Abstract Submitted
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First-Principles Study of Graphene Channel on Graphite Monofluoride[1] NING SHEN, JORGE SOFO, Pennsylvania State University, Physics Department — We propose the formation of graphene regions in a matrix of graphene monofluoride as a method to confine the charge carriers in graphene. Graphene is an excellent conductor and graphene monofluoride is a wide band gap semiconductor. Removing fluorine from graphene monofluoride creates regions of graphene where the charge carriers are confined by the band gap of the fluorinated parts. In particular, we study the electronic structure of graphene stripes drawn on monofluoride. On the basis of first-principles calculations, we show that the monofluoride regions preserve its property as good insulator while the graphene channel exhibits interesting electronic and magnetic properties. We study two high symmetry orientations, armchair and zig-zag. The armchair orientation is found to have a non-magnetic ground state with a band gap dependent on the width of the graphene channel. The zigzag orientation is found to have anti-ferromagnetic ground state while the ferromagnetic state is about 1meV higher in energy for wide channel.

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