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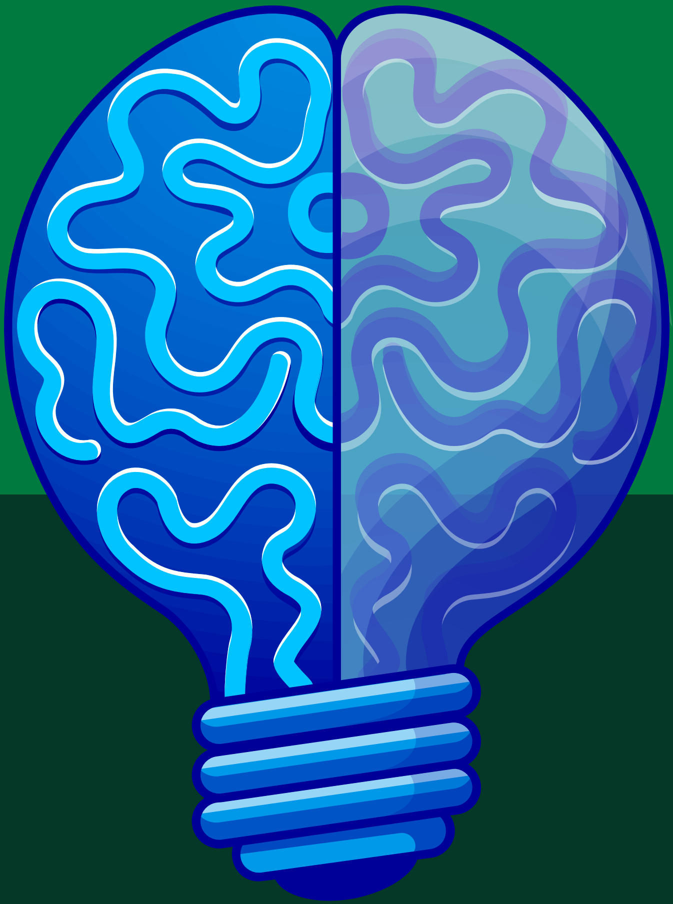

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Preface

The Scientific Project Colloquium offers a platform for publishing Diploma Science final year projects (FYP). The objective is to effectively distribute research findings throughout all scientific disciplines. The primary objective of including final year projects into the course curriculum is to encourage students to put their theoretical knowledge into practical applications.

We would like to express our gratitude to our primary establishment, the Faculty of Applied Sciences and Universiti Teknologi MARA, Perak Branch, for their invaluable assistance.

Lastly, we would like to express our gratitude to all of the authors for the tremendous help in preparing the articles, without which this undertaking would not have been completed.

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DENSITY FUNCTIONAL THEORY INSIGHTS ON THE ELECTRONIC AND OPTICAL PROPERTIES OF ZnO IN SUNSCREEN APPLICATIONS

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Abstract: The structural, electrical, and optical properties of zinc oxide (ZnO) was performed using density functional theory using CASTEP software with exchange correlation of generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE). The band gap energy of ZnO was observed at 3.27 eV after a Hubbard U correction at energy. Incorporating these corrections brought the band gap energy closer to experimental values. The absorption shows that ZnO fall in the UV region compliment with the band gap energy obtain.

Keywords: *Zinc oxide, Density functional theory, Electronic properties, Optical properties, Sunscreen*

INTRODUCTION

Zinc oxide (ZnO) is a versatile white powder widely applied across industries, with one of its most notable uses as an active ingredient in sunscreen, where it prevents the transmission of ultraviolet (UV) radiation through the skin (Kyu Bong Kim, 2017). As a physical sunscreen, ZnO acts as a broad-spectrum UV blocker and is generally considered less chemically reactive than organic UV filters. Although safer in many respects, some formulations may still cause skin irritation and pose environmental concerns (Desk, 2023). Beyond its UV-blocking function, ZnO exhibits anti-inflammatory and antimicrobial properties, making it particularly useful in sunscreens designed for sensitive or acne-prone skin. Its stability under diverse environmental conditions further strengthens its role as a reliable ingredient for daily sun protection products.

Generally, zinc oxide possesses a wide direct band gap of about 3.3–3.4 eV. These band gap energy value allow ZnO to absorb ultraviolet (UV) light effectively while maintaining good transparency in the visible spectrum, which is advantageous for applications in transparent electronics, UV photodetectors, and sunscreen formulations. ZnO most commonly crystallizes in the hexagonal wurtzite phase, which is thermodynamically stable under ambient conditions. ZnO has also attracted significant attention due to its abundance, low cost, non-toxicity, and chemical stability. Beyond traditional uses such as pigments, coatings, and cosmetics, it is now extensively studied for advanced applications including photocatalysis, gas sensing, solar cells, transparent conductive oxides, piezoelectric devices, and light-emitting diodes (LEDs).

