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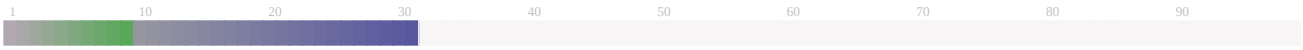

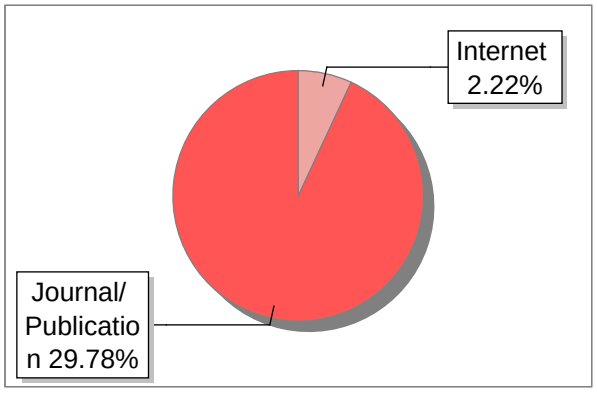

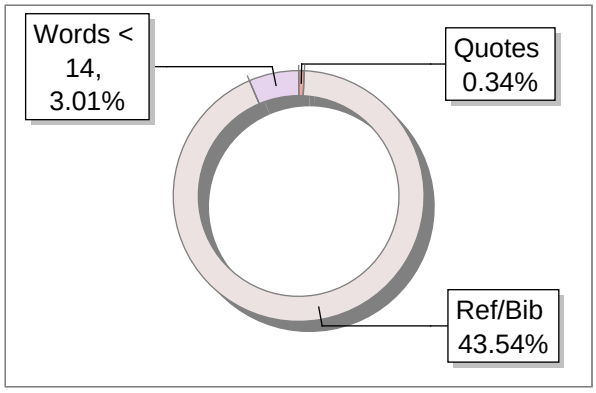

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First-principles DFT + U studies of the Nb-doped ZnO spray deposited thin films.

Experimental and Theoretical Study of Nb -Doped sprayed ZnO thin films.

The study of structural, and optical properties of sprayed Nb - doped ZnO: DFT + U and experimental approaches

Ramchandra Sapkal*[1], Rushikesh Sapkal[2], Manisha Sapkal[3], Jayashtree Waghmode[1]

1. Centre for Density Functional Theory and Research Centre , Tuljaram Chaturchand College Baramati 415123, India.
2. Department of Engineering Sustainable Technology Management Focus on Industry 4.0, SRH University of Applied Science Berlin, Berlin- 10587, Germany.
3. Department of Microbiology, Balasheb Desai College Patan 415 123 , India.

Abstract :

In present study ZnO, and Nb doped ZnO were synthesized on glass substrate by using chemical spray pyrolysis at suitable temperature. Zinc oxide (ZnO) is a n-type semiconductor material which has a wide direct band gap of energy ~3 eV. Dopant in ZnO nanostructures is an effective way to improve ZnO's structural properties in various applications. The concentration of impurities is varied from 1% to 4 mol% for (Nb-ZnO). The synthesized thin films are characterized by X-Ray diffraction method which shows hexagonal structure with 57nm crystalline size for optimized concentration of Nb and it optimized by JCPDS card number (01-079- 0208). Due to their excellent optical and electrical properties prepared films are used as a transparent window layer and electrodes in solar cell. For first principle study ,

we have performed PBE and PBE+U calculations to investigate the electronic structure of ZnO and Nb doped system . Firstly, it was found good correspondence for Hubbard parameter value using Ud,Zn = 0 to 12 eV and Up,O = 0 to 12 eV for undoped ZnO bulk system , and for Nb doped ZnO same range of Hubbard parameter value repeated with Ud (0 to 12 eV) for Nb.

