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The Electronic Properties of Hexagonal Boron Nitride and Graphene Nanoribbons ALBERT DIBENEDETTO, MAHFUZA KHATUN[1], ANTONIO CANCIO, Ball State University — Energy storage and device fabrication is an area of condensed matter physics that's widely studied by utilizing extremely tiny, two-dimensional nanostructures like hexagonal boron nitride nanoribbons (BNNRs) and graphene nanoribbons (GNRs). We are investigating the electronic properties of both materials. Results of band structure, density of states (DOS), and conductance of both materials will be presented. In addition, effects of impurities that alter their electronic behavior will be discussed. The BNNRs are insulating and on the other hand, GNRs are either metallic or semiconducting. Theories include a Tight-Binding (TB) model with Huckel theory, equilibrium Green's function method, Landauer formalism, and Density Functional Theory (DFT). The TB model is used to calculate the band structures and DOS, and the Green's function theory and Landauer formula are used to obtain the transmission function and the conductance. ABINIT computational software implements DFT to calculate the band structure of boron nitride and VMD software is used to visualize the electron density. The results of DFT will be compared with the TB model.

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