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GW study of the effect of various defects on the band gap of fluorographene YOUNG-MOO BYUN, JORGE SOFO, VINCENT CRESPI, Penn State University — Recently synthesized fluorographene, fully fluorinated graphene in a chair configuration, is a wide band-gap (E_g) semiconductor with an experimental optical band gap of ∼3 eV. However, first-principles calculations have shown that pristine fluorographene should have E_g of 5.4 to 7.5 eV. To explain this discrepancy, we have studied the effect of F vacancies, a Stone-Wales (SW) defect, C single vacancies and C double vacancies on E_g of fluorographene using density functional theory and the GW approximation. F vacancies and a SW defect are not likely to affect E_g of fluorographene, whereas a C single vacancy with a doubly fluorinated C atom, a C double vacancy, and a C double vacancy with two doubly fluorinated C atoms lead to a GW band gap of ∼4 eV, which is consistent with the optically measured E_g, and they are energetically more favorable than other C vacancies at a wide range of chemical potential of F (μ_F).

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