Despite its widespread use, a deeper understanding of ZnO in term of band gap energy, absorption edge behaviour, and dielectric response is crucial for optimizing its role in cosmetic applications. Experimental studies provide valuable insights, but density functional theory (DFT) allows a more fundamental exploration of its properties at the atomic level. Standard DFT functionals often underestimate the band gap due to limitations in describing electron–electron interactions. Thus, incorporating Hubbard U corrections (DFT+U) or hybrid functionals becomes necessary for accurate band gap prediction and optical property analysis.

This study employs first-principles calculations within the CASTEP framework to investigate the structural, electronic, and optical properties of ZnO, with a particular focus on parameters relevant to sunscreen performance: the band gap, absorption edge, and dielectric function

METHODOLOGY

First-principles calculations based on plane-wave ultrasoft pseudopotentials method were performed for hexagonal ZnO using Cambridge Serial Total Energy Package (CASTEP) module in Materials Studio (MS) 8.0 developed by Accelrys Software Inc. The structural and electronic properties of ZnO were calculated using XC functionals from generalized gradient approximation GGA of Perdew-Burke-Ernzerhof (GGA-PBE). The valence electron configurations were treated as Zn-$4s^2$ $3d^{10}$ and O-$2s^2$ $2p^4$. The optimized cut-off energy value for the plane-wave basis set of the electronic wave function was 340 eV. The integration in the Brillouin zone was performed using 5 × 5 × 4 k-points from the Monkhorst-Pack scheme. The geometrical optimization was performed using the total energy of 1.0 × 10-5 eV/atom, the maximum force of 0.03 eV/Å, the maximum stress of 0.05 GPa and maximum atomic displacement of 1.0 × 10-3 Å. The values of Hubbard U correction are U*d* =2 eV and U*p* = 10 eV was referred to this paper since to optimized the Hubaard U energy required a long time (Hamzah, 2022)

FINDINGS

The hexagonal symmetry of ZnO plays a central role in determining its polar character, which underpins many of its physical properties, particularly its semiconducting and optoelectronic behaviour. The arrangement of atoms along the c-axis of the hexagonal lattice introduces polarity, which contributes to ZnO's wide direct band gap and its exceptional ability to absorb ultraviolet (UV) radiation. This characteristic makes ZnO highly effective in blocking a broad range of UV wavelengths, a property that is particularly relevant for sunscreen applications (Desk, 2023). Furthermore, the anisotropy of the wurtzite structure influences ZnO's optical responses, as the orientation of the c-axis governs the interaction of incident sunlight with the crystal lattice, thereby ensuring broad-spectrum UV protection. The optical transparency in the visible region, combined with strong UV absorption, makes ZnO one of the most desirable physical UV filters in cosmetic formulations. In addition to its optical advantages, the low-density yet robust HCP arrangement contributes to ZnO's notable mechanical and chemical stability, ensuring its durability under diverse environmental conditions. This structural stability, along with its non-toxic and non-reactive nature, reinforces ZnO's suitability for incorporation into daily-use cosmetic and skincare products, where long-lasting performance and safety are essential (Johnson & Lee, 2020). Figure 1 shows the crystal structure of unit cell of ZnO.

