



Energetics of the Basic Allotropes of Carbon

S. G. Abdu^{1*}, M. A. Adamu² and M. Y. Onimisi³

¹*Department of Physics, Kaduna State University, Kaduna, Nigeria.*
²*Department of Physics, Federal University Dutsin-ma, Katsina, Nigeria.*
³*Department of Physics, Nigerian Defence Academy, Kaduna, Nigeria.*

Authors' contributions

This work was carried out in collaboration between all authors. Author MAA designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Authors SGA and MYO managed the analyses of the study. Author MAA managed the literature searches. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/PSIJ/2018/41778

Editor(s):

- (1) Dr. Marian Apostol, Professor, Theoretical Physics, Institute for Atomic Physics, Magurele-Bucharest, Romania.
(2) Dr. Pratima Parashar Pandey, Professor, Polymer composites, Nanotechnology Applied Sciences, College of Engineering & Technology, Integrated Institutes of Learning, Dr. APJ Abdul Kalam Technical University, Greater Noida, India.
(3) Dr. Christian Brosseau, Distinguished Professor, Department of Physics, Université de Bretagne Occidentale, France.

Reviewers:

- (1) Donald H. Galvan, Mexico.
(2) Muhammad Musaddique Ali Rafique, RMIT University, Australia.
Complete Peer review History: <http://www.sciencedomain.org/review-history/25519>

Original Research Article

Received 29th April 2018
Accepted 2nd July 2018
Published 12th July 2018

ABSTRACT

An effort was made in this work to calculate the total ground state energy and electronic band structure of Fullerenes (C₆₀), Graphite and Diamond using FHI-aims Density Functional Theory (DFT) code. The density functionals used are the local-density approximation (LDA) in the parameterization 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 obtained from the computations of the ground state energies of diamond, fullerenes and graphite were -2072.569 eV, -1027.178 eV and -2070.938 eV respectively. These results agree well when compared to the various exchange and correlation functionals used in this study. Similarly, the results obtained 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 0eV and 5.5eV. These band gaps are within reasonable overestimation errors of 0.0007 eV and 0.08 eV respectively. However, fullerenes band gap of

*Corresponding author: E-mail: sgabdul@gmail.com;

8.21131eV is not in agreement with the theoretical and experimental values of 1.83eV and 2.3eV, respectively. This is probably due to the Bucky-ball nature of Fullerenes as well as the lattice constants and physical settings used.

Keywords: DFT; LDA; GGA; Band gap; HOMO; LUMO and total ground state energy.

1. INTRODUCTION

Carbon is found naturally in the earth crust and in the atmosphere. It is abundant and forms a major part of our life. Carbon is a unique and versatile element. It exists in many forms with different structures and properties. It can also be synthesized to form new forms of materials [1]. Carbon is the basic building block of the following Carbon materials: graphite, diamond, fullerene, graphene, Carbon-fiber, Carbon nanotube, lonsdaleite, carbyne and bucky diamonds. Recently, new Carbon form called pentagraphene was discovered using the Vienna Ab initio Simulation Package (VASP) [2]. Similarly, novamene [3] was also discovered and the stable equilibrium structure was computed using Quantum Espresso code. The ability of Carbon to exist in many forms with different structures and properties led researchers into a rigorous research on Carbon nano-material.

The principal allotropes of Carbon are graphite, diamond and Fullerenes. Diamond is associated with the sp^3 hybrid orbital, all four electrons are used to form a tetravalent sigma σ bond in a 3D structure. In each unit cell, diamond has eight Carbon atoms. The bond length is equidistant between the four Carbon atoms, thereby forming a strong covalent bond with a bond angle of 109.5° . Diamond is the hardest known material, it is used in cutting, drilling and grinding. It is transparent in the visible range of the electromagnetic spectrum, making it a good candidate for jewellery. It has a high thermal conductivity (more than copper) and low thermal expansion [1,4].

Graphite has a flat layered (planar) structure. Each Carbon atom forms trivalent (sigma σ) bond with three (sp^2 hybrid orbital) other Carbon atoms in a hexagonal shape. The layers are bonded to one another by weak Van-der-Waal forces. This allows the layers to slip over each other. The p_z – orbitals electrons, do also interact: they form a π -mobile electron. Graphite is the most stable and most strongly covalently bonded Carbon allotrope (within the layer). It is soft, opaque, black, used in pencil, lubrication and in nuclear reactor moderator [1,4].

