First-principles study on optoelectronic properties for caswellsilverite mixed metal oxide MgZnO

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Preface

✓Mg_3ZnO_4 has a caswellsilverite (Rock-Salt) structure and crystallizes in the cubic $Pm\bar{3}m$ space group. Mg^{2+} forms bonds with six O^{2-} atoms, creating MgO_6 octahedra. These octahedra share corners with six other MgO_6 octahedra, edges with four ZnO_6 octahedra, and edges with another eight MgO_6 octahedra.

✓This study aims to predict the physical attributes of Mg3ZnO4 caswellsilverite materials through the ab-initio method, with the goal of conceptualizing a new thin-film solar cell structure with enhanced conversion efficiency. Initially, we utilized the Density Functional Theory (DFT) for our calculations, implementing the full-potential linearized augmented plane wave method (FP-LAPW) found in the WIEN2K software package. To determine the structural and electronic characteristics of the Mg_3ZnO_4 semiconductor materials, we employed the local density approximation (LDA), WC-GGA, and PBEsol-GGA for exchange-correlation potential. Additionally, the EV-GGA, the semi-local Becke-Johnson (mBJ) potential, and its variant by Tran and Blaha were applied to examine electronic and linear optical attributes. These findings were subsequently benchmarked against other computational studies.

✓The findings align well with existing data, suggesting that the material studied holds promise for crafting electronic and optoelectronic devices, especially in the domain of solar cells.

Computational details

- For determining structural properties, we employed the LDA, PBEsol-GGA, and WC-GGA in the exchange-correlation potential.
- However, the electronic and optical properties were evaluated using the TB-mBJ method. We set $RMT \times K_{MAX}$ at 9. We used Muffin-Tin Radii (RMT) values of 1.91, 2.05, and 1.77 atomic units for Mg, Zn, and O, respectively.
- spherical harmonics were expanded within the non-overlapping muffin tin spheres around the atoms up to l_{max}=10. The charge density, when Fourier-expanded, was cut off at G_{max}=12 $(a.u)^{-1}$. For all our materials, we utilized a k-point mesh of 1000 to depict the irreducible wedge of the Brillouin zone.
- For optical properties, a denser mesh of 2500 k-points was used. The half-width broadening was set at 0.2 eV.
- Lastly, our self-consistent computations were deemed converged once the system's total energy stabilized within a deviation of less than 10^{-4} Ryd.

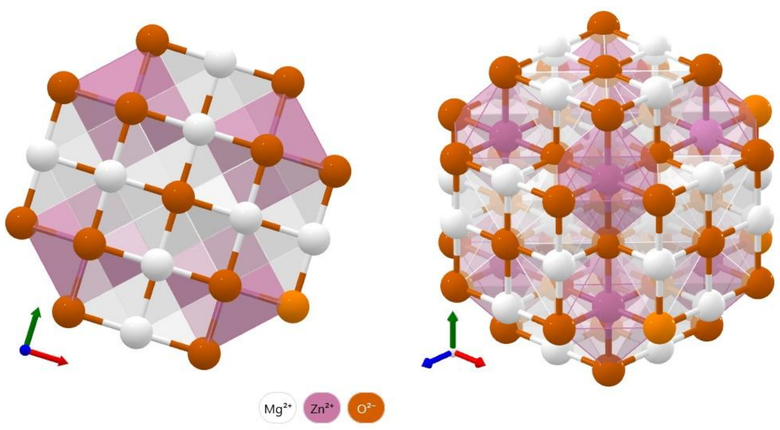

Fig. 1. Graphical presentations of the structure of Mg_3ZnO_4

WIEN2k

Fig. 2. Computational code Wien2k

The WIEN2k software package facilitates electronic structure analyses of solids through density functional theory (DFT). It harnesses the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, recognized as one of the most precise techniques for band structure computations. As an all-electron framework, WIEN2k incorporates relativistic effects and offers a multitude of features. It has been acquired by over 3600 user groups and boasts approximately 19,000 citations on Google Scholar when searched with "Blaha WIEN2k".[3]

