



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:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)



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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	The Cohesive Energy value corresponding to this minimum termed cohesive energy at balance and the minimum volume is the balance volume. Thus, the balance lattice parameter is found. Thus, the cohesive energy can be calculated using the following equation: $E_{coh} = E_{tot} - \sum_x^n E_x^{atomic};$ where E_{tot} is the compound total energy and E_x^{atomic} is the energy of each atom constituting the compound in its free state. The authors should read the references. For I not found in the paper the definition of energy cohesive energies, Y. Song, Z.X. Guo, R. Yang. D. Li. Actamater. 49 (2001) 1647–1654. B.R. Sahu. Materials Science and Engineering. 349 (1997) 74-78. DOS SANTOS, ANTÔNIO VANDERLEI; SAMUDIO PÉREZ, CARLOS ARIEL . Ab initio investigation of the	



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	substitution effects of 2p elements on the electronic structure of γ-Fe₄X (X = B, C, N, and O) in the ground state. Journal of Materials Research ^{JCR}, v. 31, p. 1-11, 2016. 2. <u>dos Santos, A.V.</u>; SAMUDIO PÉREZ, C.A. ; MUENCHEN, D. ; ANIBELE, T.P. . First principles calculations of the magnetic and hyperfine properties of Fe/N/Fe and Fe/O/Fe multilayers in the ground state of cohesive energy. Solid State Communications ^{JCR}, v. 201, p. 120-124, 2015.	
<u>Minor</u> REVISION comments		
<u>Optional/General</u> comments		

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