Structural and Electronic Properties of Rippled Graphene with Different Orientations of Stone–Wales Defects: First-Principles Study

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In this work, we used density functional theory to investigate the structural and electronic properties of rippled pristine graphene and graphene with two orientations of Stone–Wales defects. The formation of periodic ripples was induced by applying uni-axial strain on graphene sheets. The creation of pentagonal and heptagonal rings in the graphitic backbone has resulted in a dramatic modification on electronic properties at the atomic level as a consequence of modifying bond lengths. Moreover, ripples start to show up in graphene with different types of Stone.Wales defects when the strain exceeds 4%. Equally important, the strain may be used to tune the graphene wrinkling as well as graphene electronic properties. Besides, ripples induced by mechanical strain have a great impact on the electronic properties of pristine graphene and graphene with different orientations of Stone.Wales defects. This novel observation might be used to control not only graphene.s electronic properties but also graphene structural functionality.

Keywords: graphene, Stone–Wales defects, uni-axial strain, rippling, electronic properties, density functional theory.

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