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Effect of defect and temperature on the mechanical and electronic properties of graphdiyne: A theoretical study

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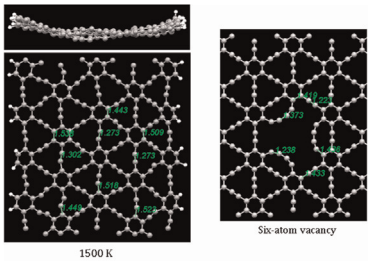
HIGHLIGHTS

- State of the art SCC-DFTB method is performed.
- The in-plane stiffness and Young's modulus of graphdiynes with various lengths are evaluated.
- A molecular dynamics simulation based on the SCC-DFTB method is used to calculate the elastic properties of graphdiyne at different temperatures.
- We also investigated the effect of different vacancies on the mechanical and electronic properties of graphdiyne.

GRAPHICAL ABSTRACT

Mechanical properties of graphdiyne decrease as the temperature of the environment and the number of removed carbon atoms increase.



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ABSTRACT

In the present work, the elastic properties (in-plane stiffness and Young's modulus) of graphdiyne, a two-dimensional lattice of sp–sp^2-hybridized carbon atoms similar to graphene, are studied using a self-consistent charge density functional tight-binding (SCC-DFTB) method. The obtained results indicate that as the length of the graphdiyne increases in the x-direction, the in-plane stiffness and Young's modulus increase and finally approach constant values for longer lengths. Furthermore, based on the calculated density of states (DOS), we observed that graphdiyne is a semiconductor with a band gap energy of 0.43 eV. A molecular dynamics simulation based on the SCC-DFTB method is also used to calculate the elastic properties of graphdiyne at five temperatures between 300 and 1500 K. Our results indicate that the in-plane stiffness and Young's modulus of graphdiyne decrease as the temperature of the environment increases. Finally, we investigated the effect of different vacancies on the mechanical and electronic properties of graphdiyne. Our results reveal that increasing the number of removed carbon atoms leads to a decrease in the elastic parameters and band gap energy of graphdiyne.

1. Introduction

Over the last decade, various types of carbon allotropes such as fullerenes, carbon nanotubes, graphene and others, known as allotropic forms or simply carbon nanoforms, have received considerable interest, primarily due to their unique physical–chemical properties and their applications in various fields of science and engineering [1–4]. Graphynes represent a new form of carbon, whose atomic structures were predicted more than 20 years ago by Baughman et al. [5]. Graphynes have a planar periodic framework that resembles that of graphene, except in the type of atomic bonds, and are composed of sp and sp^2 mixed carbon atoms. Graphyne is named after *yne* carbon, which denotes a carbon triple bond. Among the various graphyne structures, graphdiyne is one of the most synthetically approachable allotropes containing butadiyne linkages between its nearest-neighbor hexagonal rings [6]. A schematic of the chemical bonding structure and a full atomistic model of graphdiyne are presented in Fig. 1.

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Graphdiyne was reported for the first time by Haley et al. [7] in 1997, and since then, great efforts have been devoted to the synthesis of monomeric and oligomeric substructures toward constructing graphdiyne. Finally, in 2010, the first thin films of graphdiyne were synthesized through a cross-coupling reaction using hexaethynylbenzene on a copper surface [8]. Their experimental results demonstrate semiconducting properties of approximately 2.516×10^{-4} S/m for graphdiyne. Thus, the potential application of graphdiyne in future nanoelectronics is of great interest. Although some theoretical works have examined the properties of graphdiyne, such as the band gap [9,10], charge mobility [11] and lithium storage capacity [12], the mechanical properties of graphdiyne have not been explicitly determined. In 2011, Cranford et al. [13] predicted some mechanical properties of monolayer graphdiyne by employing the classical molecular dynamics (MD) method and reported that the in-plane stiffness of graphdiyne is equal to 170.4 N/m (532.5 GPa for a thickness of 0.32 nm). In the same year, Kang et al. [14] investigated the mechanical and electronic properties of graphdiyne using the density functional theory (DFT) method with the Vienna *ab initio* simulation package (VASP). These authors used the generalized gradient approximation with the Perdew–Burke–Ernzerhof (GGA–PBE) functional and reported an in-plane stiffness and band gap of 165.8 N/m and 0.46 eV for graphdiyne, respectively. Long et al. [11] used a similar approach to study graphdiyne at room temperature (300 K) and obtained an in-plane stiffness of 158.6 N/m. The band gap of graphdiyne has also been calculated by Zhou et al. [10], who used the DFT method with the GGA–PBE exchange correlation functional and the DMOL^3 package. These researchers concluded that graphdiyne with a length of 26.16 Å has a band gap of 0.49 eV.

