

Abstract Submitted  
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**First principles study of graphene nanoribbons and nanorectangles** PHILIP SHEMELLA, LI CHEN, YU ZHOU, YIMING ZHANG, SREEKALA SUBBULAKSHMI, PULICKEL AJAYAN, SAROJ NAYAK, Rensselaer Polytechnic Institute — We have studied the finite size effect on the electronic structure of graphene nanoribbons (GNRs) using first principles density functional techniques. In particular, we have computed the energy gap dependence on the width and length for zero-dimensional nanorectangles for both the armchair and zigzag ribbons; and compared to the one-dimensional (infinite length) cases. One-dimensional armchair ribbons are expected to be metallic if the number of carbon atoms across the ribbon is  $N = 3M-1$ , and non-metallic  $N \neq 3M-1$ , where  $M$  is an integer. In addition to quantum confinement along the width of the ribbon for metallic widths, an additional finite size effect emerges along the length of ribbons only for non-metallic armchair ribbons. The origin of additional quantum confinement in these structures is explained based on the energy states near the Fermi energy. The differences between zero- and one-dimensional electronic structure properties are considered with the addition of passivating groups and their effect on the electronic properties of graphenes and their impact on nanoelectronics devices are discussed.

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