Electronic and magnetic properties of triangular graphene quantum rings

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The graphene nanostructures allow the control of bandgaps and magnetic properties with size and shape[1-3]. In particular, the existence of a band of degenerate states near Fermi level of zigzag ribbons[4, 5] and triangular dots[6-8] was predicted by tight-binding model and confirmed by density functional theory calculations. In this work, electronic and magnetic properties of triangular graphene rings potentially fabricated using carbon nanotubes as masks (Fig. 1) are described as a function of their size and width. We show that many of the properties of triangular graphene quantum dots survive [7,8] and that new properties related to ring formation appear. The electronic properties of the charge neutral system are calculated using tight-binding method and interactions are treated using the mean-field Hubbard model. We show that for triangular quantum dots with a triangular hole, the magnetic properties are determined by the width of the ring, leading to ferromagnetic corners and antiferromagnetic sides. The electronic properties of graphene quantum dots as a function of additional number of electrons or holes are described by a combination of tight-binding, Hartree-Fock, and configuration interaction methods. The ground state of the outer edge is found to be maximally spin polarized for almost all filling factors. The evolution of the excitation gaps as a function of shell filling shows oscillations as a result of electronic correlations.

References

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Figure 1

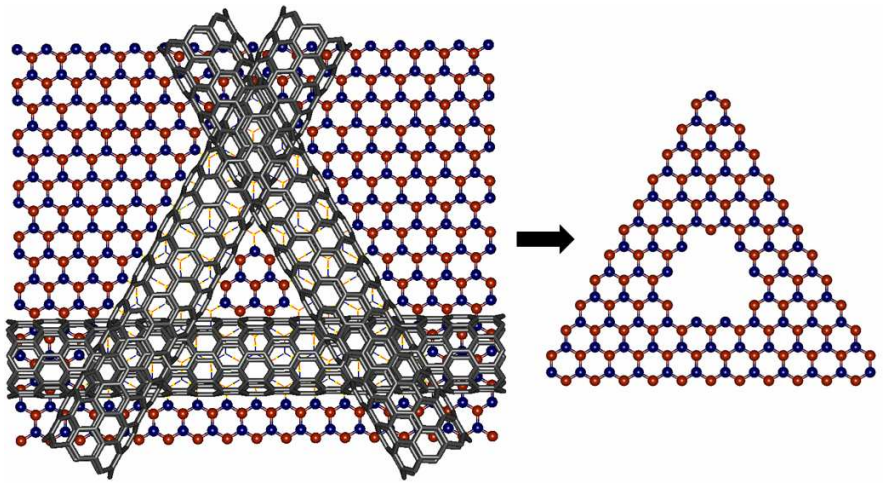

Figure 1: Experimental method for designing a TGQR. Three CNTs arranged in equilateral triangle along zigzag edges play the role of a mask. By using etching methods one can obtain TGQR with well defined edges. The circumference of CNT determines the width of TGQR. Red and blue colors distinguish between two sublattices in the honeycomb graphene lattice.