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Talk Invited Invited Talk

Strain Tunable Band Gaps of Carbon Nanotubes

G. Dereli*

Department of Physics, Yildiz Technical University, Istanbul, Turkey
* Electronic Address: gdereli@yildiz.edu.tr

The electronic energy band gap is a basic property of all semiconductors since it is responsible for the electrical transport and optical properties. Control of the size of the electronic energy band gap is important in optimizing the electronic devices. Single-walled Carbon Nanotubes (SWCNTs) represent a new class of electronic materials where the electronic properties depend upon their size and symmetry. In this talk, I will show that the mechanical deformations such as the application of tensile strain can induce changes in the density of states, modifying the size of the energy band gaps of SWCNTs. Energetics of SWCNTs are obtained using a parallel, Order N, Tight Binding Molecular Dynamic (O(N) TBMD) simulation code designed by Dereli et. al [1, 2, 3]. This code is used in SWCNTs simulations successfully and the details of the technique and the references can be followed in [4, 5, 6]. O(N) TBMD calculates the band structure energy in real space and makes the approximation that only the local environment contributes to the bonding, and hence the band energy of each atom. In this case, the run time would be linearly scaled with respect to the number of atoms [7, 8, 9, 10] . We simulated various semiconducting SWCNTs under compressive and tensile strain values. The zigzag (n,0) SWCNTs are generally semiconducting and they are quasi-metallic only when n is a multiple of 3. Applications of positive and negative strains open up the band gap causing metal - semiconductor transitions in quasi-metallic zigzag SWCNTs. On the other hand, our studies show that for the (n,0) semiconducting nanotubes, this behavior is strongly dependent on whether n mod3 is equal to 1 or 2. In semiconducting (n,0) nanotubes when n mod3 is equal to 1, compressive strain closes the band gap whereas the tensile strain opens it up. For the n mod3 equals to 2 type nanotubes, band gap closes for tensile strain and opens up for compressive strain. These results are extremely important for CNT-based electronics since one gains a mechanical control of conductance.

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