Structural properties

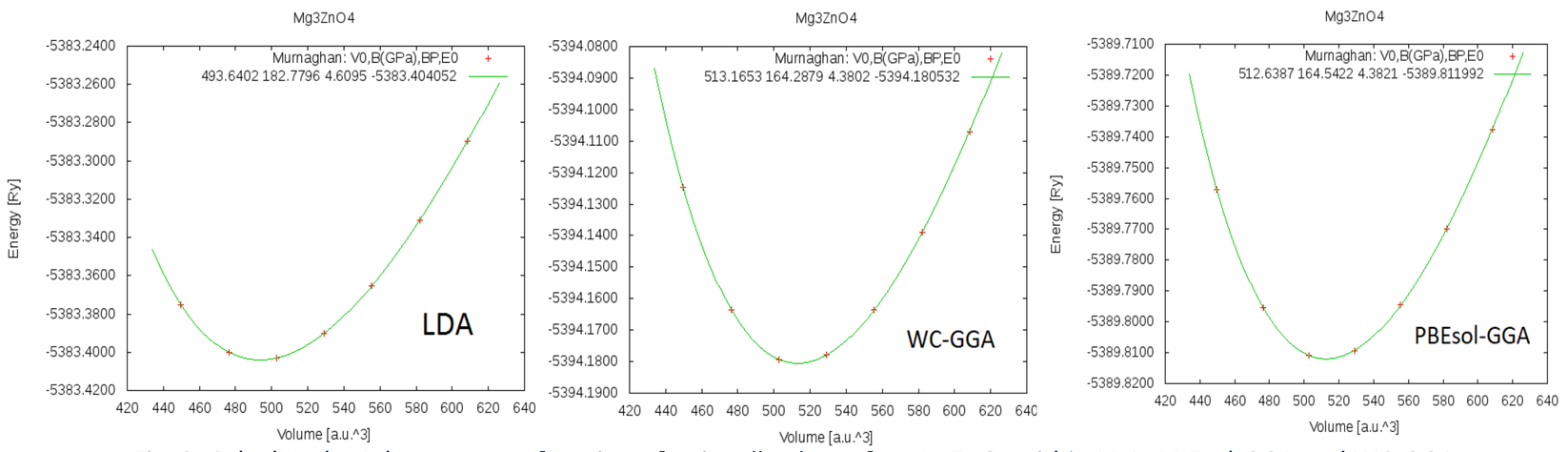

Fig. 3. Calculated total energy as a function of unit cell volume for Mg_3ZnO_4 within LDA, PBEsol-GGA and WC-GGA

TABLE 1. Calculated structural parameters within LDA ,WC-GGA and PBEsol-GGA approximations for Mg_3ZnO_4 compared with other realized works

Mg_3ZnO_4	Volume (u.a^3)	E_{min} (Ryd)	B(GPa)	B'	a (Å)	Δa (%)
LDA	493.6402	-5383.404052	182.7762	4.6095	4.1822	0.423
WC-GGA	513.1653	-5394.180532	164.2879	4.3802	4.2366	0.871
PBEsol-GGA	512.6387	-5389.811992	164.5422	4.3821	4.2352	0.838
Other works	499.9627 [2]	-	180.4 [2]	-	4.28 [1], 4.20 [2]	-

