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Research paper

# Structural parameters and electronic properties of 2D carbon allotrope: Graphene with a kagome lattice structure

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## ABSTRACT

In this paper, the electronic properties of a carbon allotrope, graphene with a kagome lattice structure, are investigated. Spin-polarized density functional theory (DFT) calculations with Grimme dispersion corrections were done. Bond lengths, electronic band structure, and projected density of states were calculated. Electronic band structure calculations show kagome flat-band formation with higher d-orbital contributed bonding behavior than the pristine graphene structure. The structural parameters and electronic band results of this 2D carbon allotrope show wider possible usage in many applications from desalination membranes to possible high-temperature superconductors.

## 1. Introduction

Because of its unique properties and possible promising applications, graphene has attracted an important amount of attention both experimentally and theoretically since its first experimental isolation and characterization reported by Novoselov et al. [1]. With the triggered interest in graphene, searching for different carbon nanomaterials, graphene-derivatives and allotropes have also gained huge interest [2,3]. These new carbon materials have superior mechanical, electronic, and thermal features, which makes them implemented in many applications of semiconductor devices, such as electronic components [4], and gas sensors [5]. In addition to these small device applications, new carbon materials, especially graphene and graphene oxide with pores, are proposed to be used as a nanofiltration membrane for desalination, drinking water production, water reuse and wastewater treatment applications [6,7]. Also, on reusable or single-use personal protective equipment (PPE) or filters in air purification and air-conditioning devices, coated with modified nanomaterials like graphene or graphene-oxide with pores can enhance the repellent SARS-CoV-2 or similar viruses [8]. With the COVID-19 outbreak, it is well understood that the usage of enhanced filters is necessarily required to prevent aerosol transmission even in daily life.

The variety of proposed and implemented applications with new carbon materials also motivates the studies on new two-dimensional (2D) carbon allotropes. Some of the novel theoretical 2D allotrope studies including radialene [9], pentaheptite [10], haekelites [11], graphdiyne [12], biphenylene [13], T-carbon [14], T graphene [15], net W and C carbon structures [16], graphenylene [17], pentahexoctite [18], penta-graphene [19], alpha-graphyne [20], twin-graphene [21], THD-graphene [22], DHP-graphene [23], tetrahexcarbon [24], net Y carbon [25] and D-Carbon [26] can be listed with respect to their date of report. In addition to these theoretical studies, T-carbon was experimentally observed as T-carbon nanowires in Zhang et al.'s study in 2017 [27]. And in 2018, D-Carbon was suggested to be experimentally possible due to satisfactorily match of previously unexplained X-Ray Diffraction (XRD) peak of a measured chimney or detonation soot [28,29] powder to calculated D-carbon XRD peaks [26].

With these recent signs of progress and possible future developments in experimental studies of new carbon allotropes, the electronic properties of the carbon allotrope with a kagome lattice [30–32], and kagome-like 2D metamaterials [33] took attention recently. In this study, the electronic properties and the structural parameters of graphene with a kagome lattice structure are investigated with implementing the density functional theory (DFT) method.

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## 2. Computational details

Our DFT calculations are carried out using the Atomistic Toolkit (ATK) software v.2017.2 [34]. Spin-polarized generalized gradient approximation (SGGA) was used for exchange-correlation (XC) functional and the double- $\zeta$  (DZ) orbital basis set is adopted. For SGGA calculations, Perdew, Burke, and Ernzerhof (PBE) [35] functionals were used purely and also with Grimme D2 dispersion correction. For further calculations, RPBE functional [36] was used with Grimme D3 dispersion correction.