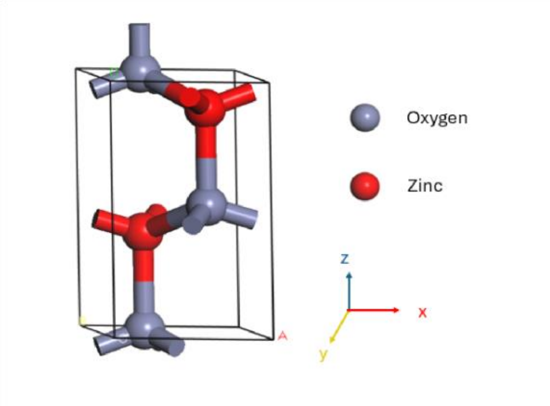

Figure 1 Crystal structure of unit cell of ZnO

The band gap of a semiconductor is defined as the energy difference between the valence band maximum (VBM) and the conduction band minimum (CBM), representing the energy range where no electronic states exist. Figure 2(a) and Figure 2(b) shows the band structure of ZnO before and after Hubbard U correction. Using standard calculation, the band gap obtained is 0.791 eV which is underestimated by 77.27% from the experimental value of 3.48 eV. After the Hubbard U correction, it shows an improvement in band gap energy of 3.27 eV, in close agreement with experimental values (3.48 eV) (Huang & Lambrecht, 2014). The improvement is due to the correction of delocalized Zn 3d state by refining the electronic structure during the Hubbard U correction. The red dashed line at E = 0 eV indicates the Fermi level, which in semiconductors lies within the band gap (Smijs & Pavel, 2011). The results confirm that ZnO is a direct band gap semiconductor, with both the VBM and CBM located at same Brillouin line. The corrected band gap of 3.27 eV corresponds to a photon wavelength of approximately 380 nm, within the UV-A (315–400 nm) and UV-B (280–315 nm) ranges (Smijs & Pavel, 2011). This allows ZnO to efficiently absorb harmful UV radiation while transmitting visible light ($\lambda > 400$ nm; $E < 3.1$ eV), explaining its effectiveness as a UV filter in sunscreens while maintaining transparency (Popov, Priezzhev, & Lademann, 2005). In sunscreen formulations, photons with energies above 3.27 eV excite electrons from the valence band to the conduction band, thereby absorbing UV radiation and preventing skin damage. Meanwhile, visible light passes through unabsorbed, minimizing the whitening effect common in earlier products. This property underpins the widespread use of ZnO in commercial sunscreens such as CeraVe Hydrating Mineral Face Sunscreen (7% ZnO), Innisfree Daily UV Defense Mineral Sunscreen (17% ZnO), and Neutrogena Sheer Zinc Face Sunscreen (21.6% ZnO), where it provides broad-spectrum UV protection with cosmetic acceptability.

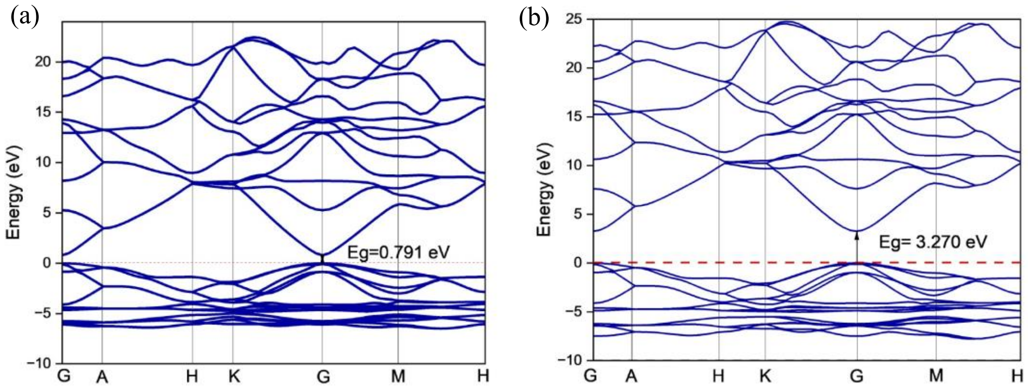

Figure 2 (a) Band gap energy before Hubbard U correction (b) band gap energy after Hubbard U correction for ZnO

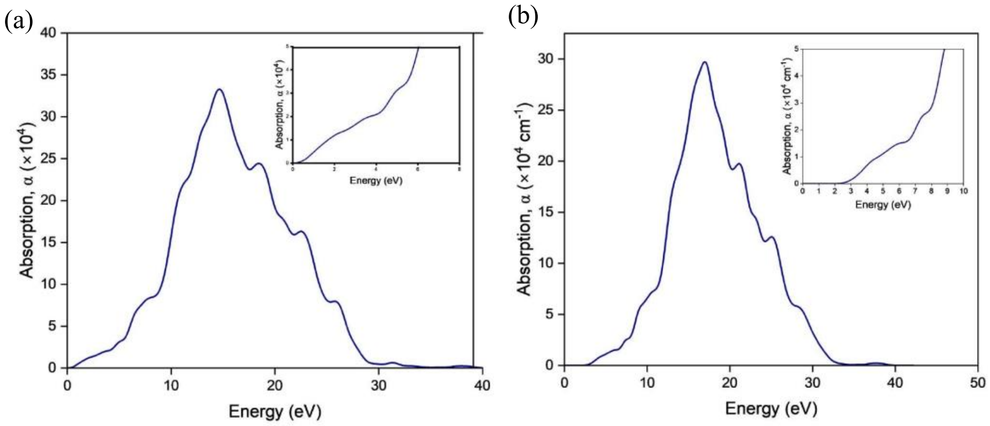

Figure 3 (a) Absorption edge before Hubbard U correction (b) absorption edge after Hubbard U correction for ZnO

Figure 3(a) and Figure 3(b) shows the absorption edge of ZnO before and after Hubbard U correction. It is observed that the improvement of absorption edge is significantly with the data obtained in the band structure. From this figure, the absorption edges fall in between ~ 3.1 eV which shows a good agreement with the band structure in previous discussion was shown in Figure 3(b). The absorption edge of 3.1 eV falls in UV spectrum which shows that this material has capability to absorb the UV light effectively. From this data, it is significant with most of the sunscreen or cosmetic product that use ZnO as one of their ingredients.

