Front. Phys. 13(5), 136105 (2018)
https://doi.org/10.1007/s11467-018-0787-x

RESEARCH ARTICLE

A novel hybrid sp-sp^2 metallic carbon allotrope

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Received March 10, 2018; Accepted April 9, 2018

In this paper, we propose a novel hybrid sp-sp^2 monoclinic carbon allotrope mC$_{12}$. This allotrope is a promising light metallic material, the mechanical and electronic properties of which are studied based on first-principles calculations. The structure of this new mC$_{12}$ is mechanically and dynamically stable at ambient pressure and has a low equilibrium density due to its large cell volume. Furthermore, calculations of the elastic constants and moduli reveal that mC$_{12}$ has a rigid mechanical property. Finally, it exhibits metallic characteristics, owing to the mixture of sp-sp^2 hybrid carbon atoms.

Keywords metallic carbon allotrope, first-principles calculations, mechanical and electronic properties

PACS numbers 62.20.-x, 63.20.-e, 74.20.Pq

1 Introduction

Carbon is one of the most fundamental elements on earth and the rich diversity of carbon allotropes is a cornerstone of modern industry. Flexible bond hybridizations of carbon atoms, such as sp-, sp^2-, and sp^3-hybridization, lead to many different and intriguing properties and have also inspired intense theoretical and experimental studies. As is well known, the only two naturally occurring carbon allotropes are graphite and diamond. In addition, the traditional graphite and fullerenes within the sp^2 network are ultra-soft and semimetallic, while sp^3-hybridized diamond and lonsdaleite are superhard and insulating. Moreover, the exploration of fullerenes [1], carbon nanotubes [2] and graphene [3], etc., which have all-sp^2 networks, in [4–11], are promising for both fundamental and applied purposes. Many three-dimensional sp^3-hybridized carbon phases, such as M-, S-, and T-carbon, etc. [12–24], show a superhard nature. The one-dimensional carbyne [25, 26], consisting of a linear chain of sp-hybridized carbon atoms, was reported to exhibit unusual electrical, optical, and catalytic properties. By compressing the sp^2 carbon allotropes, some novel hybrid sp^2-sp^3 carbon allotropes have been synthesized in previous experiments [27–29], and more phases have been predicted theoretically [30–36]. One particularly interesting carbon allotrope is the sp-sp^3 *yne*-diamond [37, 38] and its C(sp^3)-C(sp) bond, which is believed to be even stronger than the C(sp^3)-C(sp^3) diamond bond. Furthermore, the so-called graphyne [39], which possesses both the sp^2 and sp carbon atoms, was discovered to be a layered structure, and its three-dimensional structures in different stacking arrangements are metallic and semiconducting, respectively [40]. In this paper, we propose a new phase mC$_{12}$ using the particle swarm optimization method, which is a hybrid sp-sp^2 carbon allotrope. This structure is tubular, possessing a double helix, and shows metallic characteristics. Its low equilibrium density and large cell volume make it promising for hydrogen storage, similar to the recently reported T-carbon [14, 15]. Further mechanical and electronic properties are also studied in detail in this paper.

2 Computational methods

All calculations were performed based on first-principles calculations. Crystal structure searches were performed based on a global minimization of energy surfaces merging *ab initio* total-energy calculations, as implemented in CALYPSO code [41, 42]. This methodology has pre-

viously been successful in predicting crystal structures for various compounds. We searched 30 generations. For each generation, 30 structures were generated using particle swarm optimization. Structural relaxations were performed within the density functional theory and carried out within the Vienna *ab initio* simulation package (VASP) [43] in the framework of density functional theory [44] with the generalized-gradient approximation (GGA) proposed by Perdew–Burke–Ernzerhof (PBE) [45] exchange-correlation functional. The electron and core interactions were included by using the frozen-core all-electron projector augmented wave (PAW) method [46]. The electronic wave functions were expanded on a plane-wave basis set with a well-converged cutoff energy of 900 eV. Monkhorst–Pack k point meshes, with a grid of 0.02 $Å^{-1}$ for Brillouin zone sampling, were chosen to ensure that the total energies converged at values less than 1 meV/atom. The phonon frequencies were calculated using a supercell approach, as implemented in PHONOPY code [47], with the forces calculated from VASP. Finally, the electronic properties were calculated using the Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [48].