Fig. 1 (a) and (b) show the structure of the investigated structure's unit cell. The unit cell consists of 6 identical carbon atoms. All carbon atoms have a similar bonding scheme with 3 bonds like graphene. One of the mentioned bonds is represented with  $d_1$  and the other two bonds are identical and represented as  $d_2$  in Fig. 1. Bonds with  $d_2$  length resulted in a cyclopropatriene-like (CP-like) structures [37] with triangular gaps between dodecagonal structures. From a different point of view, a CP-like structure is bonding with three neighbor CP-like structures and the dodecagonal structures with  $D_p$  diameter wide "gaps" occur. In this study, the "gap" represents this wide space inside the dodecagonal structures. The equilateral triangular structure of CP-like structures requires the bond angles of  $60^\circ$  between carbon-carbon with a covalent bond nature. The cut-off energy is used as 600 Ryd and Monkhorst-Pack k-point grid is chosen as  $10 \times 10 \times 1$  to sample Brillouin zone energy calculations. The two layers are separated with a  $15 \text{ \AA}$  vacuum space, therefore the whole structure is accepted to be a two-dimensional structure. For the geometrical optimization, the maximum force on each atom is set to be smaller than  $0.005 \text{ eV/\AA}$ .

## 3. Results and discussion

The optimized structural parameters for the investigated structure with SGGA methods are summarized in Table 1. The C-C bond length between CP-like structures ( $d_1 \sim 1.36 \text{ \AA}$ ) exhibits a featured characteristic of the double bond. The C-C bonds of CP-like structure ( $d_1 \sim 1.43 \text{ \AA}$ ) represent similarity with  $sp^2$ -sp or  $sp^2$  bonding. However, unconventional bent bond angles of  $60^\circ$  and  $150^\circ$  raise questions for explaining the bonds with known hybridizations (trigonal  $sp^2$  or  $sp^2$ - $sp^5$  doublets) [38] and needs a better explanation. Also, bent bonds are known to result in the possibility of high chemical reactivity [39]. The calculated bond angles are not given in Table 1, because of obtaining perfect  $60^\circ$  and  $150^\circ$  for all three methods. The diameter of the dodecagon pores is also calculated and listed in Table 1. As can be seen from table 1, the pore diameter is found smaller with the SGGA-PBE

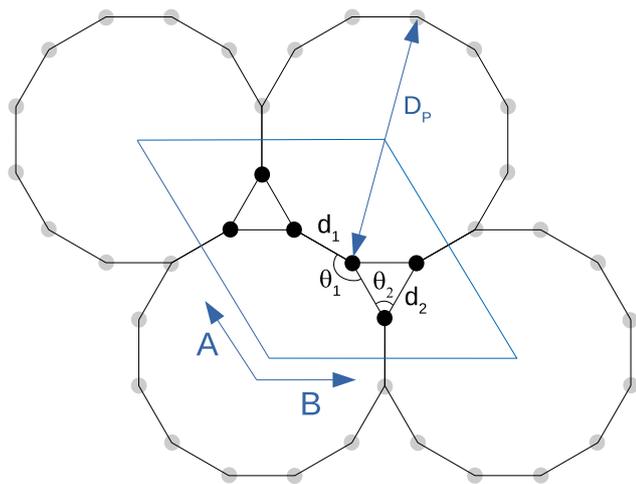
**Table 1**

Optimized lattice constant ( $a$ ), bond length ( $d$ ), and pore diameter ( $D_p$ ) values for dodecagon holes for the investigated structure for SGGA-PBE, SGGA-PBE with Grimme D2 correction, and SGGA-RPBE with Grimme D3 correction methods.

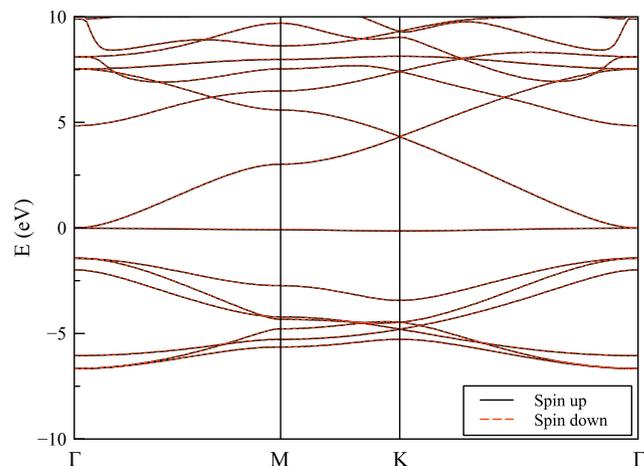
Method	$a$ (Å)	$d_1$ (Å)	$d_2$ (Å)	$D_p$ (Å)
SGGA-PBE	5.2085	1.3559	1.4305	5.3817
SGGA-PBE with Grimme D2	5.2086	1.3554	1.4304	5.3821
SGGA-RPBE with Grimme D3	5.2087	1.3567	1.4299	5.3829