Keywords: ZnO, , Nb, Structural and Optical properties, Chemical Spray Pyrolysis. DFT +U

Correspondence: rt_sapkal@yahoo.co.in

Introduction:

The ZnO materials follow the family of II-VI semiconductors and behave with a wide band gap having exciton binding energy around 60 meV [1]. ZnO has three different structures; those consist of rock salt, zinc blende, and wurtzite [2]. The semiconducting property of ZnO is used in optoelectronic applications [3]. ZnO can be used in gas sensing (4) , Furthermore, ZnO thin films are popular for use as thin film transistors. ZnO transistor thin films (TFT) work as channel layers to replace the amorphous silicon Journal Pre-proof 3 hydride in active-matrix liquid crystal displays [5,6]. ZnO thin films are used to upgrade the stability of the devices and circuits for high voltage operations when they are manufactured in the form of thin film transistors [7]. Zno based thin films can be used as Surface Acoustic Wave (SAW) [8]. Numerous scholars have studied the effects of dopants on ZnO thin films. When incorporated into the ZnO lattice, transition metal oxide dopants such as manganese (Mn [9]), chromium (Cr [10]), cobalt (Co [11]), iron (Fe) (12) and copper (Cu [13]) improve the magnetic properties. Titanium (Ti)-doped ZnO is used to improve electrical conductivity [14] because the radius of a Ti4+ ion is smaller than that of a Zn2+ ion by 30%. However, dopants like aluminium (Al [15]), magnesium (Mg [16]), tin (Ga [17]), and indium (In [18]) into ZnO films provide transparency and high conduction (TCO). Also,

rare-earth elements like neodymium (Nd) and terbium (Tb) provide high clarity, high conductivity, and a luminescence trend [19 -20]. Lanthanium (La)-ZnO thin films act as photocatalytic materials [21]. Metallic Nb has an oxidation state of 0, which changes to +2 in the case of NbO; +4 in NbO2; and +5 in Nb2O5, each of which result in different electrical conduction behaviors [22]. The presence of Nb in ZnO thin films reduces the disorder and carrier scattering because of the substitution of Nb5+ with Zn2+ [23]. Moreover, Nb-doped ZnO can be used for TCO [23], gas sensing [24], solar cell applications [27], Efficiency of Nb-Doped ZnO Nanoparticles Electrode for DyeSensitized Solar Cells Application, [28] and photocatalystsis [29]. Magnetron Sputtered Nb-Doped ZnO Thin Films switching properties for RRAM Applications [30] , Nb doped ZnO thin films an be fabricated by different methods such as Magnetron Sputtering [31], Fabrication of chemically stable hydrogen- and niobium-codoped ZnO transparent conductive films Structure, optical and electrical properties of Nb-doped ZnO transparent conductive thin films prepared by co-sputtering method [32] , radio frequency magnetron sputtering [33-34] Niobium (Nb) doping (0 at.% to 3 at.%) in ZnO thin films prepared by the chemical spray pyrolysis method [35] **The NbZnO films were deposited using atomic layer deposition. [36-37],**ZnO nanostructures containing doped with different atom % of Nb are fabricated through ultrasound assisted hydrolysis in water [38]

Many fundamental physical properties of Nb -doped ZnO such as defect energy level and relationship between doping level and energy band gap, which are of important scientific and engineering interests, are unclear. In this work, theoretical studies are performed to understand the electronic properties of undoped and Nb -doped ZnO sysytem.[39]

There are several theoretical works that use the DFT method to study ZnO structures [40 - 45]. However, it is well known that the standard DFT method largely underestimates bandgap values [46], A density functional study for structural and electronic properties of

Zinc Oxide (ZnO), in wurtzite, rock salt and zinc-blende phases has been performed [47] The conventional Density Functional Theory (DFT) method based on exchange–correlation (XC) functionals of Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) produces underestimated value of energy band gap (~0.7–1.0 eV) compared with the energy gap value (~3.4 eV) measured in the experiment.[48-49] **This** is because the standard DFT is not able to properly take into account the exchange-correlation term. The bandgap underestimation results from the usage of grossly approximated potentials in the Kohn-Sham implementation.