In recent time, a new Carbon allotrope was discovered by Curl, Kroto and Smalley at Rice University. It is spherical (soccer ball) in shape. It resembles a geodesic dome constructed by an architect in the person of Richard Buckminster Fuller. Hence, it was named in his honour as buckminsterfullerene, shortened as fullerenes (also called buckyballs). It has sixty (60) Carbon atoms arranged in both pentagonal and hexagonal shape. For it to have a spherical shape, it must satisfy the pentagon rule i.e. it must have 12 pentagons and 20 hexagons. Basic Fullerene molecular formula is C_{60} [1,4]. Unlike graphite and diamond, fullerene molecule has both sp^3 and sp^2 hybrid orbitals, i.e., It has both sigma and pi bond. Fullerene is used as a high-temperature superconductor when doped with K or Rb, it is a possible lubricating aid and is also used in medicine [1,5].

Nowadays, Density Functional Theory (DFT) is one of the leading tools used in studying the electronic structure, stability, synthesis, defects, semiconducting and superconducting properties of Carbon materials. DFT is a special computational quantum mechanical first principle method of describing and predicting the electronic structures and properties of atoms, molecules and solids. [6] used *DFT GAUSSIAN 3 software* to compute the ground state energies and stable structures of diamond, graphite and fullerenes. [7] calculated the stable atomic structure of fullerenes using FHI-aims code. They reported that the most stable structure crystallizes in fcc structure. This crystal structure was used in this study for fullerenes computations.

However, the small ($1s^2$) ionic core of Carbon couple with the hybrid orbitals degeneracy presents a challenge to computational modelling. Therefore, It is the purpose of this work to use an all-electron/full potential code (FHI-aims) that uses numeric tabulated atomic basis set to reinvestigate the electronic properties of Carbon basic allotropes. This would also assist towards checking the accuracy and efficiency of FHI-aims in comparison to other programs.

2. MATERIALS AND METHODS

First principles, or *ab initio* calculations represent the pinnacle of electronic structure calculations. Starting with the fundamental constants and Schrodinger's equation as a postulate, these methods proceed to describe the nature of atomistic systems to a degree that is almost irrefutable. The methods applied in solving Schrodinger's equation break into two main types: Hartree-Fock (HF) based methods and Density Functional Theory (DFT) methods. While both make approximations to make calculations possible, they represent the best available methods for atomistic modelling. The first task is to have a Linux based operating system (OS) (Ubuntu 16.04 version installed for this research work) on a computer. FHI-aims (Fritz Haber Institute-*ab initio* molecular simulations) is not supported on windows. Since FHI-aims is distributed in source code form, the next task is to compile a powerful executable program. For this, the following mandatory prerequisites are needed [8]:

- A working FORTRAN compiler. A good example is Intel's ifort compiler.
- A compiled version of the lapack library, and a library providing optimized basic linear algebra subroutines (BLAS). Standard commercial libraries such as Intel's mkl provide both lapack and BLAS support. Having an optimized BLAS library for a specific computer system is critical for the performance of FHI-aims.

FHI-aims requires two input files — control.in and geometry.in—located in the same directory from where the FHI-aims binary is invoked. An output file contains the basic information and result of the calculation such as the total energy, atomic forces, etc. The geometry.in file contains all information concerning the atomic structure of the system. This includes the nuclear coordinates, which are specified by the keyword; an atom, followed by Cartesian coordinates (in units of Å) and the descriptor of the species (chemical elements) [9]. The control.in file contains all other physical and technical settings for accurate and efficient convergence of the computations.

The full algorithmic framework embodied in the FHI-aims computer program package is described in [8]. The algorithms are based on numerically tabulated atom-centered orbitals (NAOs) to capture a wide range of molecular and

materials properties from quantum-mechanical first principles. FHI-aims is a very important code because, an all-electron / full-potential treatment that is both computationally efficient and accurate is achieved for periodic and cluster geometries on equal footing, including relaxation and *ab initio* molecular dynamics. The primary production method for total energies and gradients is density functional theory (LDA and GGA). Additional functionality includes quantum-chemical approaches (Hartree-Fock, hybrid functionals, MP2) and self-energy-based methods (e.g., GW) for electronic spectroscopic properties. FHI-aims allow fully quantum-mechanical simulations for a system up to thousands of atoms and performs efficiently also on massively parallel platforms with possibly thousands of CPUs [8].

However, choosing the central computational settings consistently for series of calculations greatly enhances the accuracy of any resulting energy differences (error cancellation). In FHI-aims, the key parameters regarding computational accuracy are actually sub-keywords of the species keyword of control.in, controlling the basis set, all integration grids, and the accuracy of the Hartree potential. These settings, of course, were not retyped from scratch for every single calculation; on the other hand, they remained obvious since these are the central handles to determine the accuracy and efficiency of a given calculation.

FHI-aims, therefore, provides preconstructed default definitions for the important sub-keywords associated with different species from Z=1-102 (H-Md). These can be found in the *species_defaults* subdirectory of the distribution, and are built for inclusion into a control.in file by simple copy-paste.

