



SDI Review Form 1.6

Journal Name:	Physical Science International Journal
Manuscript Number:	Ms_PSIJ_26479
Title of the Manuscript:	Computation of the Cohesive Energies of NaCl, SiO₂ and Al Using Density Functional Theory
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:

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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	For ABSTRACT. First sentence should be as "In this paper, the cohesive energies of Sodium Chloride (NaCl), Silicon dioxide (SiO₂) and Aluminum (Al) based on computer code FHI-aims were calculated using Density Functional Theory." Lines 9 and 10, "... Sodium Chloride (NaCl), Silicon dioxide (SiO₂) and Aluminum (Al) .." should be as ".. NaCl, SiO₂ and Al .." Energy values should be in the same number of digits after point, i.e. 8.38 eV, 12.32352 eV and 3.64 eV should be in the same type, for example, like 8.38 eV, 12.32 eV and 3.64 eV. For INTRODUCTION. Similarly, in lines 34 and 35, there is no need to write open name of the chemical compounds, just writing as NaCl, SiO₂ and Al is enough. If it is necessary it can be written in line 33. Again, the numbers should be in the same form in lines 37 and 38. For THEORETICAL FRAME WORK. The methodology should be clear and informative. In line 47, "Furthermore DFT is computationally very simple" is not meaningful. It should be removed or rewritten in another form.	



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	In line 77, "...one obtains an absurd result" is not a good explanation. "Absurd" is not sound any scientific saying. For MATERIALS AND METHOD. Is it necessary to explain the software and the used files in detail? Moreover, there is not any references for FHI-aims code. For RESULTS AND DISCUSSION. This part is too poor. It must be improved. Mainly, the given information and findings are in repeating form. There must be some comments depending on the various compounds. There should be information about the selection reasons for these molecules. Just giving energy values in tables and plotting their figures as functions of the iteration are not sufficient for a paper. The values given in different tables can be given in just one table. At least, values for NaCl, Na and Cl can be in the same table. For SiO₂, Si and O₂, the values can be in a second table. Similarly, the determined energy values can be tabulated in the same table for Al. Totally, 3 tables are enough. Graphes can be collected in panels in the same figure for each compound. This may be helpful to compare them. Line 172 there is "[10] (Maezono, 2003)". It must be as "[10]". Line 139 there is "obtained from the work of Linder 2012 [13]". It must be as "[13]". For CONCLUSION. The explanation "...compared to literature report of other codes reporting higher iterations before convergence" in line 262 is very poor. What is the other codes? There is not sufficient information about these codes and	
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	their findings. For REFERENCES. The references are not in the same form. Up to Ref. [7] surnames are given first and then the first letters of the authors names. For Refs. [8]-[11] and [14] the first letters of the authors names are given first and then surnames. Refs. [12] and [13] are also in different form. Moreover, in Refs. [8] and [14] there is no information about the publications. As a results, the paper in the present form have lots of lack. It should be improved in scientific point of view and in language, too.	
Minor REVISION comments		
Optional/General comments		

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