Role of silicon dangling bonds in the electronic properties of epitaxial graphene on SiC

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The graphitization of the Si terminated face of SiC is characterized by the formation of an interfacial layer between the graphene layer and the substrate commonly called "buffer layer" [1]. It consists of carbon atoms which are in the sp^2 and sp^3 configuration and covalently bound to silicon (Si) atoms of the SiC top layer in this latter case. Nevertheless, this SiC top layer still contains some Si dangling bonds (DBs). Despite its impact on the electronic properties of the buffer layer and consequently on epitaxial graphene(EG), the role of the Si dangling bonds remains controversial. While local density approximation (LDA) and local spin density approximation (LSDA) calculations on the buffer layer predict a metallic ground state with a half-filled narrow band [2-4], experimental results evidenced a vanishing local density of states (LDOS) at the Fermi energy and two localized states at ± 0.5 eV and ± 0.2 eV for the buffer layer and EG respectively [5,6].

In this work, we have performed first-principles simulations on the buffer layer and EG (Fig. 1a) based on the density functional theory (DFT) using the SIESTA code [7] within LSDA+U taking into account the Coulomb interaction between Si localized electrons. The extra Hubbard-U term is introduced following the standard Duradev implementation for an on-site Coulomb interaction between localized orbitals [8]. In contrast to LSDA, we found that LSDA+U results are in good agreement with experimental results. In the band structure, two localized states are obtained at ± 0.5 eV and ± 0.2 eV for the buffer layer and EG respectively (Fig. 1b-e). Our results indicate that Coulomb interaction is not suppressed by the presence of the buffer layer and the graphene layer as is the prediction of LSDA, but screening effects due to the interactions with the surrounding environment slightly reduce the U. This work provides a new paradigm for the study of EG based systems especially molecular sensors.

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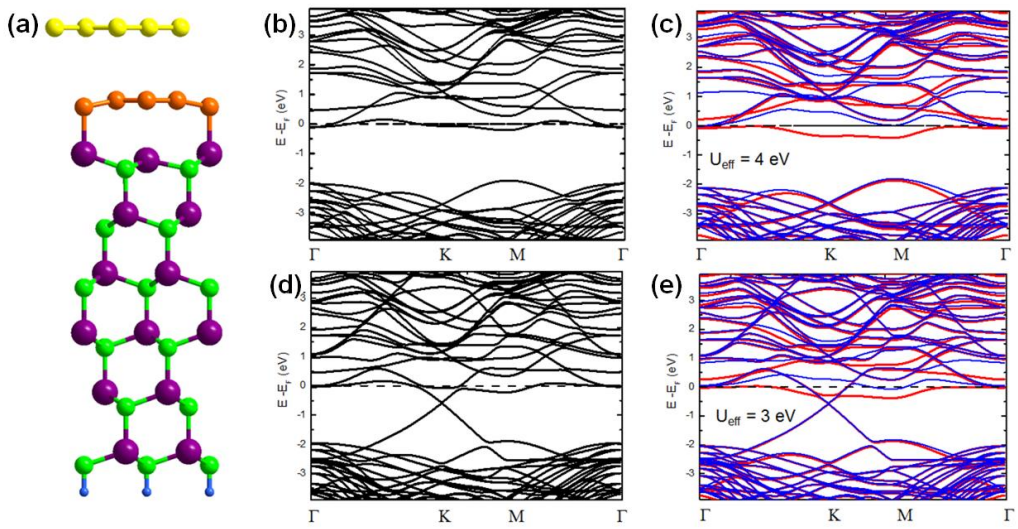

Figure 1: (a) Side view of EG on SiC. (b) LSDA and (c) LSDA+U_{eff} = 4 eV band structure of the buffer layer on SiC. (d) LSDA and (c) LSDA+U_{eff} = 3 eV band structure of EG on SiC. U_{eff} = U – J, where U and J are the Coulomb and the exchange parameters

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