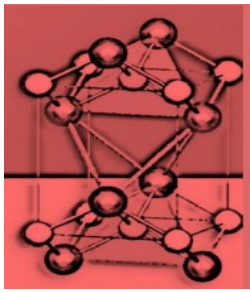

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Electronic and magnetic properties of graphene-fluorographene nanoribbons: Controllable semiconductor-metal transition

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We investigate the electronic and magnetic properties of graphene channels (2–4 nm wide) embedded within fluorographene, focusing on two distinct interfaces: the fully fluorinated α 'alpha' interface and the half-fluorinated β 'beta' interface. Density functional theory (DFT) calculations reveal that $\alpha\alpha$ systems exhibit semiconducting behavior with antiferromagnetic ordering, closely resembling pristine zigzag graphene nanoribbons. In contrast, $\alpha\beta$ systems display ferromagnetism and a width-dependent semiconductor-to-metal transition. To enable the study of larger systems, we develop and validate effective Hubbard models for both $\alpha\alpha$ and $\alpha\beta$ channels.

In order to determine the similarities and differences between graphene channels and graphene nanoribbons, where both of which have similar crystalline structure, we studied the graphene channel dependence with the degree of fluorination at the channel edges. A good observable is the localization of the states near the Fermi level. The states localized near the α interfase have almost all their weight on the graphene channel and these penetrate evanescently on the fully fluorinated graphene regions. On other hand the states localized near the β interfase, which are similar to the edge states of zigzag or Klein graphene nanoribbons, are less localized than those of graphene zigzag nanoribbons.

The effective Hubbard models were build upon DFT results and a Wannier function analysis, these models accurately reproduce the electronic structure and magnetic ordering observed in DFT calculations. Crucially, our $\alpha\beta$ model successfully captures the semiconductor-to-metal transition.

Application of this model to larger systems reveals the persistence of a ferromagnetic state with spin polarization localized at the α edge. Our results demonstrate the potential of fluorination for targeted property engineering and provide a basis for exploring graphene-fluorographene systems in device applications ranging from microelectronics to spintronics.