method. All methods result  $\sim 5.38 \text{ \AA}$  of diameter, which is a suitable value for a salt filtration application. The salt rejection ability of a graphene-like membrane is known to decrease with an increase in pore size [7]. The study of Cohen-Tanugi and Grossman shows that most salt ions can pass through graphene with pores of diameter above  $5.5 \text{ \AA}$  [40]. Therefore, the pore diameter of graphene-like 2D carbon allotropes should be below this value to successfully filter  $\text{Na}^+$  and  $\text{Cl}^-$  ions from water, where graphene with a kagome lattice structure fulfills this requirement and also have a very high porosity value of  $\sim 97\%$ . With the possible experimental proof in the future, graphene membranes with a kagome lattice structure having a very high porosity value may open the possibility of the low pressure or passive desalination applications and also can be used on reusable or single-use PPE or on filters in air purification and air-conditioning devices to prevent virus transmission. Graphene is already suggested as single flakes and sheet with defects in these applications and with the possible experimental confirmation of graphene with kagome lattice structure, there will be no need for introducing defects in the structure for increasing selective permeability.

Fig. 2 shows the spin-dependent electronic band structure of the graphene with a kagome lattice structure. Band structure in the figure is calculated with SGGA-PBE. However, other methods gave similar results and will be discussed shortly after. As seen in Fig. 2, the band structure has a similar behavior for spin-up and spin-down electrons. Therefore, it is seen that the non-interacting pristine graphene with a kagome lattice structure shows a very small magnetic nature as the pristine graphene sheet. However, it is already shown that the DFT calculations of graphene with a kagome lattice structure with doping by reducing the density of valence electrons (hole doping) makes the flat-band partially filled [30]. This type of doping can be done with the electrostatic gating, and it is highly known that graphene has a similar behavior [41]. This type of doping results in a ferromagnetic flat-band formation where it is possible to explore new exotic phases by tuning the filling factor of the flat-band. There is a graphene-like linear band formation at K-point. However, it is not located at the Fermi level ( $E_F$ ). Also, it is clear that the



**Fig. 1.** Unit cell of graphene with a kagome lattice structure. All six carbon atoms are equivalent and are connected to other atoms with one  $d_1$ -long and two  $d_2$ -long bonds.



**Fig. 2.** The spin-dependent electronic band structure of the investigated structure was calculated with SGGA-PBE functional.

kagome flat-bands emerge around the  $E_F$  [30]. This kagome flat-bands are important because the electrons are confined in a very narrow energy interval with a huge number of density of states (DOS) which may be related with Wigner-crystallization [30,42], flat-band ferromagnetism [43], fractional quantum Hall states [44] and a possibility of a high-temperature-superconductivity [45].

In Fig. 3, electronic band structure calculation for structure for SGGA-PBE, SGGA-PBE with Grimme D2 dispersion correction, and SGGA-RPBE with Grimme D3 dispersion correction methods for only spin-up states were shown. Band structures of spin-down states are similar and not shown in the figure for clarity. As can be seen from the figure, SGGA-PBE with Grimme D2 dispersion correction results are similar to legacy SGGA-PBE calculations show high similarity among the all investigated momentum and energy space. Energy values for SGGA-RPBE with Grimme D3 dispersion correction method is seemed to be shifted further away from the  $E_F$ . SGGA-PBE method is providing adequate results with a lower computational cost for the pristine graphene with a kagome lattice structure. The similarity of SGGA-PBE with Grimme D2 dispersion correction method and for SGGA-RPBE with Grimme D3 correction method results with legacy SGGA-PBE calculation results can be expected because of there is a large 15 Å vacuum space over a single layer structure where van der Waals interactions are not playing a significant role in the overall structure. In fact, showing these similarities also confirms that our results belong to an isolated single layer system.

