Theory of Magnetic Edge States in Chiral Graphene Nanoribbons

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Materials Sciences Division, Lawrence Berkeley National Laboratory — Using a
model Hamiltonian approach including electron Coulomb interactions, we systemat-
ically investigate the electronic structure and magnetic properties of chiral graphene
nanoribbons. We show that the presence of magnetic edge states is an intrinsic
feature of any smooth graphene nanoribbons with chiral edges, and discover a num-
ber of structure-property relations. Specifically, we describe how the edge-state
energy gap, zone-boundary edge-state energy splitting, and magnetic moment per
edge length depend on the nanoribbon width and chiral angle. The role of environ-
mental screening effects is also studied. Our results address a recent experimental
observation of signatures of magnetic ordering at smooth edges of chiral graphene
nanoribbons and provide an avenue towards tuning their properties via the struc-
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