Review Form 1.6

Journal Name:	**Asian Journal of Research and Reviews in Physics**
Manuscript Number:	**Ms_AJR2P_88040**
Title of the Manuscript:	**Calculation of Cohesive Energies of 3-D Bismuth Selenide (Bi2Se3) and Bismuth Antimony BiSb Topological Insulators: DFT study**
Type of the Article	**Original Research Article**

General guideline for Peer Review process:

This journal'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 guideline for Peer Review process, reviewers are requested to visit this link:

(https://www.journalajr2p.com/index.php/AJR2P/editorial-policy)

PART 1: Review Comments

	Reviewer's comment	**Author's comment** *(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*
Compulsory REVISION comments	**(1) Add bismuth antimony (BiSb), bismuth selenide (Bi2Se3) to keywords** **(2) The results obtained in this report are only for free atoms and crystalline solids. They are not topological insulators as the title implies. Explanation should be included in the Introduction to mention that the approach could be modified to predict the case of an insulator. (Just as done by other researchers, for example, Wei Zhang, et al., New Journal of Physics 12 (2010) 065013. doi:10.1088/1367-2630/12/6/065013)** **(3) Change '3 METHOD' to '3 METHOD FOR COHESIVE ENERGIES'** **(4) Define N in equation (11)** **(5) Number the equation in page 9. The format of this equation is different to (11) where the cohesive energy is defined. Some explanation is needed to show how this equation can be derived from (11)** **(6) It is recommended to rewrite the equation in page to,** $E_{coh} = E_{tot}(Bi_2) + E_{tot}(Se_3) - E_{tot}(Bi_2Se_3)$ **And the same with the second equation. Note that there is a missing + sign** **(7) Correct typos and grammar as shown in manuscript** **(8) Rewrite Conclusion to include changes made to the manuscript.**	
Minor REVISION comments	(1) Use capitals in 'density functional theory' such as in section 1 (2) Although special purpose codes have been used, more description of the model and the parameters used should be given. Some description about the optimization procedures is also needed. None of the final optimal parameters were given except the iterative cycle numbers.	
Optional/General comments	The topic discussed is a worthy one. Successful simulation will be beneficial to experimental works.	

PART 2:

	Reviewer's comment	**Author's comment** *(if agreed with 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?	*(If yes, Kindly please write down the ethical issues here in details)*	

Reviewer Details:

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