**Exploring the potential of double perovskite** **Ba₂NiWO₆** **using computer simulation**

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***Abstract***

*This study presents a comprehensive theoretical investigation of the structural, electronic, magnetic, thermal, optical, and elastic properties of the double perovskite compound Ba₂NiWO₆ using Density Functional Theory (DFT). The Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method, as implemented in the WIEN2k code, was employed. To enhance the accuracy of bandgap and magnetic property predictions, the GGA, GGA+U, and TB-mBJ approximations were incorporated.*

*The compound was found to crystallize in a cubic structure (space group*Fm3̅m*) and exhibits negative formation energies, confirming its thermodynamic stability and feasibility for experimental synthesis. Furthermore, we calculated the optimal Hubbard*U*parameter for use with the GGA+U method, determining a value of 2.32 eV.*

*Magnetic characterization revealed a net magnetic moment of 4 μB, indicating a half-metallic nature, which makes the compound a promising candidate for spintronic applications. The compound also demonstrates notable optical properties, particularly in the ultraviolet (UV) region. Additionally, it exhibits thermoelectric figure of merit (ZT) values close to unity across a wide temperature range, underscoring its potential for thermoelectric applications.*

**Keywords:** *Density Functional Theory; Double Perovskite; Optoelectronic Properties; Wien2k.*

**1. Introduction**

The demand for advanced materials with unique electronic, magnetic, and thermoelectric ‎properties has raised sharply with the growth of spintronics and sustainable energy solutions. Double perovskite compounds, specifically Ba₂NiWO₆ , ‎offer promising attributes for these applications due to their high thermal stability, diverse ‎magnetic properties, and optoelectronic potential. However, certain technological gaps persist, ‎particularly in developing materials that maintain high thermoelectric efficiency across a wide ‎temperature range and exhibit half-metallicity for enhanced spintronic performance. This ‎study aims to address these gaps by exploring the structural, mechanical, optoelectronic, and ‎thermoelectric properties of Ba₂NiWO₆ ‎.leveraging first-principles calculations. These ‎compounds exhibit impressive thermoelectric figures of merit (ZT), with values nearing unity ‎over broad temperature ranges. Additionally, the compounds demonstrate half-metallic ‎behavior and significant magnetic moments, supporting their utility in spintronic applications. ‎This study thus bridges critical gaps by providing a foundation for experimental synthesis and ‎device integration of these double perovskites. Recent advances in spintronic materials ‎highlight the value of compounds with high spin polarization and stability in varied ‎environments. Studies on similar perovskites, ‎have shown potential in specific applications but have not achieved comparable results across ‎diverse functional properties, especially thermoelectric efficiency and optical response. By ‎expanding on these findings, this work contributes a novel analysis that is essential for ‎advancing double perovskites in both sustainable energy and spintronic device applications. ‎

**II. METHODS / APPROACH**

In this study, we employed the Full-Potential Linearized Augmented Plane-Wave (FP-LAPW) method [1], as implemented in the Wien2K code [1], within the framework of Density Functional Theory (DFT) [2]. Initially, we applied the Generalized Gradient Approximation (GGA-PBE) [4], and subsequently refined our results using the GGA + U approach, which accurately describes electron correlation in partially filled outer-shell elements [3], such as the transition metals under investigation. We did not stop there; we further improved the results to achieve higher accuracy and outcomes more closely aligned with practical applications. To this end, we implemented the TB-mBJ (GGA + U) approximation [4].

**III. Results and discussions**

In fact, several key findings were obtained:

* Our results confirmed the formation of the compound in a cubic structure, and its stability was verified through calculations consistent with previous studies (***Figures 1 and 2***, and ***Table 1***).
* We found that the compound exhibits a ferromagnetic state, as illustrated in ***Figure 2***.
* We observed that the bandgap increases when applying the GGA+U and mBJ (GGA+U) approximations, ranging between 1 and 2 electron volts (***Figure 3***).
* In the optoelectronic domain, we discovered that this compound exhibits strong absorption in the ultraviolet region (***Figure 4***), making it a promising candidate for use as a wavelength-specific sensor.
* In the field of thermoelectric, we noted that our compound possesses a significant Seebeck coefficient of 3 millivolts at room temperature (***Figure 5***). Additionally, we found that it has a figure of merit very close to unity (***Figure 6***). which makes it a promising candidate for applications in thermoelectric devices, such as sensors or thermal energy-to-electricity converters.

**IV. FIGURES AND TABLES**

|  |  |
| --- | --- |
| *Figures 1* | *Figures 2* |
|  | |
| *Figures 3* | |
| |  |  |  | | --- | --- | --- | |  | **Ba2NiWO6** | | | **This work** | **Other work** | | ***T*** | 1.02 | 0.999 **[5]** | | ***Ef*** | -2.015 |  | | ***a*** | 7.829 | 7.890 **[5]**  7.832 **[6]**  7.820 **[7]** |   *Table 1* | *Figures 4* |
|  |  |
| *Figures 5* | *Figures 6* |

**CONCLUSION**

Potential developments in thermoelectric materials for effective energy harvesting and waste ‎heat recovery, as well as spintronic devices like magnetic sensors and memory storage, are ‎made possible by these discoveries. Moreover, their optical characteristics position them as ‎suitable options for use in photovoltaics, light-emitting devices, and various fields of ‎optoelectronics. In future work, conducting experimental validation of the theoretical ‎predictions would significantly improve the credibility of these findings. Investigating further ‎dopants or chemical alterations to these compounds may uncover avenues to customize their ‎characteristics for specific technological uses. This investigation, consequently, enhances the ‎existing knowledge of double perovskite materials while also emphasizing their significant ‎potential in contemporary technology.‎

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