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Novel three dimensional topological nodal line semimetallic carbon

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ABSTRACT

A new cubic three dimensional carbon phase has been predicted by first-principles calculations. This phase is constructed by triangle graphene sheets, and dubbed as sc-C_{96}. The investigation on its electronic properties has indicated that sc-C_{96} possesses a topological nodal line semimetal state, which protected by the combination of time reversal and spatial inversion symmetries, and negligible spin–orbit interaction. Due to the cubic symmetry, the Fermi surface of sc-C_{96} is constituted of three nodal line circles. From the cohesive energy and phonon spectra, we find that sc-C_{96} is dynamically stable and may be easily synthesized by polymerizing C_{96} fullerene molecules at a relatively low pressure conditions (~1 GPa).

1. Introduction

Topological semimetals, newly proposed nontrivial quantum materials [1–8], have attracted increasing attention due to their interesting quantum phenomena, physical properties (e.g. Fermi arcs on the side surfaces [9], unusually high bulk carrier mobility [10], and oscillating quantum spin Hall effect [11]) as well as great potential applications in future functional devices. As a typical example of topological semimetal carbon, graphene [12] possesses more superior comprehensive properties than other topological semimetals, such as high thermal conductivity [13], high strength [14] and chemistry stability [15], among others. Since graphene is a two dimensional (2D) topological semimetal, it is natural to ask, what is its three dimensional (3D) analogue? Recently, much effort have been devoted to explore novel carbon allotropes [16–19], and theoretical studies of 3D topological semimetal indicated that carbon also can form into 3D topological semimetal structures [6,18,20], while there is no any 3D topological semimetal carbon has been synthesized to date. Therefore, further exploring new 3D topological semimetal carbons and finding their easily synthesis paths are urgently needed.

In this paper, a simple cubic 3D carbon allotrope called sc-C_{96} has been predicted by means of the first-principles calculations. Our calculated results indicated that sc-C_{96} is a 3D topological nodal line semimetal, whose Fermi surface is protected by the time reversal and spatial inversion symmetry, and weak spin–orbit coupling (SOC) strength. In addition, sc-C_{96} is a dynamically stable phase, and the low phase transformation energy barriers from C_{96} fullerene molecules to sc-C_{96} indicated that sc-C_{96} may be easily synthesized under relatively mild conditions.

2. Computational methods

The first-principles calculations are performed on the basis of density functional theory (DFT) [21,22], as implemented in the Vienna ab initio simulation package (VASP) [23,24]. The all-electron projector augmented wave (PAW) method [25] is adopted with $2s^2 2p^2$ treated as the valence electrons. The exchange-correlation potential is described by the local density approximation (LDA) [26]. A plane-wave cutoff energy of 500 eV has been used in this work. The k-point separation in Brillouin zone of the reciprocal space is sampled as $11 \times 11 \times 11$. The conjugate-gradient algorithm is used to relax the ions in their instantaneous ground-state, and the convergence threshold is set to be within 1×10^{-6} eV/atom. The phonon dispersion curve is computed through the direct supercell method [27], and the supercell is $2 \times 2 \times 1$. It is obtained through the VASP and PHONOPY code [28]. The first-principles molecular dynamics simulations are performed in the canonical (NVT) ensemble with a $2 \times 2 \times 1$ supercell, each simulation lasted for 6 ps, with a time step of 1 fs. The climbing image nudged elastic band

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Table 1
The space group, optimized lattice parameters (a and c), mass density (ρ), cohesive energy (E_{coh}), and bulk modulus (B) for sc-C_{96}, graphite, and diamond at zero pressure, compared to the available experimental and other theoretical values.

Structure	Space groups	References	a (Å)	c (Å)	ρ (g/cm^3)	E_{coh} (eV/atom)	B (GPa)
Graphite	$P6/mmm$	Our work	2.446	6.624	2.325	8.998	284
		[30]	2.443	6.679	2.301	9.001	288
		Expt. [30].	2.460	6.642–6.716	2.770–2.280		286–319
Diamond	$Fd\bar{3}m$	Our work	3.534		3.617	9.006	461
		LDA [30]	3.530		3.625	9.004	460
		Expt. [31].	3.567		3.520		443
sc-C_{96}	$Pm\bar{3}m$	LDA	11.597		1.227	8.529	149

