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Electronic and optical properties of novel carbon allotropes

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ABSTRACT

The vibrational properties, electronic structures and optical properties of novel carbon allotropes, such as monolayer penta-graphene (PG), double-layer PG and T12-carbon, were studied by first-principles calculations. Results of phonon calculations demonstrate that these exotic carbon allotropes are dynamically stable. The bulk T12 phase is an indirect-gap semiconductor having a quasiparticle (QP) bandgap of ~5.19 eV. When the bulk material transforms to a two-dimensional (2D) phase, the monolayer and double-layer PG become quasi-direct gap semiconductors with smaller QP bandgaps of ~4.48 eV and ~3.67 eV, respectively. Furthermore, the partial charge density analysis indicates that the 2D phases retain part of the electronic characteristics of the T12 phase. The linear photon energy-dependent dielectric functions and related optical properties including refractive index, extinction coefficient, absorption spectrum, reflectivity, and energy-loss spectrum were also computed and discussed. Additionally, the chemical stability of monolayer PG and the electronic and optical properties of double-side hydrogenated monolayer PG were also investigated. The results obtained from our calculations are beneficial to practical applications of these exotic carbon allotropes in optoelectronics and electronics.
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1. Introduction

Recently, two-dimensional (2D) nanomaterials have attracted considerable experimental and theoretical interests due to the surge in graphene research [1–7] which opens an avenue for the development of 2D semiconducting materials for future multifunctional optoelectronic device applications. Many 2D materials exhibiting a variety of extraordinary properties have being explored and designed [8–14]. Because of their atomic scale thickness, the existence of quantum confinements, and other unique planar advantages, 2D materials are attractive for use in low-power, smaller, more flexible, and more efficient next-generation nanoelectronic devices, as well as for catalysis, sensing, and energy storage applications [15–20]. The unique physical and chemical properties of 2D materials are intimately related to their atomic arrangement. Most of the graphene-like 2D materials consist of hexagonal lattice and in some cases are accompanied by carbon pentagons and heptagons [1,21]. More new class of 2D materials comprised of a different topological arrangement of atoms and novel properties are desirable to provide the broadest offering available to meet virtually every application.

Following the discovery of graphene, penta-graphene (PG) [1], which is entirely composed of carbon pentagons, was predicted and reported. As depicted in Fig. 1a, monolayer PG (MPG), which consists of a packed layer of 4-coordinated C atoms (C1) sandwiched between two layers of 3-coordinated C atoms (C2), has a thickness

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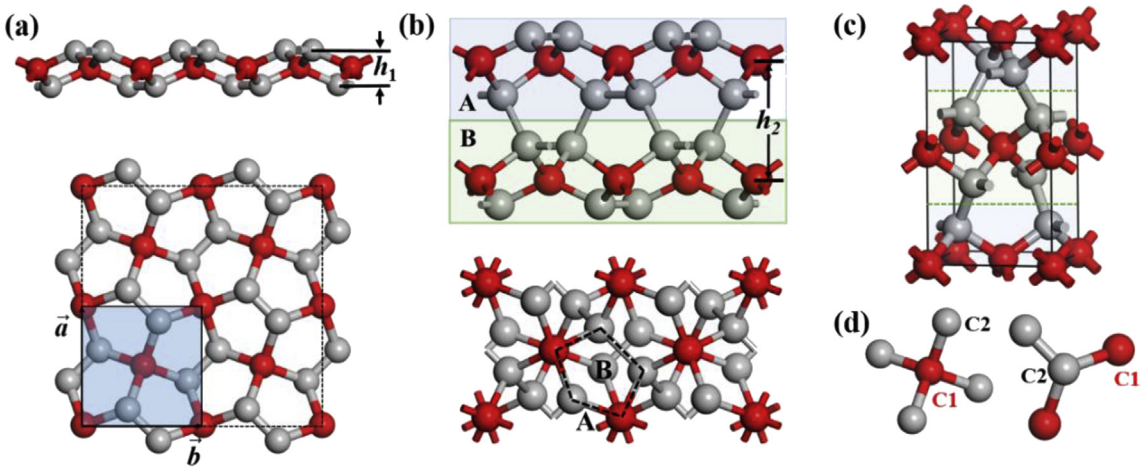

Fig. 1. Side and top views of atomic structure for (a) monolayer PG and (b) AB stacked double-layer PG. (a) shows a 2 × 2 supercell, and the primitive unit cell with lattice vectors is highlighted by a parallelogram. (b) Shows that C2 atom in layer B are located on the hollow sites of layer A. (c) The crystal structure of T12-carbon. (d) Coordination environment of C1 and C2 atoms for monolayer PG. (A color version of this figure can be viewed online.)

