Defect controlled conductivity of graphene with vacancies and N impurities

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The possibility to influence the electronic structure of graphene and hence control its conductivity by adsorption or doping with adatoms is crucial in view of electronics applications. We study electronic structure and transport properties of single and bilayer graphene with vacancy defects, as well as N doped graphene. The theory is based on first principles DFT calculations employing coherent potential approximation (CPA) to describe disorder. We show that increasing the defect concentration increases drastically the conductivity in the limit of zero applied gate voltage [1], by establishing mid-gap states and carriers in originally carrier-free graphene, a fact which is in agreement with recent observations [2]. We calculate the amount of defects needed for a transition from a non-conducting to a conducting regime (i.e. a metal-insulator transition) and establish the threshold of the defect concentration where the increase of impurity scattering dominates over the increase of carrier induced conductivity [1].

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