Novel Ba doped graphene reconstruction: a First-principles study

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Abstract
In this work, starting by experimental results, we investigate through Density Functional Theory (DFT) calculations the electronic and structural properties of Ba doped graphene grown on two different substrates. We investigate the role of the substrate in determining the electron-phonon coupling. Graphene is growth on Ni(111) substrate and then intercalated with Au or Ge monolayers, respectively (see Figures). We first demonstrate that the intercalation process is able to detach graphene from the substrate recovering the linear Dirac bands characteristic of the free-standing graphene and discuss the differences in the doping level produced by the two substrates.

Subsequent deposition of barium induces a p(2 × 2) reconstruction for both substrates, but with different adsorption site for barium. To the best of our knowledge, this is the first time in which the p(2 × 2) phase is observed for barium doped graphene. Indeed, in the bulk barium-intercalated graphite (BaC_6) the stable phase is the p(√3x√3) − R30° [1, 2] and DFT calculations predicts it is also stable for the free-standing monolayer.
Interestingly, no ordered structure is observed for identically prepared alkali and Ca-doped monolayer on Au [3, 4].

We show that the adsorption pattern of dopants is decisive for the resulting electronic band structure and related many-body effects. In addition, we calculated by first-principles the electron-phonon coupling for the E_{2g} modes at the Γ-point for the Ge- and Au- intercalated systems showing that different substrates behave in different ways: Ge substrate leads to a slightly higher charge transfer to graphene and an higher and more asymmetric electron-phonon coupling.

References

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Figures: *Top view of novel Ba doped graphene grown on Ni(111) intercalated substrate (with Au in the left panel; or Ge in the right panel).*