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New insights into the opening band gap of graphene oxides NGOC THANH THUY TRAN, SHIH-YANG LIN, MING-FA LIN, National Cheng Kung University — Electronic properties of oxygen absorbed few-layer graphenes are investigated using first-principle calculations. They are very sensitive to the changes in the oxygen concentration, number of graphene layer, and stacking configuration. The feature-rich band structures exhibit the destruction or distortion of the Dirac cone, opening of band gap, anisotropic energy dispersions, O- and (C,O)-dominated energy dispersions, and extra critical points. The band decomposed charge distributions reveal the π-bonding dominated energy gap. The orbital-projected density of states (DOS) have many special structures mainly coming from a composite energy band, the parabolic and partially flat ones. The DOS and spatial charge distributions clearly indicate the critical orbital hybridizations in O-O, C-O and C-C bonds, being responsible for the diversified properties. All of the few-layer graphene oxides are semi-metals except for the semiconducting monolayer ones.

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