Enhancement of spin-orbit coupling in doped graphene

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Using first-principles calculations, the possibility of enhancing the SOC in graphene due to its doping by cadmium and tellurium atoms has been shown. For the CdC_{15} structure, the spin splitting value was $E_{SOC} = 0.23 \ eV$. Co-doping of graphene by cadmium and tellurium leads to a lower spin-orbit splitting value $E_{SOC} = 0.08 \ eV$. At a low concentration of doped atoms, as in the case of the CdC_{31} structure, splitting of graphene energy levels is not observed. In conclusion, we note that the enhancement of SOC in graphene and a sufficiently large band gap induced by doped atoms is an important factor for the creation of a 2D topological insulator based on graphene operating at room temperatures [1].

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