For all elements, FHI-aims offers three different levels of *species_defaults*, however, we used only two of these levels of *species_defaults* in this work:

- *light*. Out-of-the-box settings for fast pre-relaxations, structure searches, etc. Actually, no obvious geometry/convergence errors resulted from these settings, and are recommended for many household tasks. For "final" results (meV-level converged energy differences between large molecular structures etc.), any results from the *light* level should be verified with more accurate post-processing calculations, e.g. *tight*.

- *tight* : Regarding the integration grids, Hartree potential, and basis cutoff potentials, the settings specified here are rather safe, intended to provide meV-level accurate energy *differences* also for large structures. In the *tight* settings, the basis set level is set to *tier 2* for the light elements 1-10, a modified *tier 1* for the slightly heavier Al, Si, P, S, Cl (the first *spdfgd* radial functions are enabled by default), and *tier 1* for all other elements. This reflects the fact that, for heavy elements, *tier 1* is sufficient for tightly converged ground state properties in DFT-LDA/GGA, but for the light elements (H-Ne), *tier 2* is, e.g., required for meV-level converged energy differences. For convergence purposes, the specification of the basis set itself (*tier 1*, *tier 2*, etc.) may still be decreased/increased as needed [8].

2.1 Computational Details

Various computations were done for the (Perdew and Wang) *pw_Ida*, (Perdew and Zunger) *pz_Ida* and (Perdew Burke Ernzerhof) *pbe_GGA* (exchange correlation) XC functionals. A Gaussian occupation broadening width of 0.01eV was selected. The convergence criterion for the SCF of eigenvalues, total energy and density were set to 10^{-2} eV, 10^{-5} eV and 10^{-4} eV, respectively. The structure geometry with a convergence minimum of 10^{-2} eV was optimized, while for the unit cell geometry optimization we selected full unit cell relaxation option. The corresponding convergence criteria for the SCF of the energy derivatives were chosen to be 10^{-4} eV.

Tier 1 basis functions of FHI-aims light *species_default* basis set was used for the geometry optimization, however, tier 2 *tight* basis set was used for the post relaxation of the relaxed geometry. BFGS (Broyden, Fletcher, Goldfarb and Shanno) structure optimization algorithm was selected for the geometry

relaxation. FHI-aims keyword *k_grid* was set to 12x12x12 *k_grid* data point. For the long-range correlation energy interaction effect, we used VdW correction based on Tkatchenko and Scheffler long-range interaction correction.

3. RESULTS AND DISCUSSION

The following tables summarize the output data obtained during FHI-aims computations and are used in discussing the minimum and stable ground state energies for the relaxed/post relaxed computations of the various XC functionals for the three bulk structures.

From Table 3.1, it can be observed that *pbe* XC functional has the minimum ground state energy for diamond bulk structure. This is in agreement with theory because *pbe* (GGA) is theoretically a better approximation to XC energy functional than the rest LDA and LSDA [10 and 11]. However, *pw_Ida* is a bit better approximation when compared to *pz_Ida*. Similarly, comparing light (relaxed) and tight (post relaxed) FHI-aims *species_default* settings computations. Tight gives efficient and accurate converged ground state energies than the light settings. This is a good indication that diamond crystalline structure has been well optimized in the relaxed/post relaxed FHI-aims computations. The following graphs summarize the output data obtained during FHI-aims computations and are used in obtaining the binding curve pattern for the total energy and the number of iterations.

The binding curve in Fig. 3.1 shows that the total energy of the bulk crystal of diamond increases as the number of iteration increases and converges steadily. The resulting binding curve indicates a stable total energy and also the best-converged energy of -2072.56851605eV for diamond. This variation pattern for diamond total energy against the number of iterations was found to be the same for the remaining XC functionals used in this study.

Table 3.1. Diamond ground state energies for relaxed/post relaxed computations

Functionals	Pw_Ida Ground State Energy (eV)	Pz_Ida Ground State Energy (eV)	Pbe_GGA Ground State Energy (eV)
Computations			
Relaxed geometry (Light)	-2056.94097548	-2056.90780088	-2072.47722687
Post relaxed geometry (Tight)	-2057.03098622	-2056.99760599	-2072.56851605

