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 $\sim3$ 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 $\sim4$ 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 ($\mu_F$).

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