

Abstract Submitted
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Electronic structure of oxygen functionalized graphene nanoribbons¹ ADAM SIMBECK, DEYANG GU, Rensselaer Polytechnic Institute, NEERAV KHARCHE, Brookhaven National Laboratory, SAROJ NAYAK, Rensselaer Polytechnic Institute — We investigate the electronic and magnetic properties of armchair graphene nanoribbons whose edges are passivated by oxygen. Using a first-principles density functional approach and the many-body GW method we find that oxygen-passivation results in a rich geometrical environment which in turn determines the electronic and magnetic properties of the ribbon. For planar systems we report magnetic ground states whose electronic structure depends upon the magnetic coupling between edges. For non-planar ribbons we report a nonmagnetic ground state with a band gap that decreases as a function of increasing ribbon width. Our results will be discussed in light of previous experimental and computational studies.

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