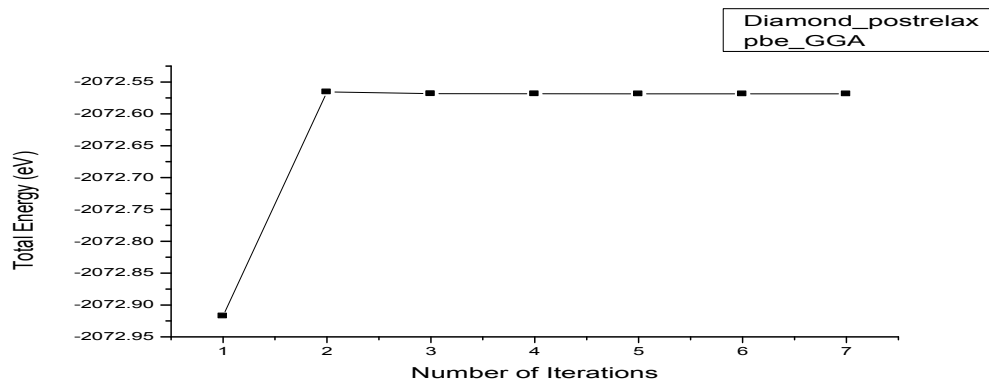


Fig. 3.1. Variations of total energy (ev) against number of iterations

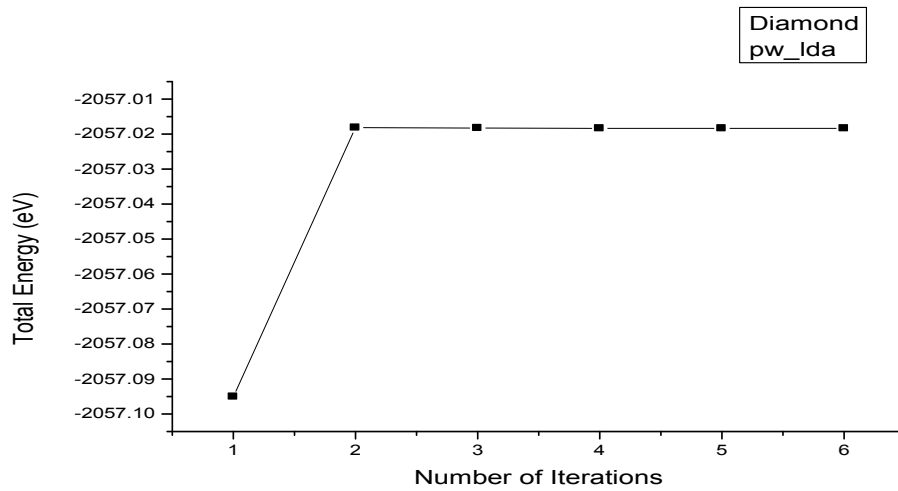


Fig. 3.2. Variations of total energy (ev) against number of iterations

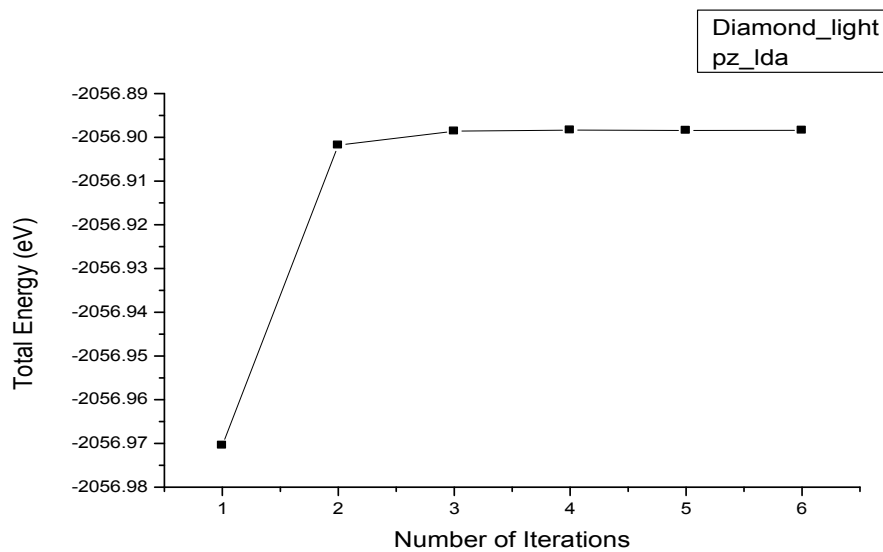


Fig. 3.3. Variations of total energy (ev) against number of iterations

Fig. 3.2 and Fig. 3.3 also illustrate the variations of diamond's ground state energies against the number of iterations. It is clear that the graphs variations are almost the same, except that the total energies values are different. In Fig. 3.2, the total energy value increases steadily from the 1st iteration to the 2nd iteration, from where this value decreases a bit and is later maintained until convergence is reached. However, Fig. 3.3 shows a slightly different trend. The total energy value rather increases in the third iteration; this value was maintained until convergence was obtained. The resulting binding curve in Fig. 3.3 indicates a stable total energy and also the best-converged energy of -2056.89840811eV for diamond.