3 Results and discussion

The novel monoclinic ($P2_1/c$) carbon allotrope structure, which contains 12 atoms in a conventional cell and then can be named as mC$_{12}$, is a sp (C1) and sp^2 (C2 and C3) mixed hybridized network. The equilibrium structure parameters within GGA level at ambient pressure are a = 8.7852 Å, b = 3.9392 Å, c = 4.8499 Å, and $\beta = 137.9°$. The new carbon phase has three inequivalent Wyckoff positions: C1 4e (0.9014, 0.5589, 0.3645), C2 4e (0.5852, 0.6203, 0.6309), and C3 4e (0.3103, 0.3143, 0.9505). As shown in Fig. 1(a), the length of C1-C1 bond is 1.251 Å, the C2-C2 bond is 1.390 Å, the C1-C3 bond is 1.352 Å, and the C2-C3 bond has two different lengths, 1.456 Å and 1.505 Å. The supercells in Figs. 1(b) and (c) indicate that the structure of mC$_{12}$ is tubular, and we found the basic building block shown in Figs. 1(d) and (e) to be a double helix structure. When viewed from different directions, the two helical carbon chains appear to be uniform in composition, while the rotational directions are clockwise and counterclockwise, respectively. The helix extends along the b-axis, and through the C2 atoms forms the C2-C2 bonds as a connection between the two chains. Moreover, Fig. 1(f) shows the finer structure of the double helix, which is a six-member carbon chain with two C1, two C2, and two C3 atoms.

The energy per atom of various carbon structures, relative to graphite at the GGA level, is listed in Table 1 to evaluate relative stability. These values show that the relative energy of mC$_{12}$ is 0.733 eV/atom, which is smaller than the previous reported values of *Tri*-C$_9$ [22] (1.093 eV/atom), T-carbon [14], (1.303 eV/atom) and K_6-carbon [21] (1.493 eV/atom) phases. Thus, this new structure should be more thermodynamically stable at ambient pressure. The lower relative energies of T_6-carbon [30] (0.587 eV/atom), C$_{64}$ [35] (0.419 eV/atom), M-carbon [12] (0.296 eV/atom), and S-carbon [13] (0.224 eV/atom) demonstrate that mC$_{12}$ is less stable than

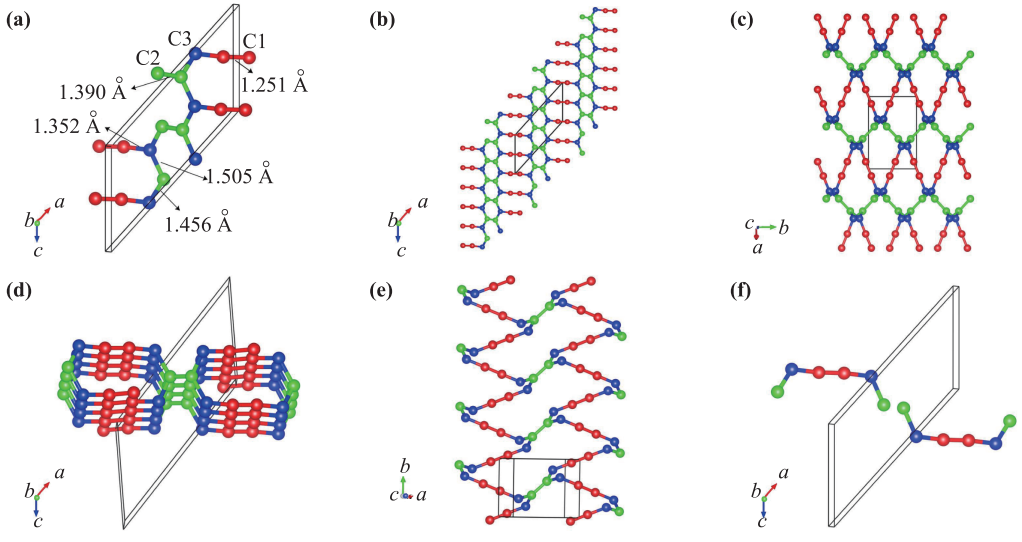

Fig. 1 Unit cell of mC$_{12}$ **(a)**. 3 × 3 × 3 supercells viewed along the b- **(b)** and c-axis **(c)**, respectively. The basic building block of double helix structure viewed along different directions **(d)** and **(e)**. The six member carbon chain **(f)**. The red, green, and blue spheres represent the three in-equivalent C1 4e (0.9014, 0.5589, 0.3645), C2 4e (0.5852, 0.6203, 0.6309) and C3 4e (0.3103, 0.3143, 0.9505) atoms, respectively.

Table 1 Calculated volume V (Å^3/atom), density ρ (g/cm^3), band gap E_g (eV), and relative energy ΔE (eV/atom). The results were calculated by the GGA method.

