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Peierls Instability and Spin Ordering in Graphene

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Peierls instability and spin ordering of zigzag graphene nanoribbons (GNR) created on a fully hydrogenated graphene (graphane) are investigated as a function of their width using first-principles density-functional calculations within the generalized-gradient approximation. For the width containing a single zigzag C chain (N=1), we find the presence of a Peierls instability with a bond alternated structure. However, for width greater than N=1, the Peierls distortion is weakened or disappears because of the incommensurate feature of Fermi surface nesting due to the interaction of C chains. Instead, there exists the antiferromagnetic (AFM) spin ordering in which the edge states are ferromagnetically ordered but the two ferromagnetic (FM) edges are antiferromagnetically coupled with each other, showing that electron-lattice coupling and spin ordering in GNR are delicately competing at an extremely thin width of N=2. It is found that, as the width of GNR increases, the energy gain arising from spin ordering is enhanced, but the energy difference between the AFM and FM (where two edge states are ferromagnetically coupled with each other) orderings decreases.

Keywords: graphene, grapane, zigzag nanoribbon, Peierls instability, antiferromagnetism