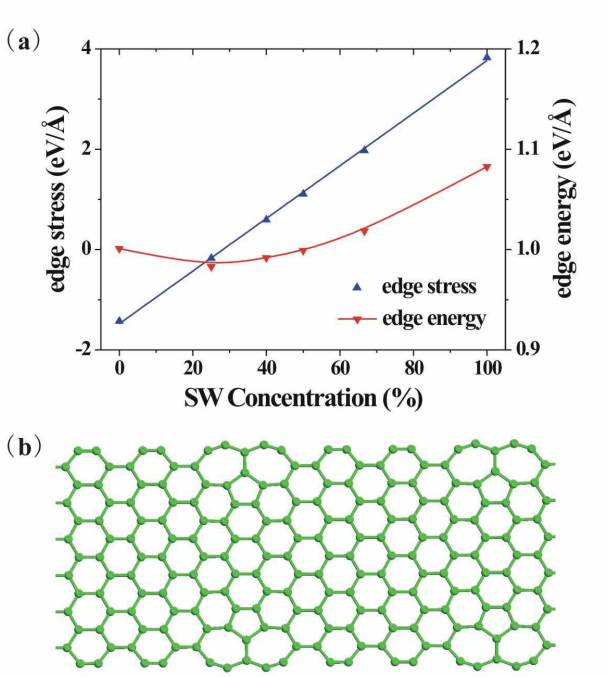

FIG. 4: (a) The armchair edge stresses (with linear fit) and edge energies of graphene nanoribbons as a function of edge SW defect concentration. (b) The optimaized ribbon structure at the 50% SW defect concentration.

armchair edge is much larger than that of zigzag edge, as shown in Figs. 3b. Third, the mechanical undulation of zigzag edges induced by compressive edge stress is comparable to thermal fluctuations[3, 4], as shown in Fig. 3b, and hence the two are difficult to distinguish. We also note that in addition to the continuum analysis we perform here, the accurate first-principles values of τ_e and E_e can be used as input parameters for the finite element simulations of large graphene systems[10].

Because the compressive edge stress is partly originated from the dangling bond, naturally, we may saturate the dangling bonds to relieve the compressive stress. We have tested this idea by saturating the edge with H that indeed confirmed our physical intuition. For armchair edge in a 1-nm wide ribbon, we found H saturation changes the edge stress from -1.42 eV/Å to -0.35 eV/Å; for zigzag edge in a 2.0-nm wide ribbon, it changes the edge stress from -0.42 eV/Å to +0.13 eV/Å. Therefore, the H edge saturation, or saturation by other molecules in general, is expected to relieve the edge compression. Especially, it can reverse the compressive stress in a zigzag edge to tensile.

Surface reconstruction has long been known as an effective mechanism in relieving surface