



The geometric and electronic transitions in body-centered-tetragonal C₈: A first principle study



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ABSTRACT

The stability, geometric structure and electronic properties of a novel body-centered tetragonal carbon allotrope Bct C₈ are systematically investigated. Bct C₈ are formed by sp³-bonded carbon atoms and can be regarded as a compressed bundle of carbon nanotubes (CNT). The transition path from CNT to Bct C₈ has been simulated, indicating a possible approach to synthesize Bct C₈. The X-Ray diffraction, phonon and Raman spectroscopies are presented as reference for experimental studies. Besides, Bct C₈ is a semiconductor with an indirect gap of 1.66 eV and will transform to semimetal when doping with boron and nitride atoms. Furthermore, considering its porous structural character, the lithium storage capability of Bct C₈ are also discussed, a directional fast lithium-ion mobility with a rather low 0.04 eV barrier is revealed. Therefore, the Bct C₈, once synthesized experimentally, would have fruitful applications in carbon-based electronics and energy storage.

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1. Introduction

Carbon materials, have various allotrope forms such as graphite, lonsdaleite, diamond, carbon nanotubes (CNT), fullerenes and so on [1–3], which points excellent electronic and mechanical properties, and have been playing important roles in materials science. The rich variety of carbon allotropes could be owed to the fact that the carbon atoms have unique capability to form sp-, sp²- and sp³- hybridized bonds [4] which can transmute to each other under certain pressure and temperature. It is well known that graphite can be transformed into cubic diamond under high pressure (> 15GPa) and high temperature (> 1300K) with sp²- bonds being transformed into sp³- bonds. Cold compressed graphite (at ambient temperature and pressure of 10 ~ 25GPa) can also form a

new super hard phase [5] and some new carbon structures are proposed to explain this new phase [6–15]. Besides graphite, fullerenes (C₆₀) under certain pressure can also be transformed into new carbon phases such as linear one-dimensional, two-dimensional (2D), tetragonal and trigonal C₆₀ polymers [16–18]. For the compressed carbon nanotubes (CNT), there are more exciting and intricate carbon phases due to the complex geometric configurations. Also other factors including diameter, chirality, length, wall number, and even hydrostatic or non-hydrostatic pressure, can lead to different carbon structures [19–23]. For example, single-wall carbon nanotube (SWCNT) can be transformed into a new superhard carbon phase under 24 GPa pressure, while multi-wall CNT under 11 GPa pressure partially formed superhard phase and completely become to a new phase at 16 GPa [24]. Besides the experimental achievements, there are also theoretical work focusing on the new carbon phases such as Cco-C8, Bct C4, R-carbon and P-carbon [25–27], as possible products of compressing CNT bundles.

In this paper, we systematically investigated the structure and properties of Bct C₈ by means of first principle calculations. Bct C₈

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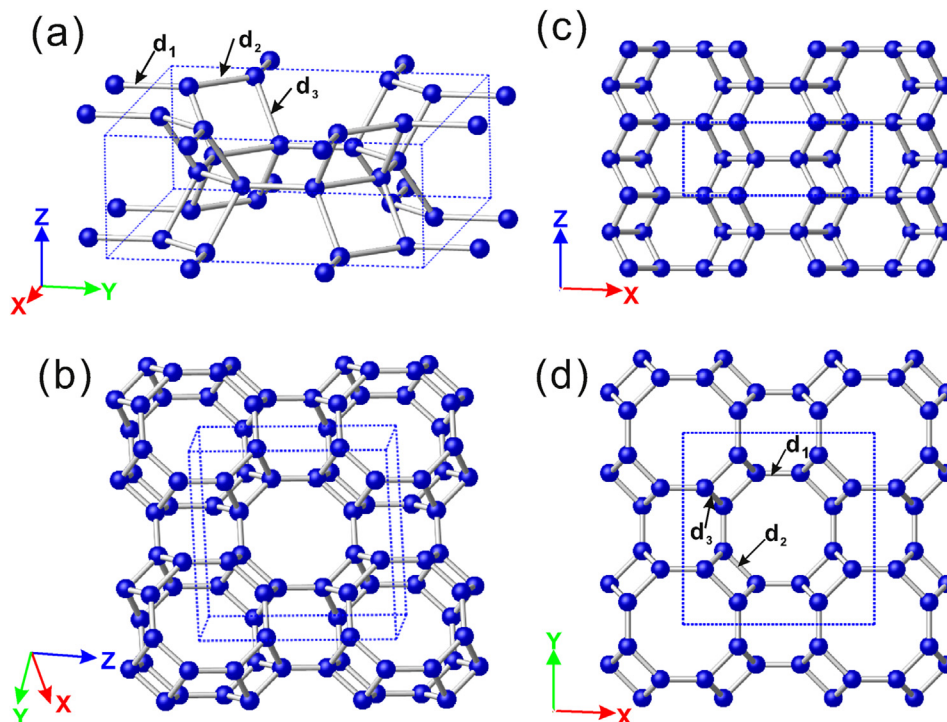