From Table 3.2, it can be observe that pbe XC functional also has the minimum ground state energy for graphite bulk structure. This is in agreement with theory, because pbe (GGA) is theoretically a better approximation to XC energy than the rest pw_lda and pz_lda [11]. However,

pw_lda is slightly a better approximation when compared to pz_lda. Similarly, comparing light and tight species_default settings for relaxed and post relaxed computations tight gives efficient and accurate converged ground state energies than the light settings. This is also a good indication that graphite crystalline structure has been well optimized in the relaxed/post relaxed FHI-aims computations.

Fig. 3.4 and Fig. 3.5 illustrate the variations of ground state energies against a number of iterations for graphite bulk structure. The trend in both Figures increases upwardly to create a curve pattern until it reaches stability at the 3rd, 4th, 5th, 6th and 7th iterations, this can be attributed to the covalent bonding and simple planar hexagonal stacking that exist in the bulk atom of graphite [12]. The resulting binding curve in Fig. 3.5 indicates a stable total energy and also the best-converged energy of -2070.93836837 eV for graphite.

Table 3.2. Graphite ground state energies for relaxed/post relaxed computations

Functionals Computations	Pw_Lda Ground State Energy (eV)	Pz_Lda Ground State Energy (eV)	Pbe_GGA Ground State Energy (eV)
Relaxed Geometry (Light)	-2044.81236553	-2044.81251118	-2061.63381564
Post relaxed Geometry (Tight)	-2054.61937938	-2054.63065901	-2070.93836837

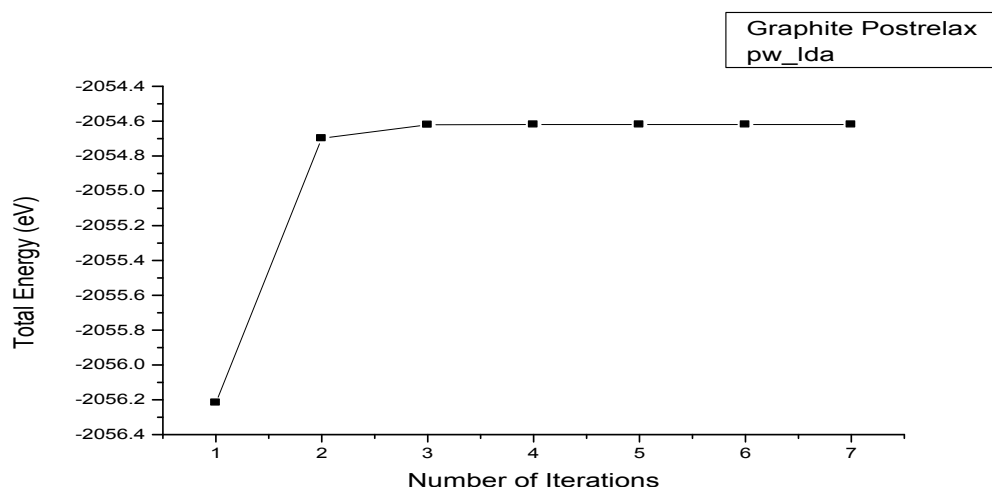


Fig. 3.4. Variations of total energy (eV) against number of iterations

Table 3.3. Fullerenes ground state energies for light and tight settings

Functionals Computations	Pw_Lda Ground State Energy (eV)	Pz_Lda Ground State Energy (eV)	Pbe_GGA Ground State Energy (eV)
Light	-1018.35981067	-1018.35683745	-1027.17026568
Tight	-1018.36680612	-1018.36379535	-1027.17849607

