عنوان مقاله:

Formulation of atomic positions and carbon–carbon bond length in armchair graphene nanoribbons: an ab initio study

محل انتشار:

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خلاصه مقاله:

In this paper, we investigate the atomic positionsof single layer armchair graphene nanoribbon for twocases, with and without hydrogen-passivate edges, accuratelyand propose a formula which either removes theneed of structural relaxation generally or decreases its timeextremely (up to seven times). We also propose a generalpattern (hyperbolic) for these positions. On the other hand,we show that edge effect influences several atoms near theedge not just one. These results can be used in software,which compute atomic positions and can increase theirefficiency. In addition, we prove that the C–C bond distancedepends on dimer number and differs in length andwidth directions, especially for narrow AGNRs. Themaximum value of these differences is about 0.017 Å.

کلمات کلیدی:

Armchair graphene nanoribbon (AGNR) Structural relaxation Atomic position Dimer C–C bond length