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Fermi level tuning of N-doped graphene by an external electric field

Graphene has been keeping a premier position in the field of nanoscale sciences and technologies owing to its unique structural and electronic properties. Indeed, graphene could be regarded as an emerging material for electronic, optical, optoelectronic, and catalytic devices in the near future, being expected to exhibit remarkable efficiency. In such devices, the Fermi level tuning of graphene is the one of important issues for controlling their functionalities and properties. External electric field and formation of hybrid structures are the possible procedure to achieve the Fermi level tuning of graphene because of the electronic structure of graphene is sensitive to the external perturbations. N-doped graphene is one of representative hybrids exhibiting unusual electronic properties being applicable for electronic and catalytic devices. Furthermore, by applying the external electric field, it is expected to further control the electronic structure of N-doped graphene. However, it is still unclear how the electronic structure of N-doped graphene is affected by the interplay between the N-doping and the external electric field. Thus, in this work, we aim to give theoretical insight into the electronic properties of N-doped graphene under the external electric field, using the density functional theory combined with effective screening medium method. Here, we consider four possible N-doped graphene as shown in Fig. 1.

Our calculations show that N-doped graphene does not possess the Dirac cone but a finite energy gap in their π electron state irrespective to the defect species. On the other hand, the electronic structures near the Fermi level are sensitive to the defect species. The external electric field normal to the sheet causes the substantial electronic states modulation near the Fermi level that depends on the distribution of wave function of these states. The electronic state associated with the dangling bonds substantially shifts under upon the electron doping by the external electric field (Fig. 2), owing to their localized nature that causes the large Coulomb energy. While the non-bonding π states are insensitive to the carrier injections by the external electric field. We also found that the Fermi level monotonically increases with increasing the electron concentration. The results indicate that the band-filling of the non-bonding π states of N-doped graphene is controllable by the external electric field.

Figures

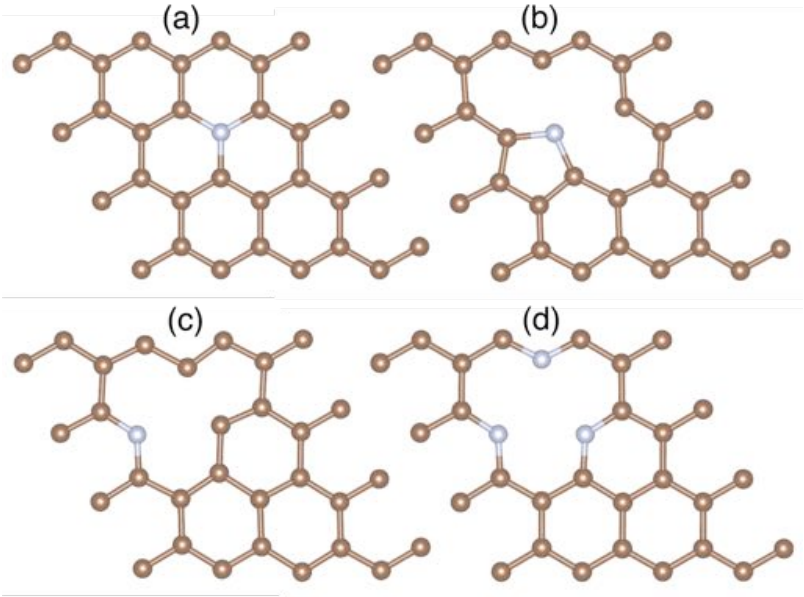

Figure 1: Optimized geometries of N-dpoed graphene with (a) graphitic, (b) pyrrolic, (c) pylidinic (pyridinic1), and (d) multiple pyridinic (pyridinic3) structures. Blown and purple circles denote C and N atoms, respectively.

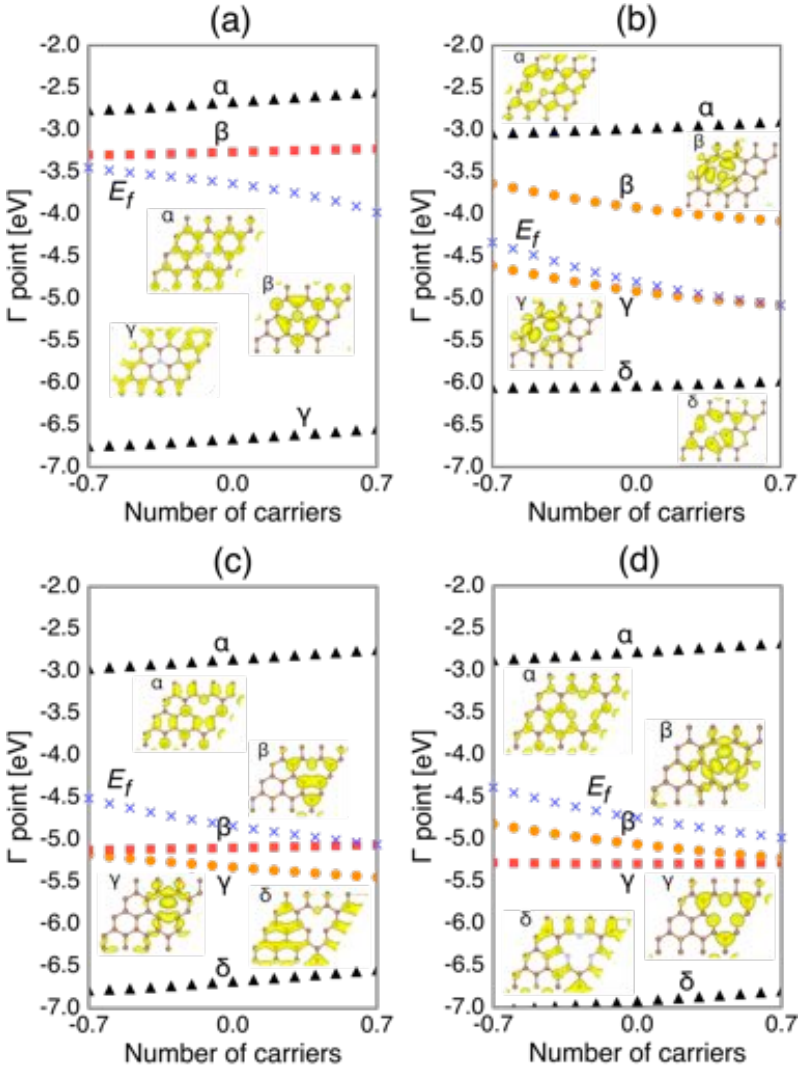

Figure 2: The Fermi level energy and eigenvalues of the electronic states near the Fermi level of N-doped graphene with (a) graphitic, (b) pyrrolic, (c) pyridinic1, and (d) pyridinic3 structures as a function of the carrier concentration. Labels assigned to wave function correspond to the eigenvalues. Crosses denote the Fermi level energy.