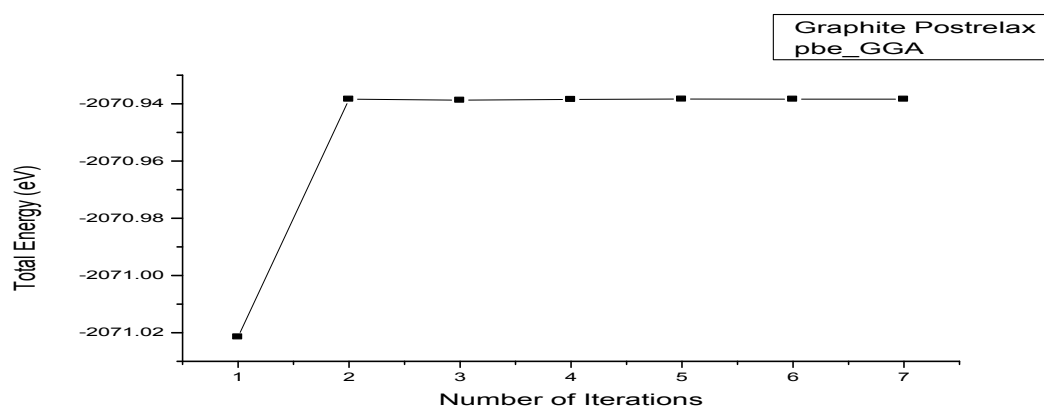


Fig. 3.5. Variations of total energy (eV) against number of iterations

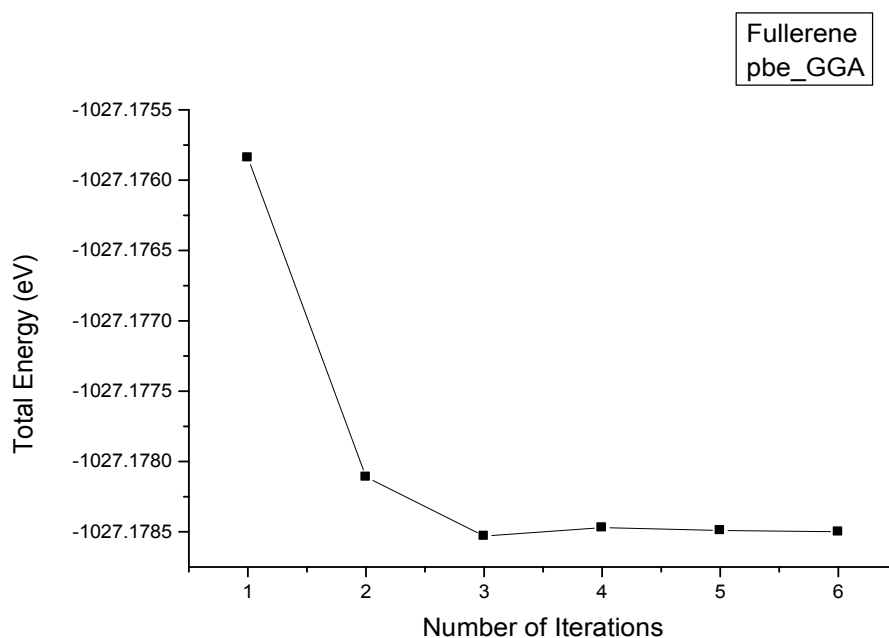


Fig. 3.6. Variations of total energy (eV) against number of iterations

For Fullerenes, ground state energies for relaxed/post relaxed computations were not successful, because FHI-aims could not write out the geometry.in_next_step file let alone post relax processing. We suggest this could be due to the dimension of fullerenes lattice constant of 14.17 \AA , physical settings used and/or its spherical shape. However, we computed the ground state energies for light/tight settings without structure optimization. Table 3.3 shows fullerenes ground state energies for the three XC functionals using light/tight default settings. The table also shows that, tight default settings give more accurate converged minimum ground state energy when compared to the light default

settings. This is in good agreement with the theory behind FHI-aims code [8]. Also looking at the XC functional total energy values, it is obvious that pbe gives the minimum ground state energy follow by pw_lda and then pz_lda. Hence, in accordance with theory pbe is much better in approximating the XC energy functional than pw_lda and pz_lda [10,11].

Fig. 3.6 illustrates the variations of Fullerenes ground state energies for the pbe XC functionals against a number of iterations. The trend in Fig. 3.6 decreases downwardly to create a curve pattern until it becomes stable at the 4th, 5th and 6th iterations; this can be attributed to the

covalent bonding and spherical shape that exist in the bulk atom of fullerenes [12,13].

In this paper, we find out that all the three variants of the total energy from FHI-aims output file are the same for diamond structure but are all different in the case of graphite and fullerenes. This shows that fullerenes and graphite have narrow and zero HOMO-LUMO (highest occupied molecular orbital - lowest unoccupied molecular orbital) gap respectively, while diamond has a wide HOMO-LUMO gap. These results are in good agreement with experimental and theoretical literature [12 and 14]. Tables 3.4-3.6 show estimated values for lowest unoccupied state (CBM), highest occupied state (VBM), overall HOMO-LUMO gap and smallest direct gap for diamond, graphite and fullerenes as obtained from the three XC functionals used in this study.

From Table 3.4, using the estimated overall HOMO-LUMO gap, FHI-aims code predicted that diamond appears to be an indirect band gap. This agrees well with the report of Pierson, 1993. The smallest direct gap of 5.57611325eV for pbe_GGA is in good agreement with theoretical and experimental values [12 and 15] with an overestimation percentage error of 1.43%. According to FHI-aims output file, since the gap value is above 0.2eV, the system is most likely an insulator or a semiconductor. This FHI-aims

output file comment agrees exactly with theoretical and experimental data. Diamond was characterized in many literatures to be an insulator [4], however, it was also considered as an indirect wide band gap semiconductor [1] that is suitable for high-temperature electronic applications. The rest XC functionals pw_Ida and pz_Ida smallest direct gap are also in good agreement with experimental values of 5.5eV [12] with an overestimation error of 1.96%.

