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As the pandemic subsides and people are getting back to workspaces, many of us are still trying to adapt to the 'new normal'. Everyone is trying to juggle between pre pandemic, pandemic and post pandemic activities. There have been significant changes in lifestyle behaviors, new trends are emerging, and healthy lifestyle practices are need of the hour. According to Ernst & Young Private limited (EY) India, Indian consumers are willing to spend more on the lifestyle activities. Around 94 percent of Indians are worried about their family's health, while 52 percent think changes in their approach to mental wellbeing will persist beyond COVID-19. Another megatrend that is influencing lifestyles is Sustainability, an Economic Times report stated that 86 per cent of individuals find that buying sustainable products makes them happy! Sustainable food choices are becoming new normal, it is evident that people are becoming eco-conscious. In fact, it has lead people turning to alternative plant-based meat free food, after all excluding meat and dairy products from diet reduces individual carbon footprint by 73 per cent. As a result, people are leaning towards veganism. Another significant change we see is demand for food transparency i.e., people are keen on knowing where their food and drinks comes from is it organic, locally sourced, natural, chemical free, sustainably sourced etc. Today we are leaning towards mindful and conscious lifestyle behavior, but are really practicing healthy lifestyle practices? What can we do to incorporate healthy behaviors into our daily lives? Here we will try to understand some of the important aspects of healthy behavior and how we can incorporate it in our daily lives. In 2018, Harvard researchers looked at factors that may increase our chances of healthy and longer life. Through data collected from men and women who were followed up for 34 years. They found that those who, exercised daily for at least 30 minutes daily, maintained healthy BMI (18.5-24.9), ate healthy balanced diet, did not smoke and moderate alcohol intake lived up to 14 years longer and healthier life than those who did not incorporate these lifestyle behaviors. In a follow up study in 2020, they found women in 50 who practiced four or five healthy lifestyle practices mentioned above lived 34 more years free of diabetes, cardiovascular diseases and cancer compared to other women who practiced none of healthy lifestyle practices. These study findings are encouraging, and it highlights importance of consistent healthy behavioral practices throughout one's life. So, lets investigate healthy behaviors mentioned above. We saw that healthy diet is an important part of a healthy lifestyle. Eating healthy diet is not about fancy foods, strict limitations, giving up the food you love. We all need to

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balance of protein, fat, carbohydrates, fiber, vitamins and minerals in our

diet to sustain healthy lifestyle, while some of the diets may suggest otherwise. Instead of eliminating certain categories of food we can replace them with a healthier alternative. Protein gives you energy, allows metabolic functions to take place and coordinate bodily functions, while also supporting mood and cognitive function. This does not mean we should consume protein blindly, on contrary it should be carefully regulated. Too much protein is found to be harmful for the kidney. Recent research suggests that some

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of us need high quality protein, especially as we age. It doesn't mean

we need to rely on animal-based protein, a variety of plant-based protein sources each day can ensure your body gets all essential protein needed.

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A small amount of fat is also an essential part of diet. It is source of essential fatty acids that body need. In addition, it also helps absorb Vit A, D and E which are fat soluble, which means they cannot be absorbed

without fat. Carbohydrates are also integral part of diet, but we should always try to consume complex carbohydrates rather than simple sugars which immediately convert into sugars which are harmful for the body. Consumption of variety of fruits and vegetable is important for ensuring we get necessary amount of vitamins ad minerals. In short, we need a diet that gives your body the nutrition it needs to function correctly, a low salt, low fat diet with plenty of fruits, vegetables and

fiber is ideal to build up physical and mental stamina and agility. In fact, it was found in research that higher sodium consumption increased risk to cardiovascular diseases (CVD). While optimal amount of potassium is found to reduce risk to CVD, so they found higher sodium to potassium ratio was associated with higher CVD risk. In recent years we have been hearing about anti nutrients, and are they harmful? Although antinutrients may block absorption of nutrients, but it is not known much about nutrition loss because effects may vary upon metabolism, how the food is cooked and prepared. In addition, these antinutrients may also have health benefits. Phytates is antinutrient found in grains, seeds and legumes it is found to lower cholesterol, slow digestion and prevent sharp rise in blood sugar. But long-term effect of these antinutrients is area of active research, but health benefits of anti-nutrients far outweigh potential negatives. It is found that some diets may work wonders for certain person, it does not mean it is appropriate for your body and lifestyle. So, one needs to tailor a diet that suits their lifestyle. But it is also recommended to incorporate regional and seasonal ingredients in diet. Another important aspect is staying active, beyond diet exercise also plays key role in our overall wellbeing.

