



SDI Review Form 1.6

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Journal Name:	Asian Journal of Physical and Chemical Sciences
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	<ol style="list-style-type: none"> 1- the authors provide a study of band structure for carbon in two different structures diamond and graphite. I ask the author what is the novelty and origin of this work. 2- the authors do not provide any structural information for this two materials 3- the huge error in this study, that the authors indicates a gap almost zero for graphite, a simple view in Figure 1.2 shows that graphite does not have a gap because we notice an overlap between the valence band and conduction . 4- so physically does not have a gap (a negative gap). Graphite a metallic behaviour.. 	<ol style="list-style-type: none"> 1- The novelty and origin of this work lies in the usage of an all electron full potential, with numeric atom centered basis functions DFT computations code to re-investigate the electronic band structure of two interesting Carbon allotropes; Diamond and Graphite. 2- We did, we mentioned the lattice constant used for each structure. However, additional structural information is now incorporated in the manuscript. The initial figure numbering of Fig. 1.1 and 1.2 now becomes 1.2 and 1.3 respectively. 3- Yes, there is an overlap between the conduction and valence bands. We also discussed it and show that graphite has a zero gap (Page 8, row 189). However, we corrected the wrong band gap value. 4- Actually, it does not have a gap and therefore have a semi metallic nature due to weak interactions between graphitic planes such that these bands split which leads to a zero-gap semimetal
Minor REVISION comments		
Optional/General comments		