Fluorinated graphene by DFTB

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Fluorographene is a two-dimensional material derived from graphene by attachment of fluorine [1]. It have attracted considerable interest over the past few years because of its potential applications in electronic devices and sensing. Moreover, it was shown that it is possible to introduce magnetism in CF by vacancy defect and/or by defect substitution [2]. Thus, it is not necessary to substitute atoms by transition metal atoms.

We present a methodology that combines density functional theory (DFT) based ground state calculation with tight binding approach. The so-called Self Consistent Charge Density Functional Tight Binding method (SCC-DFTB) which is an approximate, parametrised form of DFT [3] gives a response of the need for approximate methods. Thus, it helps to study large systems and to get a good compromise between computational efficiency and accuracy. Here, we show good performance of DFTB approach to investigate effect of the vacancy defect and substitutional doping on fluorographene with chemical group on the electronic structure and magnetic properties.

References

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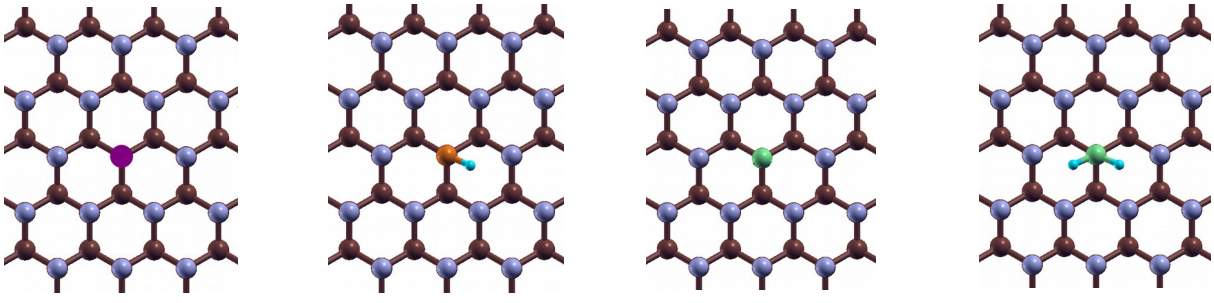
Figures



(a) (b) (c) (d)

Figure 1: Optimized structural models of (a) F defect and adsorption of (b) -OH, (c) -CN and (d) -NH_2 chemical groups on fluorographene.