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Metal-insulator transition in graphene oxide GEUNSIK LEE, KYEONGJAE CHO, Department of Physics and Department of Electrical Engineering, University of Texas at Dallas, Texas 75080, USA — Using the first-principles density-functional theory method, we show that metallic graphene undergoes a metal-insulator transition upon adsorption of oxygen, and that the fully oxidized metastable graphene has a large energy gap of 3.27 eV. Graphene oxide (GO) shows the transition at the coverage of 1/3 - 1/2 monolayer of epoxide group. Each O atom saturates two π orbitals, and the GO band structure is determined by the connectivity of metallic channels of π orbitals. Although such directional conduction is verified for most of GOs that we considered, we have found that longer range interaction between π orbitals also plays an important role in the electronic structure of GOs. We apply our results to the implication on electrical conductions in dry and wet GO samples.

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