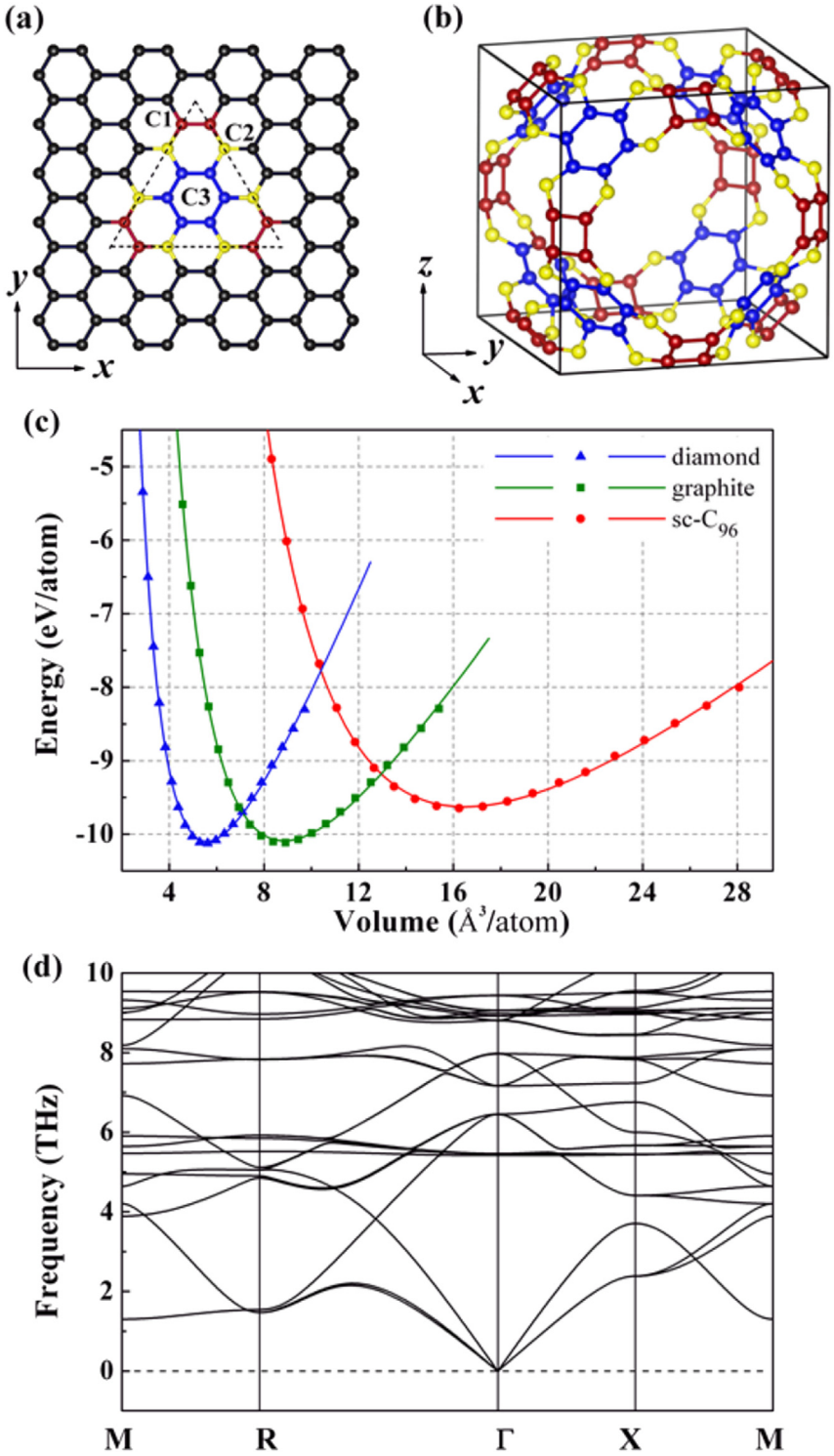

Fig. 1. (a) The basic building block of sc-C_{96} is a triangle graphene sheet (dashed area), the atoms located at the endpoints, sides and interior of the triangle graphene sheet are denoted as the C1, C2, C3 atoms and colored red, yellow, blue, respectively. (b) The optimized unit cell of sc-C_{96} that is interconnected by eight triangle graphene sheets. (c) Volume dependence of total energy for graphite, diamond, and sc-C_{96}. (d) Low-frequency part of phonon spectra for sc-C_{96}. The high symmetry q point path in the Brillouin zone is chosen as: M (1/2, 1/2, 0) → R (1/2, 1/2, 1/2) → Γ (0, 0, 0) → X (1/2, 0, 0) → M (1/2, 1/2, 0). (A color version of this figure can be viewed online.)