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Calculated Magnetic Properties of Zigzag Boron Nitride Nanoribbon¹ J. RUFINUS, Science Division, Widener University — Substantial theoretical and experimental efforts have been made in the quest to find the candidates for future spintronics devices. Recently, the search for new spintronics materials has also included two-dimensional graphene-based materials due to the theoretical prediction that this type of material may show the half-metallic property. We present the results of an ab-initio density functional theory within a generalized gradient approximation study of zigzag Boron Nitride Nanoribbon (ZBNNR). Our results show different magnetic orderings. However, we found that, in general, narrow zigzag BN nanoribbon prefers a magnetic state depending on the shape and thus the orientation of the atoms on its edges. These results are especially noticeable for very narrow ZBNNR.

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