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Band-gap opening properties of graphene binding with low-concentration fluorine YUHUA DUAN, DOE-National Energy Technology Laboratory, Pittsburgh, PA 15236, CHARTER STINESPRING, Chemical Engineering Department, West Virginia University, Morgantown, WV 25506, USA, BENJAMIN CHORPENING, DOE-National Energy Technology Laboratory, Pittsburgh, PA 15236 — To better understand the effects of low-level fluorine (F) in graphene-based sensors, the structure and impact of low-concentration of fluorine defects on the electrical properties of single- and multi-layer graphene films were investigated by density functional theory with van der Waals dispersion interactions. When F bonds to a carbon atom of graphene, the carbon atom is pulled slightly above the graphene plane creating what is referred to as a C_F defect, and a valence band (B_F) near the Fermi level is formed mainly from the p orbitals of the F atoms with some small contribution from the p orbitals of the bonded carbon atoms. Depending on the F binding sites, the B_F can serve as a valence band or a conduction band and only few configurations of the F-binding graphene can open a band gap. Such results indicate that the band gap opening for graphene with low F-adsorption level strongly depends on the F-binding configurations, which is different from the fully or highly partial fluorinated graphene. At low F-adsorption level, the interaction between neighboring pairs of F adatoms is negligible and the most important interaction is between the F and carbon atoms in the C_F defect. Such results are useful for sensor and nano-electronics developments.

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