ABSTRACT

THESIS: Electronic Properties of Functionalized GNRs with Extended Hückel Theory

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Electronic properties of graphene nanoribbons (GNRs) were investigated. Graphene nanoribbons are one-atom layer thin sheets of carbons arranged in a pattern of repeating hexagons that have a semi-infinite length and finite width. GNRs have important electronic properties, and are very useful materials in nanoelectronics and nanodevices. GNRs are either metallic or semiconducting, depending on the width of the structure and the edge structure. There are two different edge structures: armchair and zigzag. The electronic properties of these materials can be altered by functionalizing the structures. In this project, the edges of armchair graphene nanoribbons (AGNRs) were functionalized by H, N, O, F, P, S, and Cl to tune and engineer the bandgap for the application of electronic devices. A theoretical analysis via the usage of Tight-Binding Model (TB Model) with Extended Hückel Theory (EHT) and Green's Function Theory were used to calculate the electronic band structure, density of states (DOS), conductance, and local density of states (LDOS). The functionalized results are compared to the results of the perfect structure. The presence of foreign elements on the edges of graphene nanoribbons has a significant effect on the electronic properties and quantum transport.