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Inducing Magnetization by Flexing Graphene Nanoribbon RENAT SABIRIANOV, NABIL AL-AQTASH, University of Nebraska at Omaha — Zigzag graphene nanoribbons (ZGNRs) are antiferromagnetic in the ground state with zero net magnetization due to the compensation of contributions from opposite edges. The uniform deformations (both shear and axial) do not produce magnetization due to the symmetry restrictions. However, we report the results of first-principles calculations that predict that the induction of net magnetization in the graphene nanoribbon upon non-uniform strain applied to the nanoribbon. Using density functional theory (DFT) method implemented in SIESTA code, we show that the bending or twisting of nanoribbon produces magnetization because in the presence of strain gradient the induced magnetization on opposite edges are not compensating each other. We estimate an average magnetization of $\sim 3.3\mu_B$ 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). Our study suggests that the induced magnetization can be used for the control of magnetic structure in graphene including the trap of the domain walls.

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