Electronic and magnetic properties of zigzag edged triangular graphene flakes

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The graphene flakes we consider have equilateral triangular shapes with zigzag edges (n-TGF), where n denotes the number of edge hexagonal cells in one side of the triangle. Termination of these n-TGF structures with several elements (of the first two rows of the periodic table) and application of electric field to these flakes alter their electronic and magnetic properties.

In accordance with previous studies [1,2], we find that bare flakes have large spin magnetic moment values of 4(n-1) μB, whereas they reduce to (n-1) μB for full saturation of edges with Hydrogen, Lithium, Beryllium or Flour atoms. Moreover we have studied possible termination of other elements like Boron, Carbon and Nitrogen. Hydrogen and Flour atoms prefer to bind at the top of an edge Carbon atom. Unlike Hydrogen and Flour termination, the other atoms prefer to bind at the bridge sites.

Recent studies [3,4] show that the magnetic moments of triangular graphene flakes can be controlled by applied electric field. We show that the value of total spin polarization of triangular graphene flakes can be changed by tuning an applied in-plane external field. We demonstrate that, in these flakes total spin polarization can be reduced stepwise with the applied field. The electric field control of ferromagnetism in TGFs promises a new route for spintronic applications.

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