In a study it was found that people who did regular and vigorous exercise had larger brain volumes and lower risk of dementia. But it is also important that we try to exercise in pollution free environment, Dr. David Raichlen of University of Southern California said, "The better the air quality is around you as you exercise the better workout will be for your brain". Sleep is essential to our daily needs as food and water. Sleep needs change with age infants need 14-17 hours, teens require 8-12 hours and adults require 7-8 hours' sleep. Although sleep durations may vary, in studies it is found that people who slept less than 5 hours had increased risk of obesity, diabetes and cardiovascular diseases. In addition, the quality of sleep is also important because meeting recommended standards are not enough if sleep gets disrupted several times. A good quality sleep not only helps you become productive but is also important for healthy lifestyle. These are some healthy behavioral habits we can incorporate in our lives to stay productive and healthy in resent and future.

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of us need high quality protein, especially as we age. It doesn't mean

of us need more high-quality protein, especially as we age. That doesn't mean

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A small amount of fat is also an essential part of diet. It is source of essential fatty acids that body need. In addition, it also helps absorb Vit A, D and E which are fat soluble, which means they cannot be absorbed

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Modern day lifestyle has increased sedentary lifestyle affecting adversely to overall impairment of body movement. So daily moderate physical exercise and balanced diet and help reduce risk of chronic diseases.

Modern-day lifestyle has increased sedentary lifestyle affecting adversely the muscular-skeletal health leading to overall impairment of the body movement. So a daily moderate physical activity and having a balanced diet can help reduce the risk of many chronic diseases

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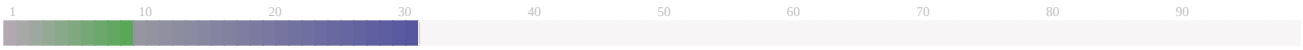

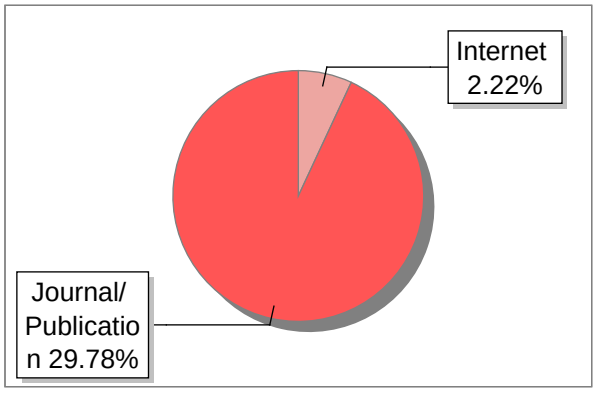

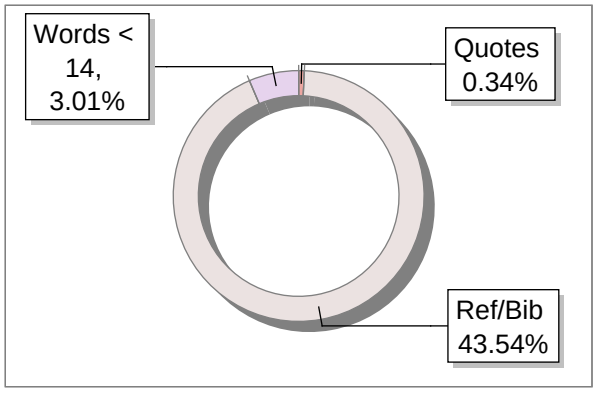

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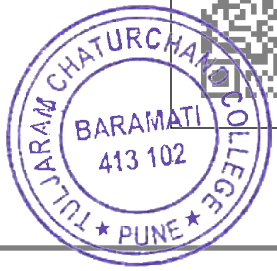

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First-principles DFT + U studies of the Nb-doped ZnO spray deposited thin films.