Electronic properties

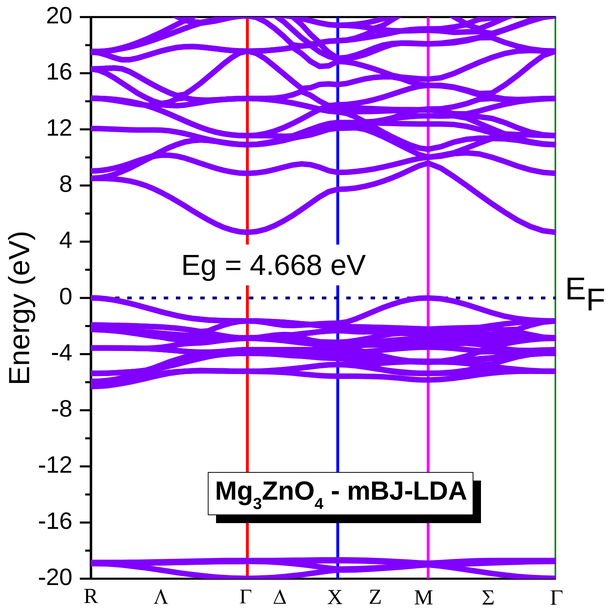

Fig. 4. Calculated band-structure for Mg_3ZnO_4 within mBJ-LDA

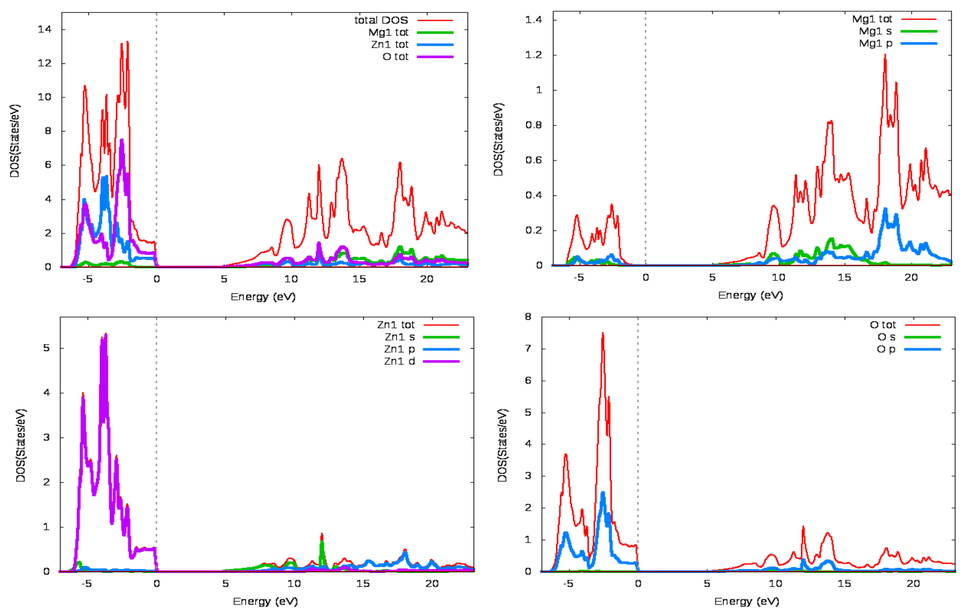

Fig. 5. Calculated TDOS/PDOS for Mg_3ZnO_4 within mBJ-LDA

Tab 2. Calculated Band-gap for Mg_3ZnO_4

Mg_3ZnO_4	LDA	WC-GGA	PBEsol-GGA	EV-GGA	mBJ-LDA	mBJ-GGA
Present work	2.456	2.217	2.217	3.033	4.668	4.476
Theoretical works	4.75 [1], 5.95 [2]					