From Table 3.5, using the estimated overall HOMO-LUMO gap, FHI-aims predicted that graphite also appears to be an indirect band gap. The smallest direct gap of 0.21308645eV for pw_Ida is in good agreement with theoretical [16] and experimental values [12]. According to FHI-aims output file, since the HOMO-LUMO gap value (0.00072958eV) is rather small (approximately zero gap) and we use a finite k-point grid, the material is most likely metallic in the sense that there are states at or near the Fermi level. This FHI-aims output comment shows that graphite is a conductor, and it agrees exactly with theoretical [16] and experimental data. Also, the approximately zero gap value of FHI-aims output file is in agreement with the literature [12]. The rest XC functionals pz_Ida and pbe_GGA smallest direct gap are also in good agreement with experimental values within small overestimation errors.

Table 3.4. Diamond electronic band structure for post relaxed computations

Functionals	Pw_Ida Ground State Energy (eV)	Pz_Ida Ground State Energy (eV)	Pbe_GGA Ground State Energy (eV)
Valence Band Maxima (VBM)	-8.54310497	-8.53387243	-8.10988403
Conduction Band Minima (CBM)	-4.34300078	-4.34356041	-3.95778618
HOMO-LUMO Gap	4.20010419	4.19031201	4.15209785
Smallest Direct Gap	5.61457427	5.60711319	5.57611325

Table 3.5. Graphite electronic band structure for post relaxed computations

Functionals	Pw_Ida Ground State Energy (eV)	Pz_Ida Ground State Energy (eV)	Pbe_GGA Ground State Energy (eV)
Valence Band Maxima (VBM) -	-7.07415413	-7.33934792	-6.81313445
Conduction Band Minima (CBM)	-7.06569011	-7.33861834	-6.80852692
HOMO-LUMO Gap	0.00846402	0.00072958	0.00460753
Smallest Direct Gap	0.21308645	0.41541884	0.30724683

Table 3.6. Fullerenes electronic band structure for tight settings computations

Bands	Functionals	Pw_Ida Ground State Energy (eV)	Pz_Ida Ground State Energy (eV)	Pbe_GGA Ground State Energy (eV)
Valence Band Maxima (VBM)		-13.60248641	-13.60706560	-13.71228408
Conduction Band Minima (CBM)		-5.39117210	-5.39539613	-5.25904269
HOMO-LUMO Gap		8.21131431	8.21166947	8.45324138
Smallest Direct Gap		8.21131432	8.21166948	8.45324139

From Table 3.6, using the estimated overall HOMO-LUMO gap, FHI-aims predicted that fullerenes also appear to be an indirect band gap. The smallest direct gap of 8.21131432eV for pw_Ida and the remaining XC functionals values do not agree with the theoretical value of 1.83eV [14] and experimental value of 2.3eV [Byun 2012, PhD Dissertation, Pennsylvania State University]. According to the FHI-aims output file, since the gap value is above 0.2 eV. The system is most likely an insulator or a semiconductor. This FHI-aims output prediction agrees exactly with theoretical and experimental data, fullerenes was reported to be a band insulator, direct band-gap semiconductor [1]. In addition, fullerenes can be converted from a semiconductor into a conductor or even superconductor when doped with alkali metals [17]. The rest XC functionals pz_Ida and pbe_GGA smallest direct gap are also not in good agreement with theoretical [14] and experimental values.

It can be easily observed that all the electronic band gaps above are overestimated by certain percentage errors. This is because generally, DFT overestimates the band gap energy of solids [10].

4. CONCLUSION

The total ground state energy and electronic band structure of Fullerenes (C₆₀) for FCC, Graphite for hcp and Diamond crystal were calculated using the local-density approximation (LDA) in the parameterization by [18-20], and PBE+vdW approach as defined by [21]. The results of the total energy required for binding/stability of the ground state during the optimized process were found to converge faster with the 12x12x12 k-grid points in the Brillouin zone of the FHI-aims code. Similarly, FHI-aims tight/post relaxed settings were found to give more accurate converged results. In terms of the XC functionals, pbe_GGA was better in approximating the XC energy functional than

LDA. The result presented above have confirmed a faster and more accurate prediction of the electronic band structure and total energies of solids considered when compared to literature report of other studies reporting similar band gaps and/or total energies. Major findings of this research are; Graphite is a zero gap conductor (0.00072958eV), diamond is a wide band gap semiconductor (5.57611325eV). These are in good agreement with experimental values of 0eV and 5.45eV, respectively. However, fullerene is also a wide band gap semiconductor (8.21131431eV). This band gap does not agree with what was obtainable in the literature (1.83eV and 2.3eV). This discrepancy might probably be due to the present DFT calculations of the solid fullerene's lattice constant, spherical shape and the optimized parameters used in the study.