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

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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

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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

effects Paul Erhart, Karsten Albe, and Andreas Klein, PHYSICAL REVIEW B 73, 205203 2006,)

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)

References :

1. Ahmed H. Hammad a b 1, M. Sh. Abdel-wahab a c, Asim jilani a d, Characterization of niobium-doped zinc oxide thin films: Structural changes and optical properties, Materials Today Communications, https://doi.org/10.1016/j.mtcomm.2020.101791, Volume 26, March 2021, 101791
2. Li T, Cai H, Li C, Liu X and Huang F (2020) Rocksalt-Zincblende–Wurtzite Mixed-Phase ZnO Crystals With High Activity as Photocatalysts for Visible-Light-Driven Water Splitting. *Front. Chem.* 8:351. doi: 10.3389/fchem.2020.00351
3. Romana Zahoor, Abdul Jalil, Syed Zafar Ilyas, Sarfraz Ahmed, Ather Hassan, Optoelectronic and solar cell applications of ZnO nanostructures, Results in Surfaces and Interfaces, Volume 2, 1 February 2021, 100003
4. Mariane A. Franco a b, Patrick P. Conti c, Rafaela S. Andre a, Daniel S. Correa, A review on chemiresistive ZnO gas sensors, Sensors and Actuators Reports Volume 4, November 2022, 100100

5. Gartner, M.; Stroescu, H.; Mitrea, D.; Nicolescu, M. Various Applications of ZnO Thin Films Obtained by Chemical Routes in the Last Decade. *Molecules* **2023**, *28*, 4674. https://doi.org/10.3390/molecules28124674
6. R.L. Hoffman,Chapter 12 - ZnO Thin-Film Transistors,Editor(s): Chennupati Jagadish, Stephen Pearton,Zinc Oxide Bulk, Thin Films and Nanostructures,Elsevier Science Ltd,
7. Kavindra Kandpal a, Navneet Gupta b, Jitendra Singh c, Chandra Shekhar b Study of ZnO/BST interface for thin-film transistor (TFT) applications, Surfaces and InterfacesVolume 23, April 2021, 100996, https://doi.org/10.1016/j.surfin.2021.100996
8. X Y Du1, Y Q Fu1, S C Tan1, J K Luo1,2, A J Flewitt1, S Maeng3, S H Kim3, Y J Choi3, D S Lee3, N M Park3 X Y Du et al 2007 J. Phys.: Conf. Ser. 76 012035DOI 10.1088/1742-6596/76/1/012035, ZnO film for application in surface acoustic wave device
9. Xu Li, Xinghua Zhu, Kangxin Jin, Dingyu yang, Study on structural and optical properties of Mn-doped ZnO thin films by sol-gel method,Optical Materials,Volume 100, 2020,109657, ISSN 0925-3467, https://doi.org/10.1016/j.optmat.2020.109657.
10. Moussa, N.M., Ebrahim, F.M., Adly, K. *et al.* Chromium doped ZnO nanoparticles for energy storage, gas and humidity sensing and spin based electronic devices applications. *Opt Quant Electron* **54**, 683 (2022).https://doi.org/10.1007/s11082-022-04075-y
11. Georgeta Voicu, Dana Miu, Cristina-Daniela Ghitulica, Sorin-Ion Jinga, Adrian-Ionut Nicoara, Cristina Busuioc, Alina-Maria Holban,Co doped ZnO thin films deposited by spin coating as antibacterial coating for metallic implants,Ceramics International,Volume 46, Issue 3, 2020, Pages 3904-3911, ISSN 0272-8842, https://doi.org/10.1016/j.ceramint.2019.10.118.
12. P.L. Hadimani, S.S. Ghosh, A. Sil, Preparation of Fe doped ZnO thin films and their structural, magnetic, electrical characterization, Superlattices and Microstructures, Volume 120, 2018, Pages 199-208, ISSN 0749-6036, https://doi.org/10.1016/j.spmi.2018.05.029.
13. Bhubesh Chander Joshi and Aadarsh Kumar Chaudhri, Sol–Gel-Derived Cu-Doped ZnO Thin Films for Optoelectronic Applications, ACS Omega 2022 7 (25), 21877-21881, DOI: 10.1021/acsomega.2c02040,
14. Vineet Kumar Pandey, C.K. Dixit, Effect of Titanium Doping on the Electrical Properties of Conducting ZnO Transparent Thin Films, Materials Today: Proceedings, Volume 24, Part 2, 2020, Pages A15-A20, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2020.04.324.
15. Bimal K. Sarma, Pradhyut Rajkumar,
16. Al-doped ZnO transparent conducting oxide with appealing electro-optical properties – Realization of indium free transparent conductors from sputtering targets with varying dopant concentrations, Materials Today Communications, Volume 23, 2020, 100870, ISSN 2352-4928, https://doi.org/10.1016/j.mtcomm.2019.100870.
17. Wei-Sheng Liu, Shen-Yu Wu, Chao-Yu Hung, Ching-Hsuan Tseng, Yu-Lin Chang, Improving the optoelectronic properties of gallium ZnO transparent conductive thin films through titanium doping, Journal of Alloys and Compounds, 10.1016/j.jallcom.2014.06.175, **616**, (268-274), (2014)