	Space group	V	ρ	E_g	ΔE
mC$_{12}$	$P2_1/c$	9.378	2.127	metallic	0.733
Graphite	$P6_3/mmc$	11.565	1.725, 1.859[a]	metallic	0.000
M-carbon	$C2/m$	5.942, 5.974[b]	3.357, 3.339[b]	3.493[c]	0.296
S-carbon	$Cmcm$	5.856	3.406, 3.399[c]	4.342[c]	0.224
T-carbon	Fd-3m	13.180	1.513, 1.50[d]	2.25[d]	1.303
C$_{64}$	$I4_1/amd$	7.785[e]	2.562[e]	1.315[e]	0.419[e]
K_6-carbon	$I4_132$	9.750	2.046	metallic	1.493
T_6-carbon	$P4_2/mmc$	6.805	2.931	metallic	0.587
Tri-C$_9$	$R32$	6.369	3.131	metallic	1.093

[a]Ref. [23]; [b]Ref. [24]; [c]Ref. [13]; [d]Ref. [14]; [e]Ref. [35].

these four allotropes. The novel structure of mC$_{12}$ shows a metallic nature; moreover, compared to the majority of carbon allotropes, it has a lower equilibrium density (2.127 g/cm^3) and a larger cell volume (9.378 Å^3/atom), except for K_6- and T-carbon, indicating its light metallic characteristics. The phonon spectra of mC$_{12}$ at 0 GPa were calculated to assess the dynamical stability. As shown in Fig. 2, there was no imaginary frequency in the whole Brillouin zone, demonstrating that this structure is dynamically stable at ambient pressure.

The elastic constants and moduli were calculated with the mechanical properties shown in Table 2, where the carbon allotropes K_6- and T-carbon are also listed for comparison. As is commonly known, monoclinic crystals have 13 independent elastic constants, and the necessary and sufficient criterion for a crystal to be stable is to determine whether the elastic constant scalar matrix is definite positive [49]. Table 2 shows that the calculated elastic constants of mC$_{12}$ satisfy this stability criterion, demonstrating its mechanical stability at 0 GPa. The elastic constant C_{11} of mC$_{12}$ is 345 GPa, larger than that of K_6- (250 GPa) and T-carbon (203 GPa). Furthermore, the C_{44} of K_6- (29 GPa) and T-carbon (70 GPa) are much smaller than that of mC$_{12}$ (115 GPa). However, these three carbon allotropes have small differences in the C_{12}, with 187 GPa, 136 GPa, and 156 GPa for K_6-carbon, T-carbon, and mC$_{12}$, respectively.

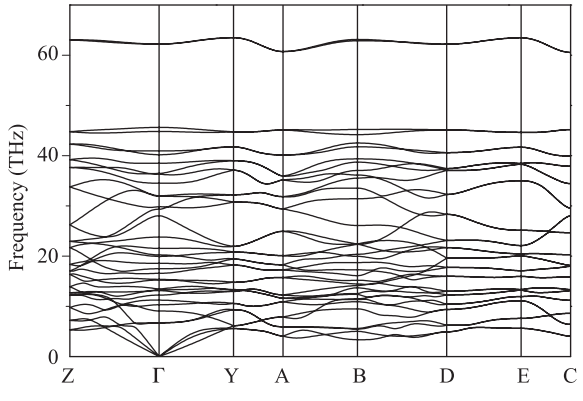

Fig. 2 Phonon spectra of mC$_{12}$ at 0 GPa.

The bulk modulus B and shear modulus G were calculated using the Voigt–Reuss–Hill approximations [50], and Young's modulus E and Poisson's ratio ν were defined by [51]: $E = 9BG/(3B + G)$, $\nu = (3B - 2G)/[2(3B + G)]$. As shown in Table 2, the bulk modulus of mC$_{12}$ is 160 GPa, which is smaller than that of K_6-carbon (209 GPa), and almost equal to that of T-carbon (159 GPa). This indicated an analogously volumetric elasticity and compression resistance. For both the shear modulus and Young's modulus, the values followed the order of mC$_{12}$ > T-carbon > K_6-carbon. The Poisson's ratio for mC$_{12}$ is 0.26, which is smaller than that of K_6-carbon (0.43) and T-carbon (0.35), revealing that mC$_{12}$ has a more rigid mechanical property than K_6- and T-carbon. The ratio of bulk to shear modulus is utilized to estimate the allotrope's brittle and ductile properties [52]. As shown in Table 2, the ratio of mC$_{12}$ is 1.71, indicating a weak brittle character ($B/G < 1.75$), while the ratios of 6.97 for K_6-carbon and 3.08 for T-carbon show

Table 2 Calculated elastic constants (GPa), moduli (GPa), Poisson's ratio, and the B/G ratio. The results were calculated by the GGA method.