Conversely, Graphite is a suitable candidate for optoelectronic and other electronic devices. Diamond is suitable for high temperature thermal electronic devices, while a fullerene is a good material for conversion into conductors and superconductors.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Pierson HO. Handbook of carbon, graphite, diamond and fullerenes. Noyes Publications, New Mexico; 1993.
2. Shunhong Z, Jian Z, Qian W, Xiaoshuang C, Yoshiyuki K, Puru J. Penta-graphene: A new carbon allotrope. PNAS. 2014;112(8): 2372–2377.
3. Larry A, Al Fasim M, Richard SW, Francesco D, Nicola M. Novamene: A new class of carbon allotropes. Materials Science, Chemistry, Heliyon 3. 2017;3(2). DOI: 10.1016/j.heliyon.2017.e00242

4. Adams W, Williams L. Nanotechnology demystified. United States of America: Mcgraw Hill; 2007.
5. Patrizia C, Gerald G, Koster AM. First-principle calculations of large fullerenes. Journal of Chemical Theory and Computation. 2009;5:29-32.
6. González JM, Ruden A, Barbosa C, Ortega C, Sequeda F. Computational study of allotropic structures of carbon by density functional theory (DFT). Ingeniería y Ciencia. 2014;10(19):145–162. Available:<http://www.eafit.edu.co/ingciencia>
7. Abdu SG, Adamu MA, Onimisi MY. DFT computations of the lattice constant, stable atomic structure and the ground state energy per atom of fullerenes (C60). Science World Journal. 2018;13(1). Available:www.scienceworldjournal.org
8. Blum V, Gehrke R, Hanke F, Havu P, Havu V, Ren X, Reuter K, Matthias S. Ab initio molecular simulations with numeric atom-centered orbitals. Comp. Phys. Commun. 2009;180(11):2175–2196.
9. Viktor A, Oliver H, Sergey L. Hands-on tutorial on ab initio molecular simulations, tutorial I: Basics of Electronic-Structure Theory. Berlin, Fritz-Haber-Institut der Max-Planck-Gesellschaft; 2011.
10. Parr RG, Yang W. Density-functional theory of atoms and molecules. Oxford University Press. New York; 1989.
11. Fiolhais C, Nogueira F, Marques M. (Eds.) A Primer in Density Functional Theory. Vol. 620, Springer-Verlag, Berlin; 2003.
12. Krueger A. Carbon materials and nanotechnology. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim; 2010.
13. Fleming RM, Hessen B, Siegrist T, Kortan AR, Marsh P, Tycko R, Dabbagh G, Haddon R. Fullerenes: Synthesis, properties, and chemistry, chapter 2: crystalline fullerenes. AT & T Bell Laboratories, Murray Hill, NJ 07974; 1992.
14. Heggie MI, Terrones M, Eggen BR, Jungnickel G, Jones R, Latham CD, Briddon PR, Terrones H. Quantitative density functional study of nested fullerenes. Physical Review B, Condensed Matter and Materials Physics. 1998; 57(21):13339-13342.
15. Belenkov EA, Brzhezinskaya MM, Greshnyakov VA. Crystalline structure and properties of diamond-like materials. Nanosystems: Physics, Chemistry, Mathematics. 2017;8(1):127-136. DOI: 10.17586/22208054201781127136
16. Charlier JC, Gonze X, Michenaud JP. First-principles study of the stacking effect on the electronic properties of graphite(S) . Carbon. 1994;32(2):289-299.
17. Katz EA. Fullerene thin films as photovoltaic material. In Sōga, Tetsuo. Nanostructured materials for solar energy conversion. Elsevier. 2006;361–443. ISBN: 978-0-444-52844-5.
18. Perdew JP, Wang Y. Accurate and simple analytic representation of the electron-gas correlation energy. Physical Review B. 1992;45(23):13244-13249. Available:<http://dx.doi.org/10.1103/PhysRevB.45.13244>
19. Perdew JP, Zunger A. Self-Interaction correction to density-functional approximations for many-electron systems. Physical Review B. 1981;23: 5048-5079. Available:<http://dx.doi.org/10.1103/PhysRevB.23.5048>
20. Perdew JP, Burke K, Ernzerhof M. Generalized gradient approximation made simple. Phys. Rev. Letter. 1997;77(18): 3865–3868.
21. Tkatchenko A, Scheffler M. Accurate molecular van der Waals interactions from ground state electron density and free-atom reference data. Physical Review Letters. 2009;102(7):073005. DOI: 10.1103/PhysRevLett.102.073005

© 2018 Abdu et al.; This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Peer-review history:
 The peer review history for this paper can be accessed here:
<http://www.sciencedomain.org/review-history/25519>