Table 1
Calculated lattice constants (a and c in Å), single layer thickness (h_1 in Å), layer distance (h_2 in Å) and cohesive energy per atom (E_c/N in eV/atom) for monolayer PG, AB stacked double-layer PG and T12-carbon.

Structural	a	c	h_1	h_2	E_c/N
MPG	3.644	–	1.205	–	−7.071
DPG	3.526	–	1.493	3.037	−7.354
TC	3.429	6.091	1.709	3.045	−7.734

of ~1.2 Å. *Ab initio* molecular dynamics simulations [1] indicate that hydrogen intercalation may be a viable way to selectively break the interlayer C–C bonds in T12-carbon (TC) and to chemically exfoliate a PG monolayer. Furthermore, the bulk T12-carbon may be synthesized experimentally via decompression from the appropriate high-pressure phase [22]. Meanwhile, the structural properties, and the electronic and phonon band structures of monolayer PG and T12-carbon were also reported in some literature [1,13,14,22–24]. For example, thorough and systematic theoretical calculations have been performed to confirm that the monolayer PG and T12-carbon are dynamically and mechanically stable. And the monolayer PG with a large intrinsic quasi-direct bandgap [1] of ~3.48 eV is a desirable candidate for optoelectronics and digital electronics. Equally important, physical properties such as energy gap, bulk modulus, shear modulus, and Vickers hardness of T12-carbon resemble those of diamond phases. Interestingly, the basic characteristics of monolayer PG can be tailored by stacking to form 2D materials, rolling to form 1D nanotubes, and even wrapping to form 0D C_{20} fullerenes [25]. These versatile carbon allotropes are expected to offer opportunities for broad applications in nanoelectronics and optical devices. In order to take full advantage of the properties of these novel materials for eventual technological applications, a better understanding of their electronic structure and optical properties is required.

In this work, we employ first-principles calculations to investigate the structural, electronic, and optical properties of monolayer PG, AB stacked double-layer PG (DPG) and T12-carbon. Additionally, the chemical stability of monolayer PG and the electronic, and optical properties of double-side hydrogenated monolayer PG are also discussed. The paper is organized as follows: in Section 2, the

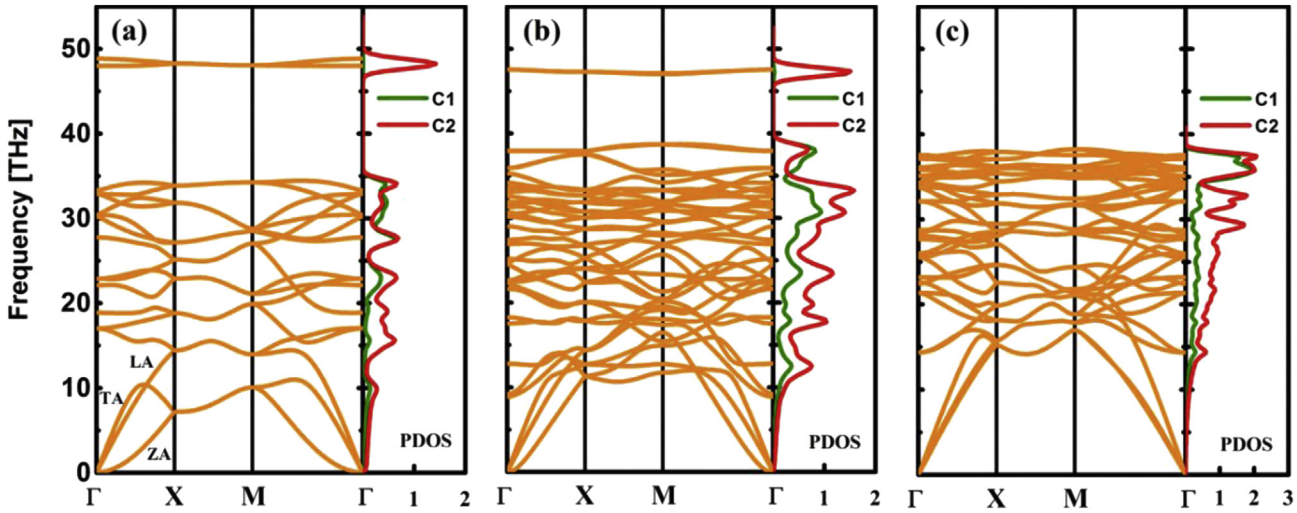

Fig. 2. *Ab initio* calculation of phonon dispersion curves along the Γ-X-M-Γ directions of the BZ and vibrational partial density of states (PDOS) for monolayer PG, AB stacked double-layer PG and T12-carbon at the equilibrium volume. (A color version of this figure can be viewed online.)

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