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Spin polarized conductance due to arrays of defects in carbon nanoribbons for electronic applications

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Abstract –The utilization of graphene nanoribbons for next generation nanoelectronics is commonly expected to depend on controlled synthesis that yields a low density of defects. We present a class of intramolecular graphene heterojunctions and show how certain defects can be used to enhance the electronic and magnetic properties of graphene nanoribbons. The hybrid graphene nanoribbons have both armchair and zigzag features which are separated by an interface made up of alternating pentagonal and heptagonal carbon rings. Our calculations indicate that depending on the transport direction and the width of the hybrid nanoribbons, these systems can exhibit spin polarized or tunnelling driven conductance.

Here, we present results obtained for nanoribbon junctions that are based on an ordered array of structural defects. Such arrays of defects have been observed experimentally, and could be visualized as grain boundaries in a graphene or graphite crystal [1]. In particular, an array of pentagons and heptagons can be used to join an armchair and a zigzag nanoribbon. Andriotis and Menon have used a similar approach to construct T-junctions with all zigzag or armchair edges, and compute junction transport properties as a function of the size of the branches [2,3]. In this work, we present a complete study on the electronic and magnetic properties of 2D hybrid armchair-zigzag graphene and 1D hybrid armchair-zigzag graphene nanoribbon systems using Density Functional Theory (DFT), as well as the electron transport for the 1D structures. We find that 2D hybrid graphene sheets have states at the Fermi level, and that hybrid nanoribbons exhibit spin polarized transport as well as unusual magnetic properties that depend on the width of the zigzag section.

Electronic and magnetic properties of hybrid graphene systems consisting of armchair-like and zigzag-like segments joined by a grain boundary formed by a linear array of 5-7-rings were fully examined using DFT calculations. The results showed that these systems exhibit electronic and magnetic properties not observed in graphene. Two dimensional hybrid systems exhibit electronic states at the Fermi level, while one dimensional hybrid nanoribbons can exhibit half metallicity without the use of an external field. Transport calculations reveal that these systems could behave as spin polarized conductors when current is applied along the HNR axis, or could exhibit tunneling driven conduction if current is applied perpendicular to the HNR axis. The grain boundaries of these systems have been found experimentally and a study of their properties is therefore important. In summary, an array of structural defects could be used in favor, and the properties of such systems could find use in electronic devices.

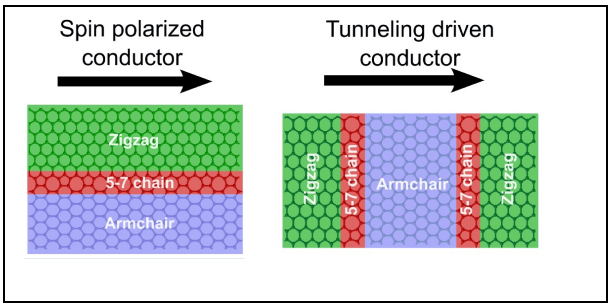

Figure 1: Schematic figure of the hybrid nanoribbons and their transport properties.

References

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