

F atoms on Graphene

Electronic properties of fluorographene

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In Short

- Exploring electronic and optical properties of fluorographene at high level of theory.
- How does different degree of fluorination influence the electronic properties?

Experimentally by exposing graphene to weak fluorination agents XeF_2 [1], fluorinated graphene can be synthesised. However, the degree of fluorination on graphene is very difficult to control and determining the exact structures in relation with experimental observables (e.g., optical and mechanical properties) remains a great challenge. Plenty of studies [2,3] of the electronic structures of fluorinated graphene using DFT functionals such as LDA and GGA functionals are available. However, the major problem presented in these commonly used DFT functionals, i.e., the so-called band gap problem, is that of their general underestimation of electronic band gaps. As a solution to this problem, we intend to focus on the electronic properties of graphene substrates fluorinated to various degrees by different levels of theory meaning employing finite grid based periodic density functional theory and plane-wave based G_0W_0 approximation [4,5] which is able to account for the effect of electron correlation on the band gap. and on optical properties of fully/partially fluorinated graphene by means of BSE calculations [6], which reincorporates electron–hole interactions into the polarisation. Our first calculations (Structures and Bandstructures are showed in Fig 1) have already showed the large influence of different degree and position of fluorination on the band structure (Fig 1 and Tab 1) Herein, we believe a systematic study of the influence of different degrees of fluorination on the band gap width with different size of the super cell will help us draw insightful of structure-function correlations.

Structure	1	2	3
G_0W_0	7.52	1.60	1.94

Table 1: Band gap width (in eV) calculated based on G_0W_0 approximation for the example fluorinated graphene.

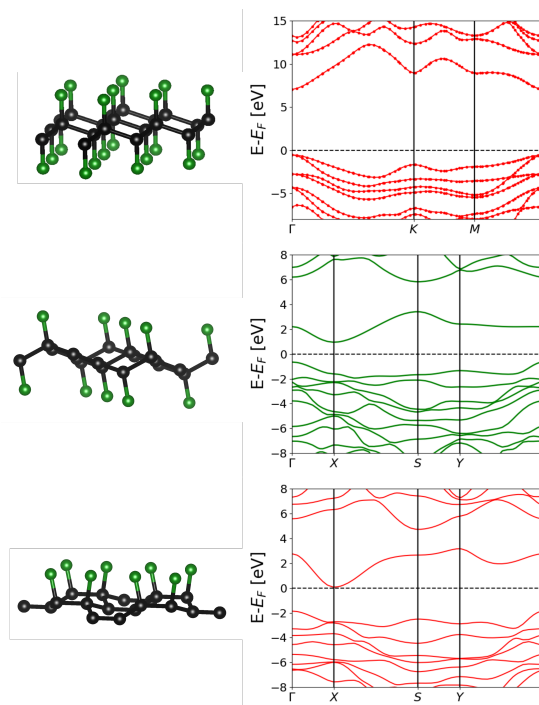


Figure 1: Examples of fully/partially fluorinated graphene and corresponding bandstructures.

More Information

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