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Electronic Properties of Graphene Nanoribbons Using Extended Hückel Theory SPENCER JONES, MAHFUZA KHATUN, Ball State University — We will present results of electronic properties of armchair and zigzag graphene nanoribbons (GNRs) calculated with extended Hückel (EHT) theory. Energy band structures and density of states (DOS) are calculated using a tight-binding TB model, and Green's function method and the Landauer formula have been implemented determining the transmission function, conductance, and local density of states (LDOS). We have investigated the effects of edge states of the ribbons where edge atoms are terminated with hydrogen atom. Results of without- and with- edge terminated structures have been studied near the Fermi level. The interesting observation is the effect of the dangling bonds at the edges. The EHT technique not only includes the Pz orbital interactions but also the other three S, Px, and Py orbital interactions We observe that there is no fundamental difference in the electronic properties near the Fermi energy for the edge terminated GNRs. The only difference between the two methods is in the conduction and valence band regions away from the Fermi level. We expect the characteristics of electronic properties will be different if the edges are terminated with heavy element (s).

Mahfuza Khatun
Ball State University

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