	K_6-carbon	T-carbon	mC$_{12}$
C_{11}	250	203	345
C_{22}			139
C_{33}			536
C_{44}	29	70	115
C_{55}			193
C_{66}			161
C_{12}	187	136	156
C_{13}			226
C_{23}			136
C_{15}			22
C_{25}			72
C_{35}			26
C_{46}			60
B	209	159	160
G	30	52	94
E	86	141	236
ν	0.43	0.35	0.26
B/G	6.97	3.08	1.71

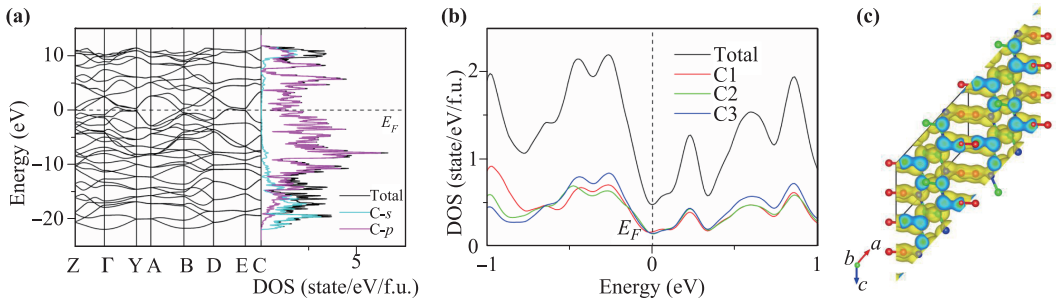

Fig. 3 Electronic band structure and density of states (DOS) calculated by HSE06 hybrid functional **(a)**, DOS between $E_F - 1$ and $E_F + 1$ eV **(b)**, band decomposed charge density between $E_F - 1$ and $E_F + 1$ eV viewed along *b*-axis, with the isosurface value of 0.005 **(c)**. The red, green, and blue spheres represent the three inequivalent types of carbon atoms C1, C2, and C3, respectively.

a strong ductile nature.

The electronic properties at 0 GPa were calculated using the HSE06 hybrid functional, as shown in Fig. 3. The electronic band structure and density of states (DOS) are shown in Fig. 3(a). Based on these values, we can see that the bands cross the Fermi level (E_F) represented by the dashed line, indicating that $m\mathrm{C}_{12}$ has a definite metallic character. From the DOS, we see that in the energy range of −22 to −17 eV, the total DOS originated mainly from the C-*s* orbital electrons. However, in the range of −17 to 10 eV, the DOS was mainly influenced by the contribution of C-*p* orbital electrons; for the higher energy range of 10 to 12 eV, the DOS originated from the mixed contributions of the C-*s* and C-*p* states. To further study the electronic properties, the DOS and the band decomposed charge density between $E_F - 1$ and $E_F + 1$ eV are shown in Figs. 3(b) and (c); the isosurface value of the band decomposed charge density was taken as 0.005. Thus, one finds that the contributions of the three inequivalent atoms were almost the same near the Fermi level, showing that the metallicity derives from the mixture of *sp*-sp^2 hybrid carbon atoms and that the band decomposed charge density also indicates the appearance of conduction around the three types of carbon atoms.

4 Conclusions

Based on a crystal structure searching technique combined with *ab initio* total-energy calculations, we have proposed a new light metallic *sp*-sp^2 hybrid carbon allotrope $m\mathrm{C}_{12}$. We studied the mechanical and electronic properties of $m\mathrm{C}_{12}$ using first-principles calculations. The elastic constants and phonon spectra were then calculated to determine the mechanical and dynamical stability at 0 GPa. The low equilibrium density and large cell volume make $m\mathrm{C}_{12}$ a promising light material. In addition, this structure possesses a rigid mechanical property. Concerning electronic properties, $m\mathrm{C}_{12}$ shows a metallic character, which originates from the mixture of *sp*-sp^2 hybrid carbon atoms.

Acknowledgements This work was financially supported by the National Natural Science Foundation of China (Grant No. 11204007), the 111 Project (B17035), the Natural Science New Star of Science and Technologies Research Plan in Shaanxi Province of China (Grant No. 2017KJXX-53), and Education Committee Natural Science Foundation in Shaanxi Province of China (Grant No. 16JK1049). Xiao-Feng Shi is acknowledged for helpful discussions and comments on the manuscript. All the authors thank the computing facilities at the High Performance Computing Center of Xidian University.

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