Fig. 1. Schematic drawing of the crystal structure of Bct C₈; (a) and (b) are the perspective views; (c) and (d) are the side view and the top view, respectively. The dash line indicate the unit cell. (A colour version of this figure can be viewed online.)

has a sp^3 - hybridized bonding character and body-centered tetragonal lattice structure as well as Bct C₄, but with 8 atoms in the primitive unit cell, which can be regarded as one of the possible products of compressing CNT bundles [28]. We found that Bct C₈ is thermodynamically and kinetically stable with no imaginary phonon modes and possesses a cohesive energy of -8.63 eV/atom. The electronic band structures and density of states are calculated, indicating that Bct C₈ is a semiconductor material with an indirect energy gap of about 1.66 eV, which is comparable to silicon. Semiconductor-semimetal transformation would occur when doping with B, N or B-N co-doping, which is very useful in electronic semiconductor devices. Furthermore, the Bct C₈ can be used as a lithium (Li) storage material for its special hollow configuration which can restrict the motion of absorbed Li atoms to a specific direction. The transforming pathway from CNT bundles to Bct C₈

has been simulated, and an energy barrier of 0.556 eV is found, indicating a possible approach to synthesize Bct C₈. The X-Ray diffraction and Raman spectroscopies are also provided for future experiment. Once Bct C₈ could be synthesized experimentally, it will be quite useful in carbon based electronics and energy storage devices.

2. Computational details

The structural relaxation, mechanical and electronic properties were calculated by using the Vienna *ab initio* simulation package (VASP) [30,31] with the projector augmented wave (PAW) method [32]. Both local density approximation (LDA) developed by Perdew-Zunger [33] and generalized gradient approximation (GGA) developed by Perdew-Wang-Ernzerhof [34,35] were adopted as

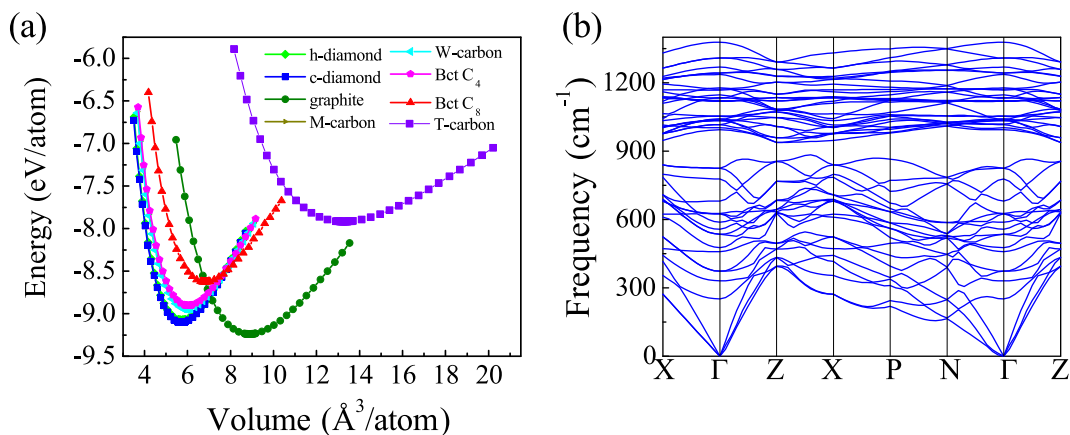


Fig. 2. (a) The total energy per carbon atom along with the changes of volume per atom for cubic diamond (c-diamond), lonsdaleite (h-diamond), graphite, M-carbon, W-carbon, Bct C₄, Bct C₈ and T-carbon, respectively; (b) The phonon spectrum of Bct C₈. (A colour version of this figure can be viewed online.)

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