Edge states and flat bands in graphene nanoribbons with arbitrary geometries

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Graphene nanoribbons (GNR), stripes of nanometric widths cut from graphene, are the subject of a growing interest. They exhibit edge-localized states, which may play an important role in transport and magnetic properties. For instance, the magnetic properties of nanoribbons are directly related to the existence of localized edge states [1]. All these edge terminations have been experimentally identified by different techniques, such as scanning tunneling microscopy [2,3], high-resolution transmission electron microscopy [4], or atom-by-atom spectroscopy [5]. It is thus important to identify general edges and nanoribbons that present localized edge states, as well as their degeneracy and characteristics.

We prescribe general rules to predict the existence of edge states and zero-energy flat bands in graphene nanoribbons and graphene edges of arbitrary shape [6]. No calculations are needed. For the so-called minimal edges, the projection of the edge translation vector into the zigzag direction of graphene uniquely determines the edge bands. By adding nodes to minimal edges, arbitrarily modified edges can be obtained (Fig. 1); their corresponding edge bands can be found by applying hybridization rules of the extra states with those belonging to the original edge. Our prescription correctly predicts the localization and degeneracy of the zero-energy bands at one of the graphene sublattices, confirmed by tight-binding and first-principles calculations (Fig. 2). It also allows us to qualitatively predict the existence of E = 0 bands appearing in the energy gap of certain edges and nanoribbons.

References

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Figures

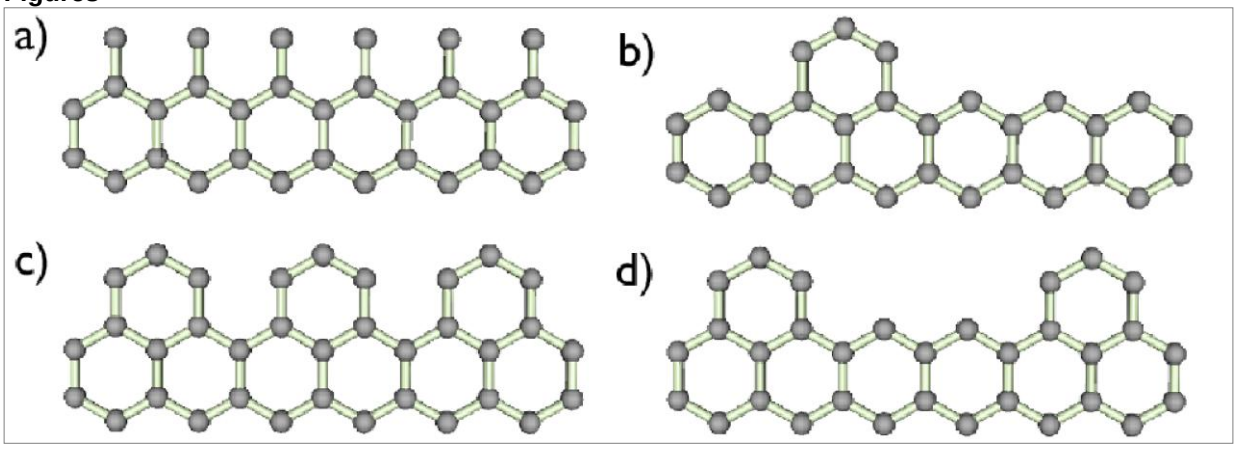

FIG. 1: Geometries of several modified zigzag graphene edges: (a) Bearded zigzag edge, composed of Klein defects; (b) a cape structure on a zigzag edge, obtained by bonding one extra atom to two adjacent Klein defects; (c) a cove edge; and (d) a periodic modified edge with a cape.