18. Auttasit Tubtimtae, Ming-Way Lee, ZnO nanorods on undoped and indium-doped ZnO thin films as a TCO layer on nonconductive glass for dye-sensitized solar cells, Superlattices and Microstructures, Volume 52, Issue 5, 2012, Pages 987-996, ISSN 0749-6036, https://doi.org/10.1016/j.spmi.2012.08.002..
19. Çolak H, Karaköse E, Sungür Ç. Niobium doping effect on electrical and optical properties of ZnO nanorods produced by ultrasonic spray pyrolysis. Physica B: Condensed Matter. 2023 Dec 15;671:415455.
20. Malyutina-Bronskaya V, Zalesski V, Zhyhulin D, Mudryi A. Structural, optical and photoelectric properties of Tb doped ZnO thin films for device applications. Optical Materials. 2022 May 1;127:112305.
21. Roguai S, Djelloul A. ZnO and La-doped ZnO films by USP method and their characterizations for ultraviolet photodetectors and photocatalysis applications. Inorganic Chemistry Communications. 2023 Nov 1;157:111372.
22. Zhussupbekov K, Walshe K, Bozhko SI, Ionov A, Fleischer K, Norton E, Zhussupbekova A, Semenov V, Shvets IV, Walls B. Oxidation of Nb(110): atomic structure of the NbO layer and its influence on further oxidation. Sci Rep. 2020 Mar 2;10(1):3794. doi: 10.1038/s41598-020-60508-2. PMID: 32123233; PMCID: PMC7052221.
23. Jingzhen Shao, Weiwei Dong, Da Li, Ruhua Tao, Zanhong Deng, Tao Wang, Gang Meng, Shu Zhou, Xiaodong Fang, Metal-semiconductor transition in Nb-doped ZnO thin films prepared by pulsed laser deposition,Thin Solid Films, Volume 518, Issue 18, 2010, Pages 5288-5291, ISSN 0040-6090, https://doi.org/10.1016/j.tsf.2010.04.068
24. Yantao Liu*,z , Wenxia Wang*, Jianping Ma*, Ying Wang*, Wei Yey , Chao Zhang*, Jingjing Chen*, Xinyu Li* and Yan Du* JOURNAL OF ADVANCED DIELECTRICS Vol. 9, No. 6 (2019) 1950048 (6 pages) © The Author(s) DOI: 10.1142/S2010135X19500486
25. Seong-Hwan Kim, Gyu-In Shim, Se-Young Choi,
26. Fabrication of Nb-doped ZnO nanowall structure by RF magnetron sputter for enhanced gas-sensing properties, Journal of Alloys and Compounds,Volume 698, 2017, Pages 77-86, ISSN 0925-8388, https://doi.org/10.1016/j.jallcom.2016.11.377.
27. Anuntahirunrat J, Sung YM, Pooyoding P. Efficiency of Nb-doped ZnO nanoparticles electrode for dye-sensitized solar cells application. InIOP Conference Series: Materials Science and Engineering 2017 Sep 1 (Vol. 229, No. 1, p. 012019). IOP Publishing.
28. Jirapat Anuntahirunrat1 , Youl-Moon Sung1, * and Pattarapon Pooyoding1 1 Electrical Engineering, Kyungsung University, Busan 608-736, Korea, IOP Conf. Series: Materials Science and Engineering 229 (2017) 012019 doi:10.1088/1757-899X/229/1/012019]],
29. Byun JM, Choi HR, Do Kim Y, Sekino T, Kim SH. Photocatalytic activity under UV/Visible light range of Nb-doped titanate nanostructures synthesized with Nb oxide. Applied Surface Science. 2017 Sep 1;415:126-31.
30. Dr. Amit K. Chawla, Dr. Ratnesh Pandey, Akula Umamaheswara Rao, Archana Singh Kharb, Avaani Chanana, Kifayat H. Mir, Pramod Kumar, Dr. Tarun Garg, Dr. Vipin Chawla, Dr. Ravish Jain, Charu Pant, Dr. Sanjeev Kumar … See fewer authors , Volume8, Issue39 October 20, 2023, e202302882]

