Tunable electronic and magnetic properties in fluorographene and Titanium carbide via vacancy-defect and functionalization: A DFTB perspective

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Two dimensional monolayers have attracted considerable interest over the past few years due to their use on diverse applications. In addition, defects and adsorption of some chemical groups have been reported to modulate the electronic properties and the magnetic ordering in fluorographene [1] and Titanium based Mxene [2, 3], which can facilitate the use of these materials in optoelectronic and spintronic applications.

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 [4] that 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 functionalization of fluorographene and Titanium carbide Mxene on the electronic structure and magnetic properties.

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