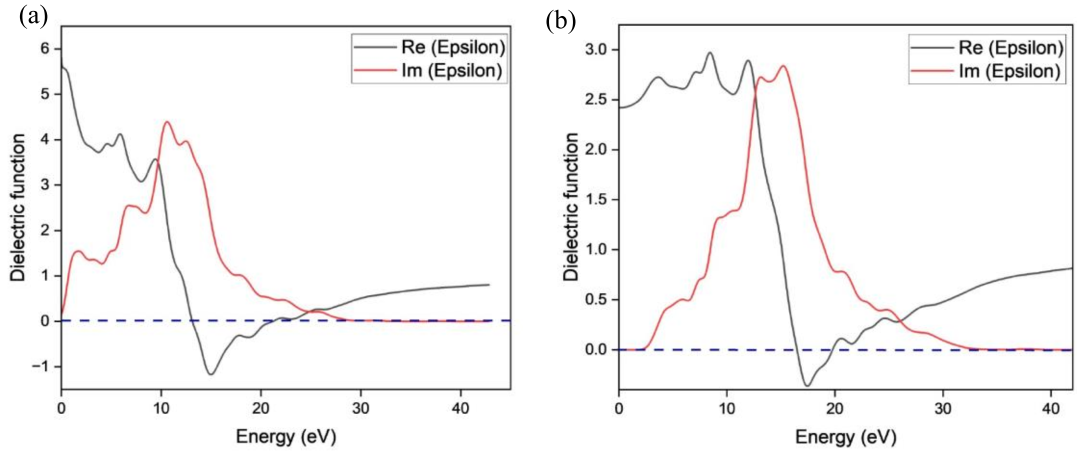

Figure 4 (a) Dielectric function before Hubbard U correction (b) dielectric function after Hubbard U correction for ZnO

Figure 4(a) and 4(b) shows the dielectric function of ZnO before and after Hubbard U correction. It clearly seen that there is an improvement in dielectric after Hubbard U correction. The dielectric function can be split into two parts: the imaginary part, Im (ε), represented by the red line, and the real part, Re (ε), represented by the black line. The imaginary part describes how much energy is dissipated in the material by the absorption of light, the real part describes how the ZnO plant affects the speed of propagation of electromagnetic waves due to a change in the refractive index that changes the light dispersion (Smith et al., 2023). The real part of the dielectric function, Re (ε), shows a static dielectric constant of approximately 2.5–3 at low photon energies, which gradually decreases and becomes negative in the range of 15–20 eV, indicating the occurrence of plasmon resonance. Beyond this energy, Re (ε) stabilizes toward positive values, suggesting weaker dispersion effects at higher energies. The imaginary part, Im(ε), reveals the optical absorption edge at ~3.2 eV, in agreement with the corrected band gap of 3.27 eV. A strong absorption peak is observed around 12–14 eV, attributed to interband transitions from O 2p to Zn 4s/4p states, followed by a gradual decline in absorption beyond 20 eV. The onset of absorption within the ultraviolet region confirms that ZnO is a direct band gap semiconductor capable of efficiently blocking UV-A and UV-B radiation, while its transparency to visible light (λ > 400 nm) ensures its cosmetic appeal in sunscreen formulations. These results demonstrate that DFT+U provides an accurate description of ZnO's optical behaviour, thereby reinforcing its role as a safe and effective broad-spectrum UV filter.

CONCLUSIONS

In this work, the electronic, and optical properties of ZnO were investigated using density functional theory with Hubbard U correction. The corrected band gap of 3.27 eV aligns closely with experimental values, confirming ZnO as a wide direct band gap semiconductor. The corresponding absorption edge at ~3.0–3.2 eV indicates strong absorption in the UV-A and UV-B regions while maintaining transparency in the visible spectrum. Analysis of the dielectric function further supports this behaviour, showing a static dielectric constant of 2.5–3 and pronounced absorption peaks arising from interband transitions. These findings emphasize ZnO's dual advantage as an efficient UV-blocking material and a transparent component in sunscreen formulations, underscoring its potential for safer and more effective cosmetic applications.

COMPLIANCE OF ETHICAL STANDARDS

Not applicable.

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