There are three approaches to compensate for the bandgap underestimation of DFT: (1) the GW approximation [50] that takes into account the self-energy of a many-body system of electrons, (2) hybrid exchange-correlation functionals like HSE 51], PBE0 [52], and B3LYP [53] The two functionals assessed are the Tao-Perdew-Staroverov-Scuseria, a nonempirical metageneralized gradient approximation (meta-GGA) functional and the Heyd-Scuseria-Ernzerhof (HSE), a screened exchange hybrid functional.[54] and (3) the DFT+U formalism that includes the Hubbard on-site Coulombic U term [55- 60]. Among the three approaches, hybrid functionals and DFT+U are widely used in theoretical works. While hybrid functionals are computationally expensive, the DFT+U method is comparable to the standard DFT method in terms of the computational cost. In the following, we will present a summary of both approaches [60-61] Moreover, the DFT–LDA+U approach can significantly improve the calculation including transition metal localization [62] The obtained supercells of pure and Mn-doped ZnO materials are optimized using DFT. The generalized gradient approximation (GGA) in the scheme of Perdew–Burke–Ernzerhof (PBE) was used to treat the exchange-correlation function [63-64]

In this work we have performed PBE and PBE+U calculations to investigate the electronic structure of ZnO and Nb doped system . Firstly, it was found good correspondence

for Hubbard parameter value using Ud,Zn = 0 to 12 eV and Up,O = 0 to 12 eV for undoped ZnO bulk system , and for Nb doped ZnO same range of Hubbard parameter value repeated with Ud (0 to 12 eV) for Nb.

Theoretical development of First principle Theory :

The foundation of first-principles method relied on quantum mechanics that describe the behavior of electrons and atomic nuclei in any situation [20]. The Schrodinger equation serves as the basic equation in this topic, which can be expressed as follows (Eq. (1)):

$\hat{H}\,\Psi = E\,\Psi$ ----------(1)

where $\hat{H}$ is the Hamiltonian operator, Ψ is the wavefunction, and E represents the energy of the system. The Hamiltonian operator consists of kinetic and potential energies due to the Coul

$$\hat{H} = \sum_{I=1}^{N} \frac{P^2(a)}{n!}(z-a)^n$$

Apparently, the Schrodinger equation is too complex to be solved and would lead to uncontrollable computation in a system containing more than one electron. This is largely due to the nature of electrons that strongly interact which each other, which leads to many-body problem [16,20]. Several approximations are then developed to solve the Schrodinger equation, of which the first useful one is the wellknown Born–Oppenheimer approximation

The idea in Born–Oppenheimer approximation is that the electron motion and nuclear motion are separated [16]. This is due to the fact that the mass of the nucleus is way larger than that of the electron, and the nuclei are principally fixed particles. By having this approximation in mind, the problem of interacting electron, ions and nuclei vanishes and eventually enables the possible application of the Schrodinger equation in a complex system

Density functional theory

In 1964, Hohenberg and Kohn [23] have developed a theorem that defined the electron density as a unique function for ground state energy of a system with N-electron. Later, a set of independent-particle equation has been established by Kohn and Sham [24]. They have introduced a Schrodinger-like equation with a modified effective potential that is much easier to calculate than the original Schrodinger equation.

The Hohenberg–Kohn theorems

Kohn–Sham method

Exchange–correlation functional

Local density approximation

Generalized gradient approximation

Hubbard-U scheme

Experimental Methods:

1) Fabrication of Undoped and Nb doped ZnO thin films:
2) Computational :

The experimental structural parameters of wurtzite ZnO at a = 3.2427 Å and c = 5.1948 Å with wurtzite parameter z = 0.3826 as discovered by Sabine and Hogg [13] using X-ray crystallography method is used as the reference structural data in this work. A standard DFT geometrical optimization is first performed on the primitive wurtzite ZnO unit cell, followed by a self-consistent DFT calculation to study its electronic properties. Hubbard term Ud is then added to the d-orbitals of the Zn atoms, ranging from 2 eV to 14 eV in the interval of 2 eV. The second part of this research studies the effect of including both Hubbard term Ud to Zn d-orbitals and Up

