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First-Principles Studies of Oxidation Functional Groups on Graphene JIA-AN YAN, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — Opening a band gap in monolayer graphene is of special interest for the graphene-based electronics applications. Inspired by the potential applications of graphene oxide, we have systematically investigated the effects of the oxidation functional groups (epoxy and hydroxyl) on the structural, energetics, and electronic properties of graphene by first-principles calculations. Our energetics calculations show that the OH group tends to aggregate to the neighboring carbon sites of an epoxy group, resulting in the formation of several possible building units. We find that the epoxy group strongly hybridizes with the extended π (π^*) bands, giving rise to a shift of the Dirac point in the momentum space and a decrease in the Fermi velocity. In contrast, the adsorption of a single hydroxyl group leads to the formation of a localized state and a gap opening near the Fermi level. The oxidation concentration dependence of the energy gap is investigated.

Jia-An Yan
School of Physics, Georgia Institute of Technology, Atlanta, GA 30332

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