Unraveling the electronic properties of graphene with substitutional oxygen

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Oxygen (O) is of undeniable importance in organic chemistry, being involved in a vast range of carbon (C)-based compounds. However, despite its wide variety of bonding configurations, scenarios involving O atoms with three C neighbors are rare in organic chemistry. In graphene, O plays an important role in the development of technological applications, but usually as part of out-of-plane functional groups [1]. For these reasons, the recent observation of substitutional O in the π-conjugated C honeycomb lattice [2] has generated great interest. Nevertheless, a detailed characterization of its electronic properties and an in-depth analysis of their potential novelty with respect to other type of impurities is still missing.

In this work, a combined theoretical and experimental exploration of in-plane substitutional O in monolayer graphene is presented [3]. The O implantation was realized via a controlled plasma-based process, allowing thorough atomic- to device-scale characterization. Using Density Functional Theory (DFT), we show that in-plane oxygen n-dopes graphene and we determine the distinctive character of the scattering potentials introduced in the most common impurity cases. Our simulations are combined with transport and scanning tunneling microscopy (STM) experiments, which serves to confirm the successful implantation of O, and to establish comparison with more conventional impurities like nitrogen (N)[4,5] or out-of-plane functional groups containing oxygen [1].

These achievements set up a cross-field understanding of a novel type of chemical doping in graphene and pave the way towards its implantation in other elaborate carbon nanostructures, such as graphene nanoribbons.

References

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Figures

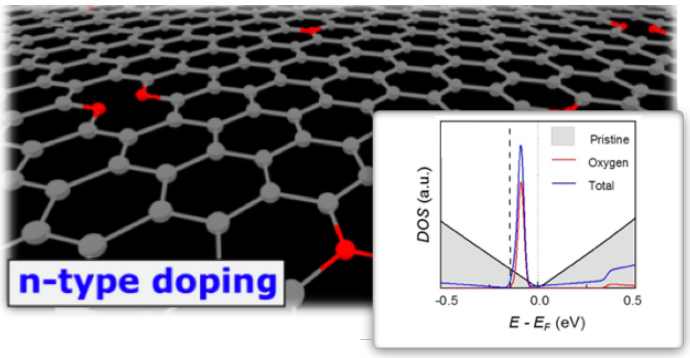

Figure 1: Illustration of different substitutional oxygen configurations, together with the effect of graphitic oxygen in the electronic structure of graphene.