31. Bing Hana, Jianmin Songb, Junjie Lia, Yajuan Guoa, Binting Daia, Xudong Menga, Weiye Songa, Fu Yanga and Yanfeng Wang*a
aInstitute of New Energy Science and Technology of Hebei North University, Zhangjiakou 075000, China. , DOI: 10.1039/C9RA01231A (Paper) RSC Adv., 2019, 9, 12681-12688]
32. L. Sun, J. G. Jones, and P. R. Stevenson, "Tuning the Optical Properties of Niobium-doped ZnO Films," in *Optical Interference Coatings Conference (OIC) 2022*, R. Sargent and A. Sytchkova, eds., Technical Digest Series (Optica Publishing Group, 2022), paper TD.4.

https://opg.optica.org/abstract.cfm?URI=OIC-2022-TD.4]] ,

33. [, Lin, Chun-Cheng , Chu, Sheng-Yuan , , Huang, Chih-Yu , Hong, Cheng-Shong , Effects of Nb doping on switching-voltage stability of zinc oxide thin films, Journal of Applied Physics, Volume 128, Issue 17, article id.175308, 2020]
34.] [Gokulakrishnan, V., Parthiban, S., Jeganathan, K. et al. Structural, Optical, and Electrical Properties of Nb-Doped ZnO Thin Films Prepared by Spray Pyrolysis Method. J. Electron. Mater. 40, 2382–2387 (2011). https://doi.org/10.1007/s11664-011-1755-1]

35. **]| Çolak a b, Ercan Karaköse c, Çiğdem Sungür , Niobium metal doped ZnO nanorods were fabricated on a glass substrate using an ultrasonic spray pyrolysis system**
Physica B: Condensed Matter, Volume 671, 15 December 2023, 415455
36. A. Shaw , J. S. Wrench , J. D. Jin , T. J. Whittles, I. Z. Mitrovic , M. Raja; V. R. Dhanak; P. R. Chalker and S. Hall ,
37. **Atomic layer deposition of Nb-doped ZnO for thin film transistors ,** *Appl. Phys. Lett.* 109, 222103 (2016) https://doi.org/10.1063/1.4968194
38.] Pal U, Morales-Flores N, Rubio-Rosas E. Effect of Nb Doping on Morphology, Optical and Magnetic Behaviors of Ultrasonically Grown Zno Nanostructures. Mat.Sci.Res.India;14(2). Available from: http://www.materialsciencejournal.org/?p=6010]

39. (First-principles LDA + U studies of the In-doped ZnO transparent conductive oxide X. H. Zhou, Q.-H. Hu, and Y. Fu Citation: Journal of Applied Physics 104, 063703 (2008); doi: 10.1063/1.2978324),

