



SDI Review Form 1.6

Journal Name:	Asian Journal of Physical and Chemical Science
Manuscript Number:	Ms_AJOPACS_41779
Title of the Manuscript:	First-Principles theoretical study on electronic band structure of Diamond and Graphite
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)
Compulsory REVISION comments	<p>The author's present the total ground state energy and electronic band structure for Graphite and Diamond using FHI-aims Density Functional Theory (DFT) code. The density functional used was the generalized gradient functional PBE, and PBE+vdW approach as defined by Tkatchenko and Scheffker. The results reported from the computations of the ground state energies of diamond and graphite were -2056.898408114 eV and -2061.703700984 eV respectively. Similarly, the results presented from the computations of the electronic band gaps of graphite and diamond were 0.00451936 eV and 5.56369215 eV, respectively. These are in good agreement when compared to the experimental values of 0 eV and 5.48 eV. These gaps are within reasonable percentage errors of 0.0% and 1.46% respectively.</p> <p>The article is a good work, well written and yields good information on Diamond and Graphite.</p> <p>Furthermore, the results presented are good enough as to provide relevant information that deserves to be accepted for publication at AJOPACS. Before continuing with the publication acceptance, I would like to address the following questions:</p> <ol style="list-style-type: none"> 1) Page 1, row 2, Define FHI-aims? 2) Page 2, row, First principles calculations represent the pinnacle of electronic structure calculations. Authors exaggerate with these remarks. 3) Generally, it is known that DFT overestimates the calculations for E_g obtained as is in this case for some structures. The authors should have mentioned this important fact. 	<ol style="list-style-type: none"> 1- We have now define it. 2- The exaggeration has been rectified. 3- We mentioned the variation of our computed band gap as an increment in comparison with other literatures (Page 8, row 171). However, we now included the overestimation problem in our abstract.
Minor REVISION comments		
Optional/General comments		