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Electronic properties of one-dimensional graphene quantum-dot arrays

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ABSTRACT

Using the first-principles method based on density functional theory, the electronic properties of various one-dimensional graphene quantum-dot arrays (1D GQDAs) are systematically studied. It shows that arrays present semiconducting behaviors when their edge structure is armchair-type, however, if their edge structure is zigzag-type, arrays are either metallic or semiconducting depending on the type of *edge units*: AA-type or AB-type. Punching nanoholes in quantum-dots would lead to an increase of the band gap for semiconducting arrays, but does not change a metallicity significantly for metallic arrays. Moreover, we find that the band gap of 1D semiconducting GQDAs decreases oscillatorily with size increasing, which means that the bandgap size is closely related to the quantum confinement and size effects. Our studies show that constructing various kinds of 1D GQDAs can effectively regulate the electronic behaviors of the graphene structure and obtain abundant electrical properties.

1. Introduction

Since graphene, a single-layered two-dimensional crystal composed of sp^2 hybridized carbon atoms, was successfully fabricated in experiment [1], its unique properties in mechanics, electronics, and magnetics have attracted much attention. In particular, it is predicted that it would have promising applications in nanoelectronics based on its unusual electronic properties [2–6]. Two-dimensional graphene can be tailored into other shapes as well, such as one-dimensional graphene nanoribbons (GNRs) [7], graphene quantum dots (GQDs) [8,9], and graphene quantum rings (GQRs) [10–12], by using different techniques [13]. Among them, GNRs are the most popular structure investigated, and they have two typical families: zigzag-edged GNRs (ZGNRs) and armchair-edged GNRs (AGNRs), which can be achieved by cutting a two-dimensional graphene along different crystallographic directions. Due to different edge structures, ZGNRs always present metallic behaviors while AGNRs is semiconductor [14], if they are passivated by hydrogen atoms and neglecting the spin effects of electrons simultaneously.

Seeking for high-performance graphene-based devices is a challenging work. The key technique for graphene to be applied widely to nanoelectronic devices is how to make them have a suitable bandgap, especially for developing field effect transistors (FETs). However, two-dimensional graphene is a semimetal with a zero bandgap. Therefore, lots of methods, such as edge modification [15], heteroatom doping [16], introducing mechanical deformation [17] and topologic defects [18], are used to modulate the electronic structure of graphene, especially for a bandgap opening. Recently, an interesting approach proposed to engineering bandgaps is to punch periodic nanoholes on two-dimensional graphene or GNRs [19–21], which changes the electronic structure by forming

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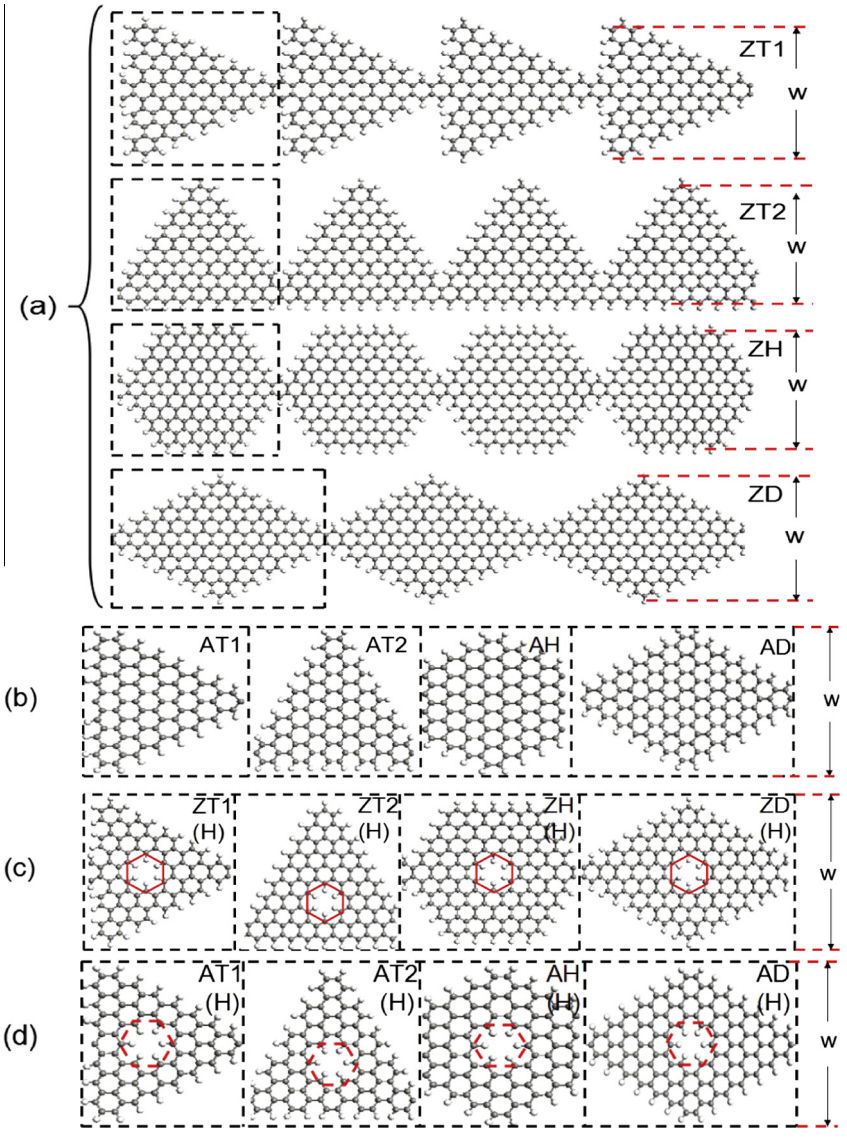

Fig. 1. One dimensional graphene quantum-dot arrays. (a) 1D QDAs derived from ZGNRs ($W = 10$), the dotted box indicates the quantum-dot (unit cell). (b) 1D QDAs derived from AGNRs ($W = 15$), (c) and (d) indicate the quantum-dots which come from punching nanoholes in the eight quantum-dots as shown in (a) and (b), and the nanoholes shape is highlighted with red lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

inner edge structures to realize the transformation of the metal or semimetal to semiconductor. These studies indicate that the bandgap size of graphene or GNRs is closely related to the density of nanoholes punched, thus it is possible to effectively control their electronic structure by adjusting the density of nanoholes. It is worth noting that to obtain the favorable electronic properties of GNRs, except for introducing the well-defined inner edges and changing their shapes properly, an alternative pathway is to alter their outer edge structures, namely, introducing edge defects artificially. Due to the effects of edge states, it might be more effectively to regulate the electronic structure of nanoribbons significantly.

In this paper, we consider a special nanostructure, one-dimensional (1D) graphene quantum-dots arrays (GQDAs), which can be viewed as a long chain through connecting graphene nanoflakes with different geometrical shapes (triangular, hexagonal, and diamond-shaped) each other in some artificial way at one infinite line, or regarded as a special derivative of GNRs by tailoring edges of GNRs and introducing larger edge defects periodically. Relative to single graphene quantum-dot, the periodic potential is introduced when graphene nanoflakes are connected regularly into 1D GQDA, its electronic properties will be changed correspondingly. The calculated results show that due to the edge structure effect, size effect, and quantum

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