



**SDI Review Form 1.6**

Journal Name:	<a href="#">Physical Science International Journal</a>
Manuscript Number:	Ms_PSIJ_41778
Title of the Manuscript:	ENERGETICS OF THE BASIC ALLOTROPES OF CARBON
Type of the Article	Original Research Article

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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)
<b>Compulsory</b> REVISION comments	<p align="center"><b>Physical Science International Journal</b></p> <p>Manuscript Number: Ms_PSIJ_41778</p> <p>Title: Energetics of the basic allotropes of carbon.</p> <p>Reply:</p> <p>The author's calculate the total ground state energy and electronic band structure for Fullerenes (C<sub>60</sub>), Graphite and Diamond using FHI-aims Density Functional Theory (DFT) code. The density functional used are the local-density approximation (LDA) in the parametrization by Perdew and Wang 1992, Perdew and Zunger 1981, the generalized gradient functional PBE, and PBE+vdW approach as defined by Tkatchenko and Scheffler. The results presented from the computations of the ground state energies of diamond, fullerenes and graphite were -2027.569 eV, -1027.178 eV and -2070.938 eV respectively. These results agree well when compared to the various exchange and correlation functional used in this study. Similarly, the results presented from the computations of the Kohn Sham electronic band gaps of graphite and diamond were 0.00072 eV and 5.57611 eV, respectively. These are also in agreement when compared to the experimental values of 0 eV and 5.45 eV. These band gaps are within reasonable percentage errors of 0.0% and 1.43% respectively. However, fullerenes band gap of 8.21131 eV is not in agreement with the theoretical and experimental values of 1.83 eV and 2.3 eV, respectively. This is probably due to the Bucky-ball nature of Fullerenes as well as the lattice constants and physical settings used.</p> <p>The article is a very good work, well written and explains with clarity the main purpose of the investigation. Moreover, the results presented are good enough as to provide relevant information that deserves to be accepted for publication at PSIJ. Before continuing with the publication acceptance, I would like to address the following questions:</p> <ol style="list-style-type: none"> <li>1) Page 3, row 57, Define FHI-aims?</li> <li>2) Page 3, row 75, eicient should be corrected to efficient.</li> <li>3) Page 12, row 215, University] should be corrected to University.</li> <li>4) Generally, it is known that DFT overestimates the calculations for E<sub>g</sub> obtained as is in this case for some structures. The authors should have mentioned this important fact.</li> </ol> <p>D. H. Galvan.</p>	<ol style="list-style-type: none"> <li>1. Noted. It has now been defined.</li> <li>2. Noted.</li> <li>3. Also noted.</li> <li>4. Overestimation of the E<sub>g</sub> is now incorporated.</li> </ol>
<b>Minor</b> REVISION comments		
<b>Optional/General</b> comments		