Tuning graphene's electronic structure via unbalanced disordered sublattices and defect superlattices

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Graphene, a single carbon plane arranged on a honeycomb lattice, has received a lot of attention in the last few years due to its very appealing physical properties as the room temperature quantum hall effect, a large coherence length or a high electronic mobility [1]. These basic properties hold a high application potential for graphene in nanoelectronics. Nevertheless the future of this field strongly depends on the possibility to control the electronic properties of this material.

On the basis of extensive tight-binding and ab initio calculations, we demonstrate the possibility to tune graphene's electronic structure via realistic atomic defects (epoxide and hydroxyl groups chemisorbed on graphene).

For example we report on the bandgap opening in graphene monolayer induced by unbalanced disordered sublattices. Our findings show that the bandgap width depends on the nature, the concentration and the distribution (random, semi-random, periodic) of the impurities. We also perform an indepth study about the special case of periodic distribution of atomic defects. We demonstrate the existence of three different families of defect superlattices which conduct to specific band structures and therefore could lead to different electronic and transport properties [2].

References

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