First-principles calculations of electrical conductivities in edge-modified graphene nanoribbons

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Abstract

We chose pristine armchair graphene nanoribbons with 7 zigzag edges (7aGNRsH), boron doped armchair graphene nanoribbons with 7 zigzag edges (7aGNRsH-B) and armchair graphene nanoribbons with 7 zigzag edges that has one carbon atom vacancy (7aGNRsH-V). We investigate the influence of strain on the electrical properties of graphene nanoribbons that have potential applications in making sensors and other optoelectronic devices. Based on first-principles calculations, results show that pristine unstrained 7aGNRsH is electrically inactive but turns to be electrically active in a wide range of energy spectrum, e.g., from IR to visible to UV, due to the application of strain engineering. In metallic unstrained and strained 7aGNRsH-B and 7aGNRsHV, non-vanishing electrical conductivity in the IR, visible and UV energy spectrum regimes are observed. We also investigate the influence of strain on the Berry curvature of 7aGNRsH, 7aGNRsH-B and 7aGNRsH-V nanoribbons. The results show that fermions are spread through out the Brillion zone in the reciprocal space for semiconducting unstrained 7aGNRsH but localized near the Γpoint for strained 7aGNRsH that has out-of-plane deformations due to strain engineering. For metallics 7aGNRsH-B and 7aGNRsH-V, Berry curvature plots show that fermions are localized far away from the Γ-point. In two atom boron doped p-type armchair graphene nanoribbons with 7 zigzag edges (7aGNRsH-2B), large peaks in electrical conductivity at IR energy spectrum regimes can be observed. These peaks of electrical conductivities in 7aGNRSH-2B may be detectable in experimentally synthesized structure in Reference, JACS 137, 8872 (2016).