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Study of partial oxidation of zigzag graphene 1-d ribbons S. SREEKALA, Y. ZHANG, P.M. AJAYAN, S.K. NAYAK, Rensselaer Polytechnic Institute — We study the effect of partial oxidation of graphene 1-d ribbons using the first principle- density functional theory. We have considered zigzag graphene, n=8 with four dangling carbon on each edge. The zigzag graphene 1-d ribbon is a zero bandgap material, when it is functionalized completely with hydrogen atoms. However, when two of these hydrogen atoms are replaced by oxygen, the band gap opens. This is due to the fact that the oxygen forms double bond with the carbon and hence disrupts the delocalization of the π and π^* bond. This functionalization does not induce magnetization. On further increase of oxygen, the band decreases. When oxidation is more than 75% on one side of the graphene ribbon or on either sides, the lone pair of electrons of the oxygen induces magnetization to some of the carbon atoms. Also some configurations of partially oxidized graphene show that antiferromagnetic order is the stable ordering in these systems.

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