

Abstract Submitted
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Isotope dependence of the electronic structure in graphene¹

TAKASHI KORETSUNE, RIKEN CEMS, SUSUMU SAITO, Tokyo Institute of Technology — It has been known that the effect of electron-phonon couplings on the electronic structure of diamond is not negligible and recently, it has been confirmed that the experiments are well reproduced using first-principles calculations. In case of graphene, the renormalization of the Fermi velocity due to the electron-phonon couplings has been predicted. Thus, we theoretically study the possibility of band structure engineering in graphene using the electron-phonon couplings and the isotope effect. First, we consider the difference of pure ¹²C graphene and ¹³C graphene. On the basis of density functional theory, it is found that the depth of so-called Dirac point, that is, work function of graphene, shows isotope dependence, indicating that it is possible to shift the depth of the Dirac point locally without using a gate voltage. We also discuss the possibility of band-gap opening by a periodic patterning of the carbon isotope.

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