Quantum Confinement Effect in Armchair Graphene Nanoribbons: Effect of Strain on Band Gap Modulation Studied Using First-principles Calculations

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Tsan-Chuen Leung

National Chung Cheng University

The quantum confinement effect may play an important role in the gap modulation of armchair graphene nanoribbons (AGNRs) under strain. Using the phase accumulation model, the speaker and his research group have investigated the energy dependent phase shift $\phi(\varepsilon)$ at the point of AGNRs under various strains using first-principles calculation. The calculation results show that although the energy dispersion of the phase shift is modified by strain, the phase shift near the Fermi level is close to 0.75π, indicating that strain has little effect near that energy level. The speaker and his research group can approximate the energy-dependent phase shift by a constant, $\phi(\varepsilon) = 0.75\pi$, for AGNRs under various x strains. Due to the structural similarity between AGNRs and zigzag carbon nanotubes (ZCNTs), the electronic properties of AGNRs should be similar to those of ZCNTs. The quantization condition of the wave vector of ZCNTs governed by the periodic boundary condition along the circumference direction is similar to that of AGNRs except that the phase shift is equal to zero, $\phi(\varepsilon) = 0$. Using the zone-folding (ZF) method, the speaker and his research group can calculate the band gap of any strained AGNR (ZCNT) from the phase shift $\phi = 0.75\pi$ ($\phi= 0$) and the electronic structure of the strained graphene. The AGNR shows a zigzag behavior of the dependence of the band gap on strain which is very similar to the ZCNT. The zigzag patterns are significantly shifted by different phase shifts. The peak value of the band gap and the period of the pattern decrease as the width of the ribbon increases. For a given AGNR, the peak value and the period of the pattern increase as the strain increases. A flattening of the peaks appears at the strain where the maximum band gap occurs due to large compressive strain. All these observations can be understood easily from the speaker and his research group's ZF calculations. The agreement between the speaker and his research group's model and real local-density approximation calculations indicates that the speaker and his research group's model can provide an efficient and accurate method to estimate the band gap of AGNRs and ZCNTs under strain, and therefore can provide a better understanding of the effect of quantum confinement on the electronic properties of AGNRs.