Linear optical properties

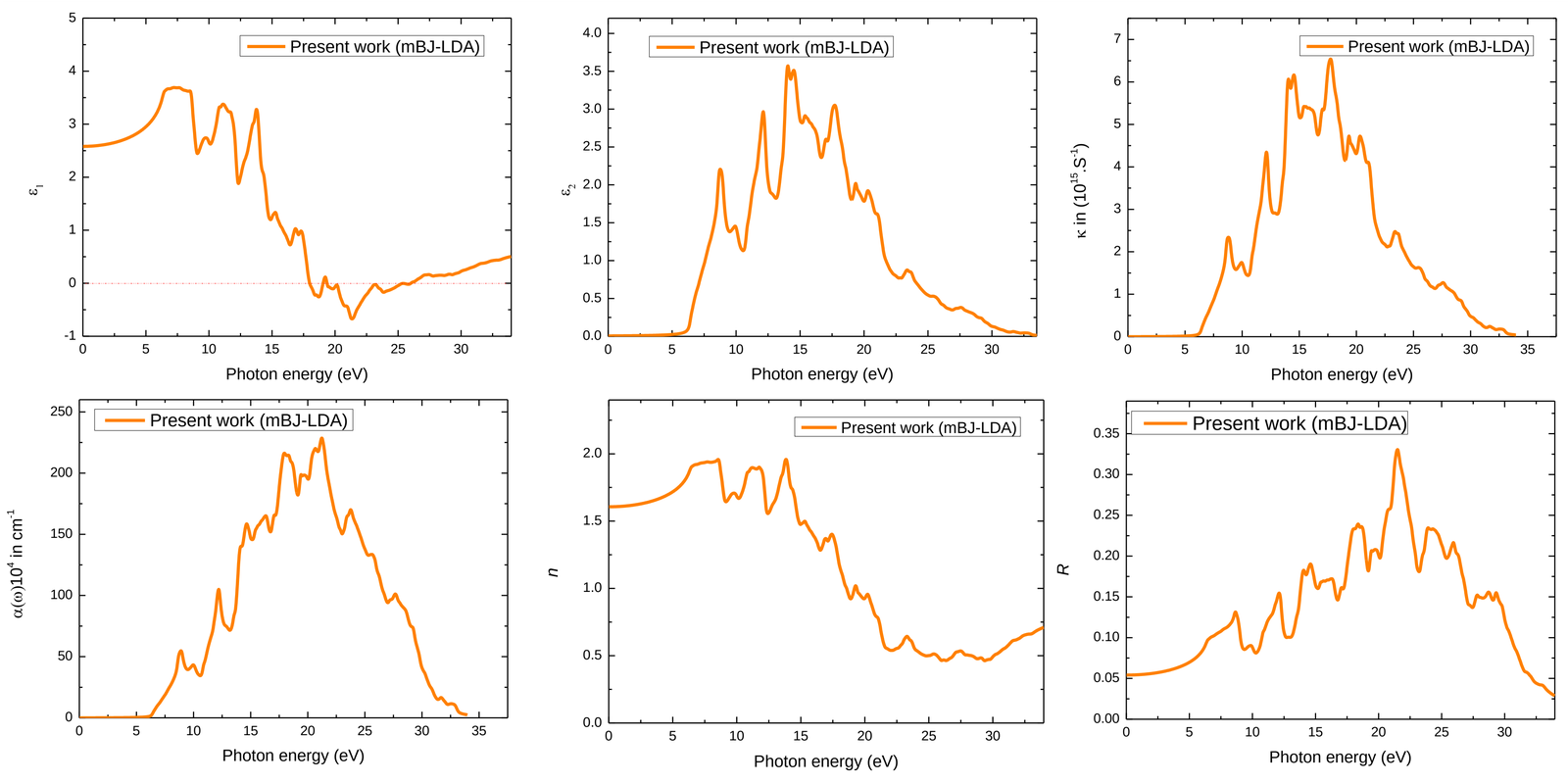

Fig. 6. Calculated opticale properties of Mg_3ZnO_4 within mBJ-LDA

Conclusion

✓ In this research, we delve into the structural, electronic, and optical attributes of caswellsilverite. Employing the all-electron FP-LAPW technique, we optimized the lattice constants (a, b, and c), the corresponding bulk modulus (B), and its primary pressure derivative (B') using LDA, PBEsol-GGA, and WC-GGA. The outcomes for the structural constants align exceptionally with theoretical predictions. For assessing the energy band gap and total density of states, we adopted the modified semi-local mBJ-LDA approximation. This method notably refines the calculated energy gap in comparison to prior simulations. Building on this concurrence, we projected the optical dielectric function, refractive index, reflectivity, and absorption coefficient using the mBJ-LDA. Our findings highlight the potential of the caswellsilverite Mg_3ZnO_4 compounds in the realm of optoelectronic devices, particularly for solar cell applications.

References

[1] Data retrieved from the Materials Project for Mg_3ZnO_4 (mp-1024045) from database version v2022.10.28.
[2] A. Zaoui and M. Ferhat, Superlatices and Microstructures, 145 (2020) 106623 https://doi.org/10.1016/j.spmi.2020.106623
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