (b) bandgap and total energy w. r. t. cutoff energy.

Table 1
The calculated equilibrium Lattice parameters (a and c) (Å), Energy gap Eg (eV), Volume V, Bulk modulus B0 (GPa) of rutile-type SnO_2.

Methods	A (Å)	C (Å)	B_0 (GPa)	References
LDA (CA-PZ)	4.6807	3.1534	236.6	Present
LDA	4.695	3.160	242.4	[13]
GGA-PBE	4.928	3.288	204.5	[13]
GGA-PBE	4.830	3.236	173	[28]
Others	4.776[a], 4.826[b]	3.212[a], 3.237[b]	179[a]	[a] [29], [b] [30]
Experiments	4.737[c], 4.746[d]	3.186[c], 3.189[d]	205[c]	[c] [7], [d] [8]

[a] Ref. [29]; [b] Ref. [30]; [c] Ref. [7]; [d] Ref. [8].