to O p-orbitals, where the Up values ranges from 5 eV to 9 eV. The changes to lattice constants and wurtzite parameter z as well as the band gap and valence band width are investigated. All calculations in this work are completed using the ABINIT electronic package [14] within the framework of projectoraugmented-wave (PAW) potentials [15] and LDA exchange correlation functionals. The PAW potentials used are from the datasets provided by Jollet et al. [16]. The plane wave basis sets are expanded to kinetic energy cutoff of 34 Hartree whereas the Monkhorst-Pack k-point mesh is set to an array of 8 8 6 at gamma centred grid. Cutoff energy is selected with convergence tolerance of 0.005 eV/atom whereas k-point mesh array is selected so that band gap is converged with 0.0004 eV tolerance. The LDA + U calculations are performed using full localized limit (FLL) double-counting correction [8]. The double-counting correction is necessary in a LDA + U calculation to avoid double counting of correlation part in localized electrons. The Hubbard term J is set to zero for all calculations; the rotationally invariant LDA + U form proposed by Dudarev et al. [9] is equivalent to the FLL method with J = 0 and U in place of U ——————————J [17]. **(E.S. Goh ⇑, J.W. Mah, T.L. Yoon, Effects of Hubbard term correction on the structural parameters and electronic properties of wurtzite ZnO,** Computational Materials Science Volume 138, October 2017, Pages 111-116)

To simulate the doping effect in the system, a 32-atoms 2×2×2 supercell was used in our calculations, as shown in Fig. 1. Firstly, one Nb atom dopant is introduced to substitute one Zn atom, which yields to a dopant concentration of 6.25%. Secondly, to determine the magnetic ground state, a 32-atoms supercell with two replaced Zn atoms were constructed. This was necessary for calculations of the relative energies,

the ferromagnetic (FM) and antiferromagnetic (AFM) spin alignments, the difference between these two energies per RE ion is defined as ΔE= EAFM–EFM, which indicates the magnetic stability in ZnO: Nb systems. However, the configuration with two dopants in the nearest neighbors called near configuration was evaluated. On the other hand, as the distance increased, far configuration was also considered. Finally, The Brillouin-zone integration was performed using a Mokhorst-Pack 2×2×2 (1/Bohr radius, a.u.) k-points mesh in the first Brillouin zone[22]. Thus, the computational scheme was appropriate for describing the electronic structure and the magnetic properties of Nb- doped ZnO.

Result and Discussion :

A) **Experimental**

B) **Theory**

BAND STRUCTURE OF ZINC OXIDE :

Experimentally, the electronic structure of zinc oxide has been investigated in some detail see Ref. 19 and references therein. Typically, the density of states reveals two primary bands between 0 and −10 eV measured from the valence band maximum. The upper band is primarily derived from O 2p and Zn 4s orbitals, while the lower band arises almost solely from Zn 3d electrons with a maximum between −7 and −8 eV. The measurements reveal a strong dispersion of the upper valence bands and a smaller dispersion of the Zn 3d levels. In general, DFT calculations yield too small band gaps compared to experiment. This effect is further enhanced in ZnO due to the underestimation of the repulsion between the Zn 3d and conduction band levels, which leads to a significant hybridization of the O 2p and Zn 3d levels and eventually to an overestimation of covalency. Schröer et al. have performed an

analysis of the wave functions obtained from self-consistent pseudopotential calculations and determined a contribution of 20%–30% of the Zn 3d orbitals to the levels in the upper valence band to be compared with the experimental estimate of 9% covalency cited above. For zinc oxide the band gap calculated with LDA or GGA is about 0.7– 0.9 eV, which is just about 25% of the experimental value 3.4 eV. The insufficient description of strongly localized electrons such as those occupying the Zn 3d states in ZnO and the underestimation of their binding energies is a generic problem of DFT within the LDA or GGA, and at least partially a result of unphysical self-interactions. In fact, it has been found that calculations based on the Hartree-Fock or the GW approximation give much more tightly bound d-electrons and significantly larger band gaps. An alternative approach is the explicit correction of self-interaction.29 Vogel et al. have developed this idea further and devised a scheme, which allows one to incorporate self-interaction corrections SIC and electronic relaxation corrections SIRC already during the construction of pseudopotentials PP. 27 Thereby, they were able to reproduce the experimental band gap as well as the position of the 3d levels in several II-VI compounds with remarkable precision. In fact, the thus obtained band structure for ZnO compares better with experiment than calculations within the Hartree-Fock and GW approximations.21,28 SIC-PPs have also been used by Zhang et al. in the calculation of the formation enthalpies of a few neutral point defects in zinc oxide.3 Unfortunately, as they point out, the SIC scheme cannot be transferred unambiguously to charged defect calculations and is therefore not applicable in the present situation