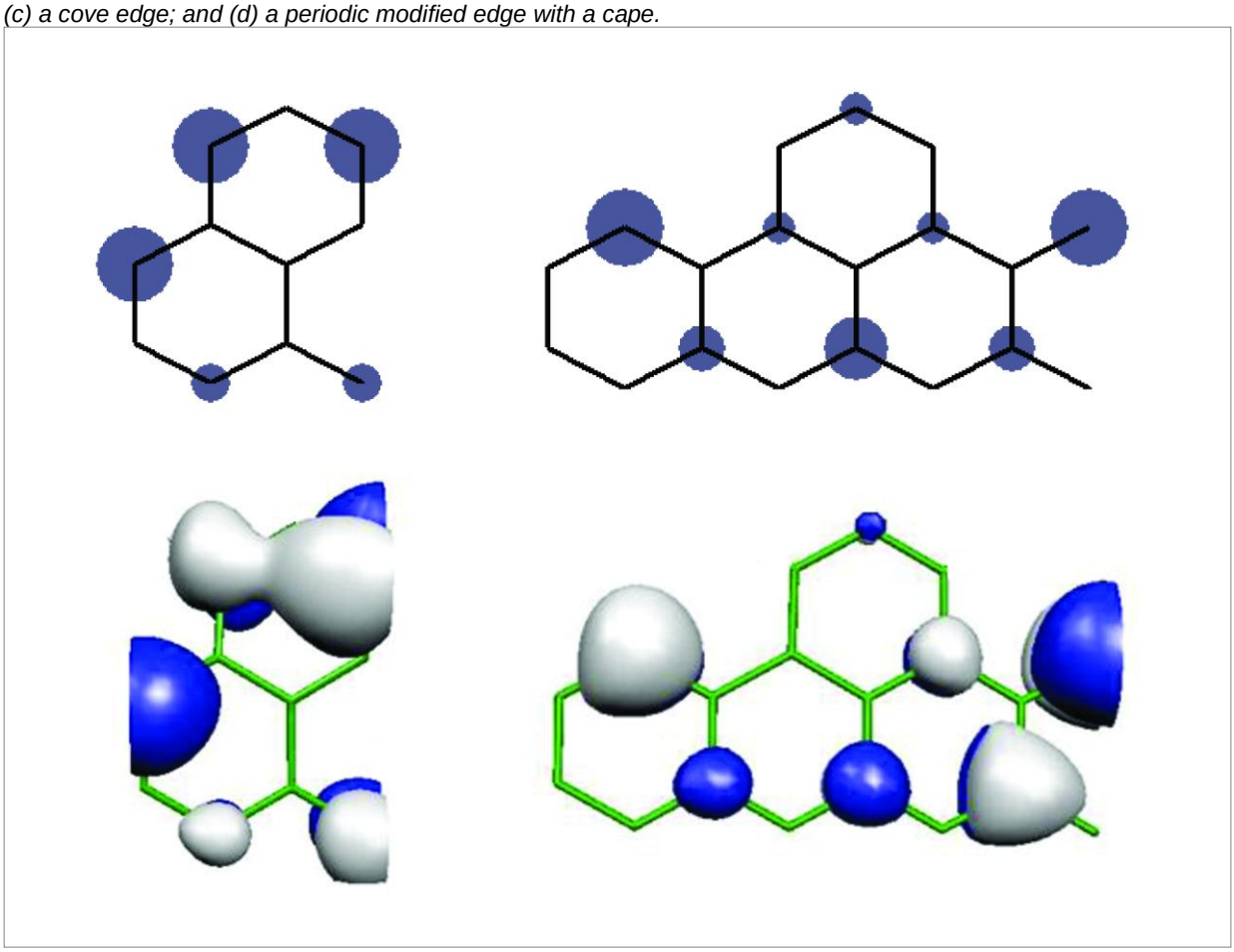

FIG. 2: (Color online) Localization of the wave functions corresponding to the E = 0 band at k = π for 40(2,0) (left) and 40(4,0) (right) GNR with a cape structure at the edges. The corresponding edges are shown in Figs. 5(c) and 5(d), respectively. Only an edge and a few neighboring nodes in the GNRs unit cells are shown. Upper panel: Results obtained using tight-binding method. Bottom panel: Results of first-principles calculations. The dot diameter in the upper panel reflects the TB density at the nodes. No dot means that the wave function is exactly zero at this node.