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An Effective Tensional Strain View on the Bandgap Tunability of Helical Graphene Nanoribbons with Open and Closed Edges DONG-BO ZHANG, TRAIAN DUMITRICA, University of Minnesota — Despite the scientific importance of graphene nanoribbons, little is known about their electronic structure other than in the flat-form presupposition. To quantify the strain stored in helical graphene nanoribbons and fractional carbon nanotubes, we supplement the standard elasticity concepts with an effective tensional strain. Using π-orbital tight binding and objective molecular dynamics coupled with density functional theory, we develop a unified theory for the electromechanical response in which the consequences of the torsional deformation are taken into account via the effective tensional strain. In spite of the open and closed edges as well as the inverse Poynting effect exhibited by these nanostructures, from the effective strain perspective the twist-induced bandgap modulations appear strikingly similar with those exhibited by carbon nanotubes in tension. Our theory may be useful for designing new electromechanical devices and experiments using carbon nanocomponents, and for establishing edge-chemistry driven nanofabrication principles for helical graphene nanoribbons with tunable bandgaps.

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