

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.

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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	Author performed the cohesive energies of NaCl, SiO₂ and Al based on computer code FHI-aims 6 were calculated using Density Functional Theory. The code has several input parameters in 7 which some of the variables were optimized. The cohesive energies of NaCl, SiO₂ and Al were 8 calculated within Local Density Approximation (LDA) of Perdew Wang of the density 9 functional theory. I think it is a good effort, still I have some queries: 1. First of all in the title author selected NaCl, SiO₂ and Al, why these different types of materials like AB, AB₂ and an element has been chosen for a same approach? 2. Author performed only the cohesive energy for different iteration taken. This is the basic calculation only we have used for optimization. 3. Why the band structure and density of states or other ground state properties are not studied? Author should add the study of other properties also?	1. The different materials were selected to enable the author carry out a comparative analysis in solids with different cohesion 2. yes 3. the band structure and density of the states were not considered because we are just interested in the cohesive energies. And our future paper will be considering the band structures and the density of states
Minor REVISION comments	1. LDA fails to explain some properties of material. The better approach like GGA, GGA+U, LSDA and many more. Why author have not taken these? 2. The representation of all the graphs is very poor. Author should study other related published paper to correct it? 3. Author has presented the same data in tables and graphs. If it is presented by graphs there is no need to give the tables and vice-versa.	1. LDA was chosen so we can be able to compare the results obtained here with similar studies carried out by other researchers using other approaches. 2. Ok 3. ok
Optional/General comments	1. The graphs are plotted for Si and O₂ separately why? The authors should give proper explanation of above mentioned.	The graphs were plotted separately to illustrate the individual element that make up the compound that we are interested in calculating its cohesive energy