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Exciton states in metallic zigzag single-walled carbon nanotubes under uniaxial strain

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ABSTRACT

The exciton energy spectrum and its binding energy under the uniaxial strain have been theoretically studied by using the tight-binding model in the metallic zigzag single-walled carbon nanotubes (SWNTs). It is found that the energy of M_{11}^{-} and M_{22}^{-} excitons and their binding energies increase with the increase of uniaxial strain, but the energy of M_{11}^{+} and M_{22}^{+} excitons and their binding energies decrease as the uniaxial strain increase. So, we can deduce that the splitting of M_{11} and M_{22} exciton will disappear as the uniaxial strain increases up to some degree, which is expected to be detected by the future experiment. On the other hand, it is interesting to calculate the exciton energy spectrum and binding energies of the bands that nearest to the Fermi level, with a narrow gap under the uniaxial strain. The obtained results show that they increase with increasing the uniaxial strain, based on which a supplemented tool is offered to detect the deformation degree of a metallic SWNT under uniaxial strain. In addition, we expect the results obtained here can offer some useful information for the future THz applications.

1. Introduction

Carbon nanotubes can be viewed as rolled up strips of graphene. The structure of a single-walled carbon nanotube (SWNT) is consequently defined by the chiral indices (n,m), which can provide much

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information on the physical properties of the SWNTs [1]. For example, the SWNTs are metallic or semiconducting when their n–m values are multiples of 3 or not [2,3], resulting in that one third of all possible carbon nanotube is metallic. Owing to their extraordinary structures, there has been much interest in their physical and chemical properties, especially their optical properties, which have been theoretically and experimentally studied by a number of groups in semiconducting CNTs by considering the exciton effects.

Excitons, which are fundamental to our understanding of optical transitions in semiconductors and insulators, are not expected to exist in the metallic systems because of strong screening by free carriers [4]. However, the situation can be very different in one-dimensional materials, especially in the single-walled carbon nanotubes (SWNTs) where the effectiveness of screening is significantly reduced. What's more, the possibility of forming bound excitons in the metallic SWNTs was recently predicted [5–8], and then the experiments have proved that the optical transitions in the SWNTs are dominated by the excitons and its binding energies can be as large as 50 meV [9–11], which agrees well with the theoretical predictions. However, due to the trigonal warping effect, the calculated excitonic Rayleigh scattering spectra [8] and linear optical spectra [12] are split into two corresponding ones, coming from two split excitons. In addition, the splitting depends on both the chirality and the transition energy.

On the other hand, it is unavoidable that the SWNTs may cause various mechanical deformations in the experiments, which can change their electronic structures and corresponding transport and optical properties [13–19]. For example, a metal-semiconductor transition of the SWNTs could be induced by the deformation, or the energy level degeneracy may be destroyed by the symmetry breaking induced by the deformations. The different mechanical deformations in the carbon nanotubes mainly include torsion, uniaxial strain and bending, among which the uniaxial strain is the most popular one. According to the previous calculations in Ref. [19], the influence on the electronic structure induced by the uniaxial strain is the largest for the zigzag tubes. More important is that the metallic zigzag SWNTs will open a gap by applying the uniaxial strain, which are often called the narrow-gap carbon nanotubes. With the development of using this type carbon nanotube for THz applications, the analysis of the long-wavelength properties of narrow-band nanotubes is becoming very interesting. Theoretically, the stability of excitons in metallic carbon nanotubes subjected to Aharonov–Bohm magnetic flux was considered in Ref. [20] and the exciton binding energy of narrow-gap was discussed in Ref. [21], the main conclusions of which are that the binding energy scales with the band gap.

However, up to now, there is no theoretical study to calculate the exciton energy spectrum and its binding energy for the metallic zigzag carbon nanotubes under the uniaxial strain by taking into account the exciton effects. So, it is very interesting to know the influence of uniaxial strain on the exciton states in the metallic zigzag carbon nanotubes. In this paper, we have studied the excitons of three nearest bands to the Fermi lever in the metallic zigzag carbon nanotubes, from which we can find that both of the energy of M_{11}^{+} and M_{22}^{+} excitons decrease with increasing the uniaxial strain, while the energy of M_{11}^{-} and M_{22}^{-} excitons increase with increasing the uniaxial strain, displaying two different variations. Furthermore, their corresponding binding energy shows the same variation trend, which are expected to be detected by the future experiment.

The paper is organized as follows. In Section 2, the model and method used to study the excitons in metallic SWNTs are introduced. The obtained results and discussions are given in Section 3. And the conclusions are presented in Section 4.

2. Physical model and formulation

The Hamiltonian of metallic SWNTs under uniaxial strain is written as:

$$H = H_0 + H_{e-e} \tag{1}$$

where the first term represents the simple tight-binding model Hamiltonian, given in the following

$$H_0 = \sum_{\langle i,j\rangle,s} t_{ij} C_{i,s}^{\dagger} C_{j,s} + H.c. \tag{2}$$