40. heoretical study of structural and optical properties of ZnO in wurtzite phase, Y. Benkrima a* , S. Benhamida b , D. Belfennache, Digest Journal of Nanomaterials and Biostructures

41. Ammar, H. Y., H. M. Badran, Ahmad Umar, H. Fouad, and Othman Y. Alothman. 2019. "ZnO Nanocrystal-Based Chloroform Detection: Density Functional Theory (DFT) Study" *Coatings* 9, no. 11: 769. https://doi.org/10.3390/coatings9110769

42. Der Pharma Chemica (2018) Volume 10, Issue 1A Comprehensive DFT Study of Wurtzite ZnO**Benkrima Yamina1*, Achouri Abderrahim1, Bentouila Omar2 and Benmebrouk Lazhar3**
43. Vu Ngoc Tuoc Tran Doan Huan1,2, Nguyen Viet Minh1 , Nguyen Thi Thao1 et al 2016 J.Phys.: Conf. Ser. 726 012022
44. Fatima A. Hasan, Mohammed T. Hussein, Study of some electronic and spectroscopic properties of ZnO nanostructers by density functional theory, Materials Today: Proceedings, Volume 42, Part 5, 2021, Pages 2638-2644, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2020.12.593.
45. *J. Phys. Chem. C* 2022, 126, 16, 7000–7011 Publication Date:April 13, 200 https://doi.org/10.1021/acs.jpcc.2c00152
46. Zhongyu Wan, Quan-De Wang, Dongchang Liu, Jinhu Liang, Effectively improving the accuracy of PBE functional in calculating the solid band gap via machine learning, nComputational Materials Science, Volume 198, 2021, 110699, ISSN 0927-0256, https://doi.org/10.1016/j.commatsci.2021.110699.
47. BAKHTIAR UL HAQ*,†, A. AFAQ*, R. AHMED†,‡ and S. NASEEM* A COMPREHENSIVE DFT STUDY OF ZINC OXIDE IN DIFFERENT PHASES International Journal of Modern Physics C Vol. 23, No. 6 (2012) 1250043 (10 pages) DOI: 10.1142/S012918311250043X
48. Ahmad Azmin Mohamad, Muhammad Syafiq Hassan, Muhamad Kamil Yaakob, Mohamad Fariz Mohamad Taib, Fadhlul Wafi Badrudin, Oskar Hasdinor Hassan, Muhd Zu Azhan Yahya First-principles calculation on electronic properties of zinc oxide by zinc–air system, Journal of King Saud University - Engineering Sciences, Volume 29, Issue 3, 2017, Pages 278-283, ISSN 1018-3639, https://doi.org/10.1016/j.jksues.2015.08.002.
49. Mahlaga P. Molepo* and Daniel P. Joubert , Computational study of the structural phases of ZnO, Phys. Rev. B 84, 094110 – Published 19 September 2011 https://doi.org/10.1103/PhysRevB.84.094110
50. Mitsutake Oshikiri and Ferdi Aryasetiawan , Band gaps and quasiparticle energy calculations on ZnO, ZnS, and ZnSe in the zinc-blende structure by the GW approximation Phys. Rev. B 60, 10754 – Published 15October 1999 https://doi.org/10.1103/PhysRevB.60.10754
51. Anderson Janotti* and Chris G. Van de Walle, LDARU and hybrid functional calculations for defects in ZnO, SnO2, and TiO2 , Phys. Status Solidi B 248, No. 4, 799–804 (2011) / DOI 10.1002/pssb.201046384
52. Frédéric Labat; Ilaria Ciofini; Carlo Adamo Modeling ZnO phases using a periodic approach: From bulk to surface and beyond, *J. Chem. Phys.* 131, 044708 (2009) https://doi.org/10.1063/1.3179752
53. Zaragoza IP, Soriano-Agueda LA, Hernández-Esparza R, Vargas R, Garza J. Analyzing ZnO clusters through the density-functional theory. Journal of Molecular Modeling. 2018 Jul;24:1-3.
54. Jamal Uddin and Gustavo E. Scuseria Theoretical study of ZnO phases using a screened hybrid density functional Phys. Rev. B 74, 245115 – Published 18 December 2006, https://doi.org/10.1103/PhysRevB.74.245115
55. X.J. Zhang, W.B. Mi, X.C. Wang, H.L. Bai, First-Principles Prediction of Electronic Structure and Magnetic Ordering of Rare-earth Metals Doped ZnO, *Journal of Alloys and Compounds* (2014), doi: http://dx.doi.org/10.1016/j.jallcom.2014.07.218

