



SDI FINAL EVALUATION FORM 1.1

PART 1:

Journal Name:	Physical Science International Journal
Manuscript Number:	Ms_PSIJ_26479
Title of the Manuscript:	Computation of the Cohesive Energies of NaCl, SiO ₂ and Al Using Density Functional Theory
Type of Article:	Original Research Article

PART 2:

FINAL EVALUATOR'S comments on revised paper (if any)	Authors' response to final evaluator's comments
For ABSTRACT. In Lines 6 and 7. "The code has several input parameters in which some of the variables were optimized." Is this sentence necessary? In Line 11 and 12. "to the experimental values of 8.18 eV for NaCl, 12.94 eV and 3.39 eV for SiO₂ and Al respectively." May be written as "to the experimental values of 8.18, 12.94 and 3.39 eV for NaCl, SiO₂ and Al respectively." For THEORETICAL FRAME WORK. I still keep the following point: In line 102, "...one obtains an absurd result" is not a good explanation. "Absurd" is not sound any scientific saying. For MATERIALS AND METHOD. I still keep the following point: 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 should be improved. There can be some comments depending on the various compounds. Just giving energy values in tables and plotting their figures as functions of the iteration are not sufficient for the 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, if possible. This may be helpful to compare them. Or author can make a critical comments to compare these findings with each other. For CONCLUSION.	Yes Okay. corrected Okay. Corrected It is not necessary to explain the software as it was only used to get the computed values. I have also included the reference for FHI-aims code. The different compounds or materials were selected to enable the author carry out a comparative analysis in solids with different cohesion. The energy values were NOT just been given in tables and plots The authors prefer leaving the graphs separated instead of panels collection.



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The explanation “..compared to literature report of other studies reporting higher iterations before convergence” is still poor. There is not sufficient information about those findings. Whole paper should be improved.	Okay, amended Okay, amended
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