Carbon allotropes named \( \alpha \)-graphynes (\( \alpha \)Gy), with \( sp^2 \) and \( sp^3 \) bonded carbon atoms (Fig. 1), have been shown to display graphene-like electronic structures with the characteristic Dirac cones. Here, we discuss the lattice stability and gap opening in hydrogenated and oxidized forms of \( \alpha \)-graphynes, and show that in both cases, the planar form is unstable against soft-phonon modes with off-plane displacements of hydrogen (oxygen) and carbon atoms. Two mechanisms of mass generation in the Dirac fermion spectrum of \( \alpha \)-graphynes are discussed: symmetry breaking and \( sp^2 - sp^3 \) rehybridization.

We also consider the stability and electronic properties of topological line defects in boron nitride (Fig. 2) and graphene. Recent experimental work has revealed the occurrence of line defects in graphene with zigzag chirality and a core structure consisting of topological defects in the form of pentagons and octagons. Moreover, finite segments of an armchair oriented defect, with squares and octagons in its core, have also been produced by electronic irradiation in graphene. Here, we compare the relative stability and the electronic properties of the zigzag and armchair line defects, in graphene and boron nitride, with an emphasis on the issue of stability versus stoichiometry of the defects in boron nitride. Stoichiometry of the defect-core periodic unit is shown to be crucial in order to determine the stability and electronic structure of the defects [1].

Furthermore, the most basic topological defect in graphene layers is the so-called Stone-Wales defect (SW), which results from a 90-degree rotation of a carbon-carbon bond, commonly referred to as a Stone-Wales transformation (SWT). We consider the effects of functional groups in lubricating the SWT in graphene and show that two hydrogen atoms in next-nearest neighbor positions in graphene lead to a strong reduction of the SWT, from 9.3 eV in the pristine case to 3.9 eV [2].

References


Fig. 2