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Induction of Magnetization in Zig-Zag Graphene Nanoribbons by Bending NABIL AL-AQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha — We study the induced magnetization in the zig-zag terminated graphene nanoribbon (ZGNR) by applying strain gradient. In-plane sinusoidal gradient is shown to produce measurable magnetization localized around the location with the largest strain gradient. We discuss it from the point of view of flexomagnetic effect. By symmetry, the magnetization induction is forbidden in infinite system. However, it appears in the finite system due to the removal of the time-reversal symmetry. We performed ab initio Density Functional Theory (DFT) calculations for 4-ZGNR and show that local magnetic moments are decreased at the edges with inward curvature and increase at the edges with outward curvature. Due to antiferromagnetic arrangement of magnetization of two edges a net magnetization is induced by strain. We estimate an average magnetization of ~ 3.3 μB that produced from the bending of nanoribbon with the sinusoidal profile δx=Asin(2πz/L) with A= 3Å and L=87.4 Å (z=0..L/2, i.e. the half of the period). The appearance of net local magnetization is due to asymmetry of magnetic moments induced at two edges when nanoribbon is subjected to non-uniform deformation, i.e. the presence of the strain gradient. The magnetic moments vary as function of local curvature due to the charge redistribution on the curved edges.

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