

Review Form 3

Book Name:	Science and Technology: Developments and Applications
Manuscript Number:	Ms_BPR_4078
Title of the Manuscript:	Comprehensive Analysis of Electronic Band Structure, Structural Phase Stability, and Optical Properties in AgMX2 Compounds (M = Al, Ga, In; X = S, Se, Te)
Type of the Article	Book chapter

General guidelines for the Peer Review process:

This Book’s peer review policy states that **NO** manuscript should be rejected only on the basis of ‘**lack of Novelty**’, provided the manuscript is scientifically robust and technically sound. To know the complete guidelines for the Peer Review process, reviewers are requested to visit this link:

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Important Policies Regarding Peer Review

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PART 1: Comments

	Reviewer’s comment	Author’s Feedback (Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.	The authors of this manuscript investigate the electronic structure, high-pressure phase transition, and optical properties of chalcopyrite compounds AgMX2 (M = Al, Ga, In; X = S, Se, Te) using the self-consistent Tight-Binding Linear Muffin-Tin Orbital (TB-LMTO) method. Although the problem addressed is intriguing, several aspects require clarification to fully appreciate the significance of the findings. Specifically, the manuscript would benefit from: 1. A clearer explanation of the study's contributions and significance in relation to existing research. It is essential to articulate how this work advances our understanding of the topic beyond the current state of knowledge. 2. To enhance the accuracy and reliability of the results, the authors are encouraged to implement updated exchange-correlation potentials. This would ensure that the findings are aligned with current methodological standards.	
Is the title of the article suitable? (If not please suggest an alternative title)	In my opinion the title should be"Optoelectronic Properties of AgMX2 Compounds (M = Al, Ga, In; X = S, Se, Te) Under High Pressure: Phase Transition Investigations" This title effectively conveys the main focus of the study, which is the investigation of optoelectronic properties and high-pressure phase transitions in AgMX2 compounds.	

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Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here.	The abstract is well-written and effectively conveys the overall scope of the manuscript. However, to further enhance its impact, it would be beneficial to highlight the key findings related to phase transition and optical parameters. Emphasizing these significant results will provide a clearer understanding of the manuscript's contributions and relevance to the field.	
Is the manuscript scientifically, correct? Please write here.	After carefully reviewing the manuscript, I found that the scientific content is generally sound and well-supported by the data presented. The authors have employed a suitable methodology and provided a clear explanation of their results. However, I do have some minor suggestions for improvement: 1. The authors' use of LDA approximation is noted; however, this method is known to have limitations in accurately computing electronic band gaps and optical properties, often resulting in underestimated or overestimated energy band gap values. To improve the accuracy of their results, the authors may consider employing the Tran-Blaha modified Becke-Johnson (TB-mBJ) potential, which has been shown to provide more reliable predictions of electronic band gaps and optical properties. 2. Additionally, to enhance clarity and reproducibility, the authors are encouraged to provide a more detailed explanation of their methodology, specifically: - Expanding the definitions of TB-LMTO and FP-LMTO - Specifying the k-mesh used in their calculations By addressing these suggestions, the authors can strengthen the validity and reliability of their findings. Overall, I believe that the manuscript is scientifically correct and provides a valuable contribution to the field. With some minor revisions, it has the potential to be a strong publication.	
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form. =	The reference list provided is comprehensive; however, it is noticeable that the majority of citations are from older studies. To enhance the manuscript's relevance and credibility, it is recommended that the authors supplement the reference list with more recent publications that are pertinent to the research topic. Incorporating updated references will not only strengthen the manuscript's argument but also demonstrate the authors' awareness of the latest developments in the field.	
Is the language/English quality of the article suitable for scholarly communications?	The language and English quality of the article are generally good, but there are some areas that require improvement to make it suitable for scholarly communication. Some minor errors in grammar, punctuation, and sentence structure were noticed.To enhance clarity and readability, I recommend a thorough proofreading to address these issues and ensure that the language is concise, precise, and free of errors.	
<u>Optional/General</u> comments		

PART 2:

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	Reviewer’s comment	Author’s comment (if agreed with the reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Are there ethical issues in this manuscript?	No, there are no apparent ethical issues in this manuscript. The authors have presented their research in a transparent and objective manner, and there is no indication of any unethical behaviour. The manuscript appears to adhere to standard ethical guidelines for scientific research and publication.	
Are there competing interest issues in this manuscript?	No competing interest issues were observed in this manuscript. The authors do not appear to have any financial or personal relationships that could potentially influence their research or the conclusions drawn from it. The manuscript seems to be free from any conflicts of interest.	
If plagiarism is suspected, <u>please provide related proofs or web links.</u>		

PART 3: Declaration of Competing Interest of the Reviewer:

I declare that I have no competing interest as a reviewer

PART 4: Objective Evaluation:

Guideline	MARKS of this manuscript
Give OVERALL MARKS you want to give to this manuscript (Highest: 10 Lowest: 0) Guideline: Accept As It Is: (>9-10) Minor Revision: (>8-9) Major Revision: (>7-8) Serious Major revision: (>5-7) Rejected (with repairable deficiencies and may be reconsidered): (>3-5) Strongly rejected (with irreparable deficiencies.): (>0-3)	Minor Revision: (>8-9)

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Editorial Comments (This section is reserved for the comments from book editorial office and editors):

	Author's Feedback

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