56. PHYSICAL REVIEW B **86**, 235113 (2012) **Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for *d* band shift in oxide semiconductors** Linda Y. Lim,[1,2] Stephan Lany,[3] Young Jun Chang,[4] Eli Rotenberg,[5] Alex Zunger,[6] and Michael F. Toney[2] DOI: 10.1103/PhysRevB.86.235113

57. Ahmed Badreldin, Ahmed Abdel-Wahab, and Perla B. Balbuena , Local Surface Modulation Activates Metal Oxide Electrocatalyst for Hydrogen Evolution: Synthesis, Characterization, and DFT Study of Novel Black ZnO, *ACS Applied Energy Materials* **2020** *3* (11), 10590-10599 DOI: 10.1021/acsaem.0c01642

58. Gui-Yang Huang a,∗, Chong-Yu Wang a,b, Jian-Tao Wang , Detailed check of the LDA+U and GGA+U corrected method for defect calculations in wurtzite ZnO, mputer Physics Communications 183 (2012) 1749–1752

59. R. Amari, B. Deghfel, A. Mahroug, Ahmad Azmin Mohamad, A. Boukhari, N.Selmi, Effects of Mn doping on the structural, morphological, electronic and optical properties of ZnO thin films by sol-gel spin coating method: An experimental and DFT+U study, Physica B: Physics of Condensed Matter (2019), https://doi.org/10.1016/j.physb.2019.411766

60. Anthony Consiglio & Zhiting Tian , Importance of the Hubbard correction on the thermal conductivity calculation of strongly correlated materials: a case study of ZnO, Scientific Reports | 6:36875 | DOI: 10.1038/srep36875

61. : Shokri A, Yazdani A, Rahimi K, Possible bandgap values of graphene-like ZnO in density functional theory corrected by the Hubbard U term and HSE hybrid functional, Materials Today Communications (2019), doi: https://doi.org/10.1016/j.mtcomm.2019.100756),

62. Zhanhong Ma 1,2, Fengzhang Ren 1,*, Xiaoli Ming 1 , Yongqiang Long 1 and Alex A. Volinsky Cu-Doped ZnO Electronic Structure and Optical Properties Studied by First-Principles Calculations and Experiments, , Materials 2019, 12, 196)

63. R. Amari, B. Deghfel, A. Mahroug, Ahmad Azmin Mohamad, A. Boukhari, N.Selmi, Effects of Mn doping on the structural, morphological, electronic and optical properties of ZnO thin films by sol-gel spin coating method: An experimental and DFT+U study, Physica B: Physics of Condensed Matter (2019), https://doi.org/10.1016/j.physb.2019.411766)\

64. Thickness effect on the properties of Mn-doped ZnO thin films synthesis by sol-gel and comparison to first-principles calculations Ammar Boukhari a,b,c , Bahri Deghfel a,* , Abdelhafidh Mahroug a,b , Rabie Amari a,b , Noureddine Selmi e , Soorathep Kheawhom f , Ahmad Azmin Mohamad c,d,** Ceramics International 47 (2021) 17276–1728)

65.

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. 2020 Apr 21;152(15):154105.
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"P. Giannozzi et al., J. Chem. Phys. 152 154105 (2020);

1. Lukas Schmidt-Mende, Judith L. MacManus-Driscoll, ZnO – nanostructures, defects, and devices, Materials Today, Volume 10, Issue 5, 2007, Pages 40-48, ISSN 1369-7021, https://doi.org/10.1016/S1369-7021(07)70078-0.