Theoretical Approach and Computational Details:

32 we employed the rotationally invariant approach proposed by Dudarev et al. 33 The Hubbard U term corresponds to the mean-field approximation of the on-site Coulomb interaction, which is added to the exchange-correlation functional. We used an effective Hubbard parameter, i.e., the difference between the Coulomb U and exchange J parameters is

taken into account, Ue f f = U −J. Among the Ue f f combinations that could yield the correct description of the itinerant or localized behavior, we have also properly described the relative orbital positions with respect to the Fermi level. Thus, we have considered Ue f f values from a self-consistent linear response procedure, 32 which describe the correct band gap value for ZnO (3.3 eV) and attend simultaneously the correct position of the d- and p-states in the valence band (VB). In this work, Firstly, it was found good correspondence for Hubbard parameter value using Ud,Zn = 0 to 12 eV and Up,O = 0 to 12 eV for undoped ZnO bulk system , and for Nb doped ZnO same range of Hubbard parameter value repeated with Ud (0 to 12 eV) for Nb.

The calculations are performed using the plane-wave pseudopotential method as implemented in the Quantum ESPRESSO package 36. Electron-ion interactions were described using the projector-augmented wave (PAW) method37. A cutoff energy of 140 Ry and 1140 Ry were used for the plane-waves expansion and for the electronic density, respectively. For the Brillouin-zone integration, we have applied the Monkhorst-Pack method38, with a k-mesh of 6×6×6 and 6×1×6 k-points for the bulk and surface. The convergence criteria for the energy and force were 10−4 Ryd and 10−3 Ryd/Bohr, respectively

we have decided to benchmark our calculations using the band structure calculated by Vogel et al. employing their self-interaction and relaxation-corrected SIRC pseudopotentials, which reproduces the experimental band gap as well as the position of the Zn 3d levels.27 Values for $U^{-} - J^{-}$ between 0 and 10 eV were considered. As $U^{-} - J^{-}$ is raised the Zn 3d states are shifted downwards and the band gap increases. At the same time the equilibrium volume decreases while the bulk modulus varies only slightly. Eventually, we settled for $U^{-} - J^{-} =$ 7.5 eV. With this value the valence band energy levels as well as the (First-principles study of intrinsic point defects in ZnO: Role of band structure, volume relaxation, and finite-size

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Conclusion:

To perform this study, we have employed density functional theory (DFT) calculations, considering the Perdew-Burke-Ernzerhof (PBE) functional. However, it is well-known that the plain DFT fails to describe strong electronic correlated materials, where in general, the band gap underestimation is obtained. Thus, to the correct description of the electronic properties was employed a Hubbard correction, i.e., PBE+U calculations. The PBE+U methodology has provided the correct electronic structure properties for bulk ZnO in good agreement with the experimental values (99.4%) (Efracio Mamani Flores,∗a Rogério Almeida Gouvea,∗a Maurício Jeomar Piotrowskia and Mário Lucio Moreiraa, Band Alignment and Charge Transfer Predictions of ZnO/ZnX (X = S, Se, Te) Interfaces Applied to Solar Cells: A PBE+U Theoretical Study, : E. M. Flores, R. A. Gouvea, M. J. Piotrowski and M. L. L. Moreira, Phys. Chem. Chem. Phys., 2018, DOI: 10.1039/C7CP08177D)

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Paolo Giannozzi1,2, Stefano Baroni1,3, Nicola Bonini4, Matteo Calandra5, Roberto Car6, Carlo Cavazzoni7,8, Davide Ceresoli4, Guido L Chiarotti9, Matteo Cococcioni10, Ismaila Dabo11Show full author list

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Affiliations expand

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