In Fig. 4 (a) and (b), the projected density of states (PDOS), which are calculated with SGGA-PBE functional, are shown for only spin-up states. As pointed before, the values of spin-down states are similar and not shown in the figure for clarity. High numbers of states are observed at kagome flat-band located at the  $E_F$ . In the near vicinity of  $E_F$ , only states of  $p$  and  $d$  orbitals are found.

To understand the nature of the bonds in the graphene with a kagome lattice structure, DOS is projected onto orbitals of carbon atoms for SGGA-PBE calculations as shown in Fig. 5 (a). The main peak at the  $E_F$  is mostly consisting of electronic states of the  $p_z$  orbital ( $l = 1, m_l = 0$ ). The main peak at the  $E_F$  is also consisting of electronic states of  $d_{xz}$  and  $d_{yz}$  orbitals ( $l = 2, m_l = \pm 1$ ).  $p_z$  do hybridize with  $d_{xz}$  and  $d_{yz}$  orbitals, forming together the  $\pi$  band [46]. The contribution of  $d_{xz}$  and  $d_{yz}$  orbitals to the total electronic states at  $E_F$  is more significant in graphene with a kagome lattice structure than the pristine graphene structure. With the same calculation parameters, the each  $d$ -orbital's states near to Dirac point in pristine graphene structure are found to be 7% of total  $p_z + d_{xz} + d_{yz}$  states. However, in graphene with a kagome lattice structure, the

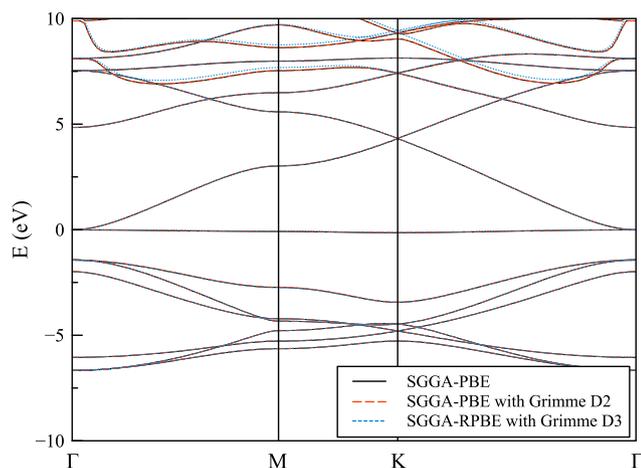


Fig. 3. Electronic band structure calculation for structure for SGGA-PBE, SGGA-PBE with Grimme D2 dispersion correction, and SGGA-RPBE with Grimme D3 dispersion correction methods. For clarity, only spin up states were shown.

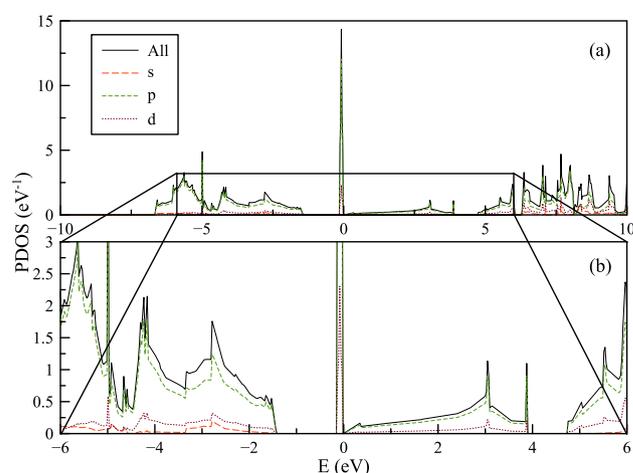


Fig. 4. (a) PDOS for graphene with kagome lattice structure, (b) details of the PDOS between  $-6$  and  $6$  eV.