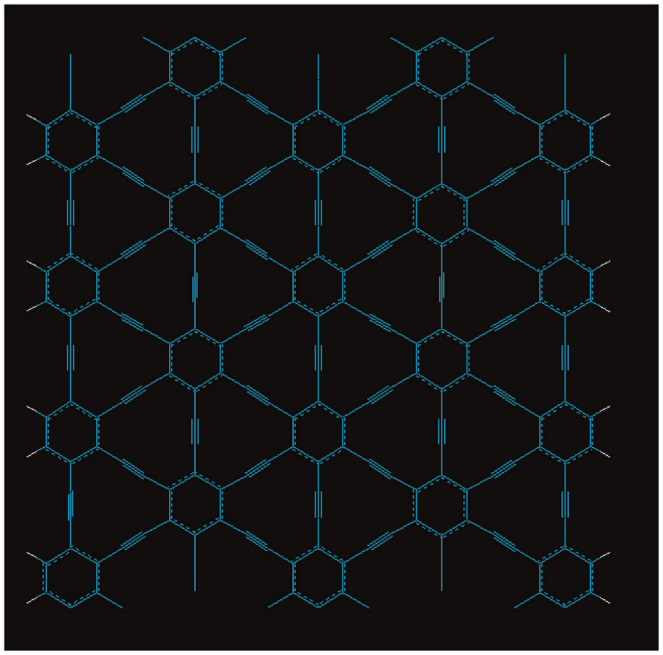

Fig. 1. Schematic representation of the chemical bonding structure of a graphdiyne sheet. The chemical structure of graphdiyne consists of a uniform lattice of two-dimensional sp–sp^2-hybridized carbon atoms, in which the aromatic carbons are bonded by single–triple–single carbon bonds.

In the present work, we first employed the self-consistent charge density functional tight-binding (SCC-DFTB) method to optimize the structure and calculate the elastic properties (in-plane stiffness and Young's modulus) of graphdiyne for various lengths (L=8.35, 14.29, 20.23, 26.16, 32.1, 38.04 and 43.98 Å). Then,

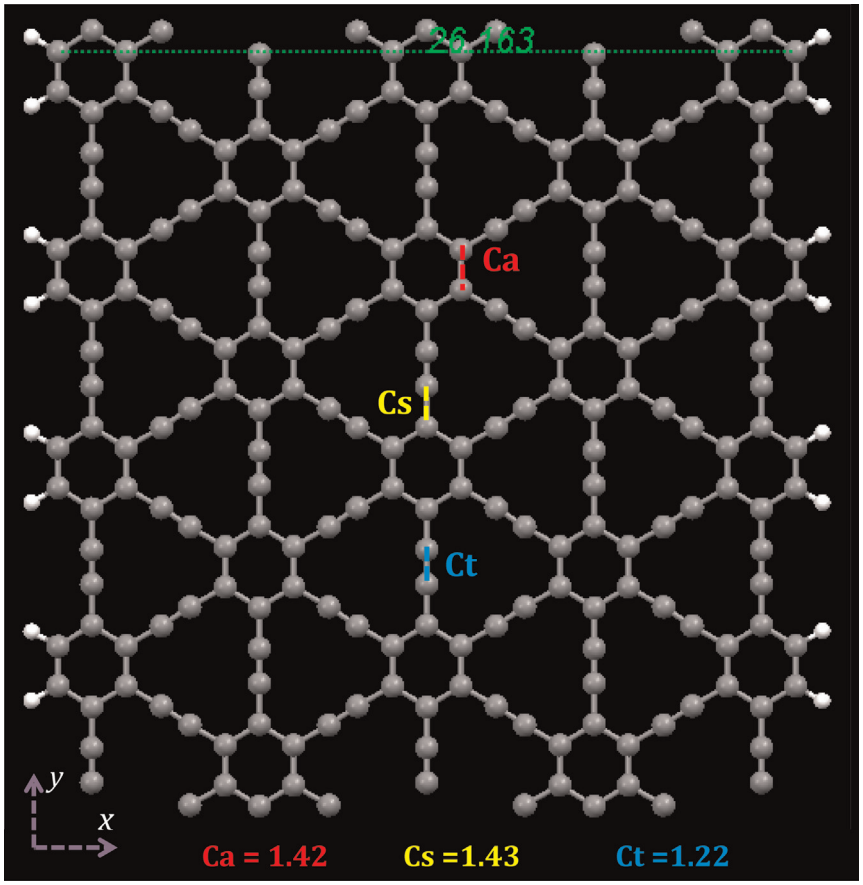

Fig. 2. The optimized structure and geometrical parameters of graphdiyne with a length of 26.16 Å.