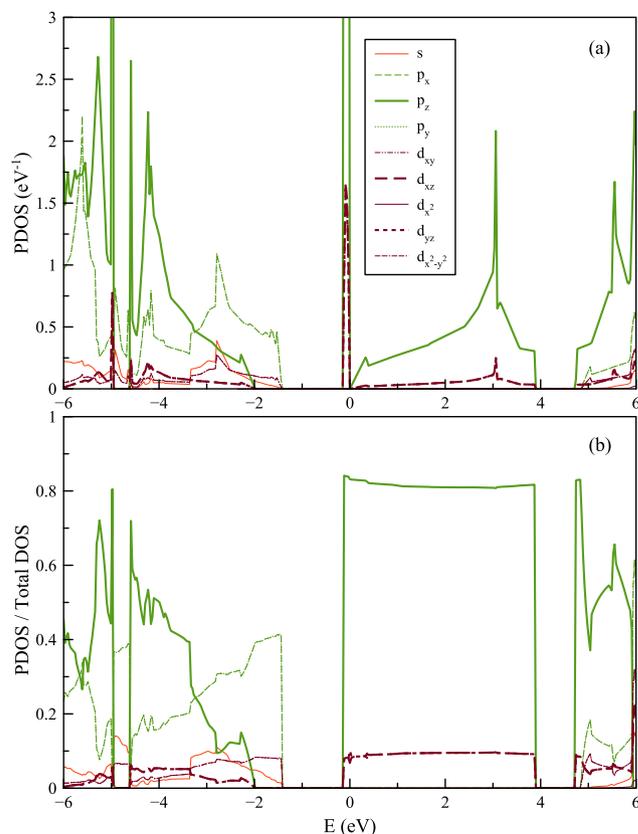


Fig. 5. (a) PDOS onto orbitals of carbon atoms in Graphene with Kagome lattice structure (b) Normalized PDOS onto orbitals concerning total DOS.

each  $d$ -orbital's states at  $E_F$  is found to be 9% as can be seen in Fig. 5 (b). From Fig. 5 (b) the long-range unvarying  $\pi$  bonding ( $p_z$  hybrid with  $d_{xz}$  and  $d_{yz}$  orbitals) behavior can be observed between 0 and 4 eV and also can be observed in the near vicinity of Dirac point which is located at 4.31 eV. It is important to point that the density of states with  $d_{xz}$  and  $d_{yz}$  orbitals follows in shape that of  $p_z$ , which results the long-range unvarying  $\pi$  bonding mentioned above. The similarity of the shape of density of states of  $d_{xz}$  and  $d_{yz}$  orbitals to the  $p_z$ , is found to in agreement with Gmitra et al.'s study for the pristine Graphene [47].

#### 4. Conclusion

In this study, structural parameters and the electronic band structure of graphene with kagome lattice structure is theoretically studied. Spin-polarized DFT calculations were done with SGGA-PBE, SGGA-PBE with Grimme D2 correction, and SGGA-RPBE with Grimme D3 correction methods. All methods resulted in similar bond lengths and similar electronic band structure and density of state distributions. A kagome flat-band structure is observed near the  $E_F$  and high number of electronic states at this kagome flat-band is mostly consisting of  $p_z$  orbital and also  $d_{xz}$  and  $d_{yz}$  orbital contributions with a  $\pi$  bonding behavior. Also,  $d$ -orbital contribution near K-point in graphene with a kagome lattice structure is found to be larger than the related contribution observed in the pristine graphene. The reason for the high contribution of  $d$ -orbital states between 0 and 4 eV needs more quantitative investigation that the plane-wave approach can be utilized in addition to the already implemented linear combination of the atomic orbitals approach. This 2D carbon allotrope, which has a novel electronic structure, can be a promising structure for many possible electronic device applications or it may be used mechanically in desalination applications because of suitable pore size and density of dodecagons in its structure.

#### CRediT authorship contribution statement

**B. Sarikavak-Lisesivdin:** Conceptualization, Formal analysis, Methodology, Writing - original draft. **S.B. Lisesivdin:** Visualization, Writing - original draft. **E. Ozbay:** Software, Project administration, Supervision. **F. Jelezko:** Resources, Supervision.

#### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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