Electronic-Structure Engineering of Graphene by Semiconductor Intercalation

Shixuan Du[1], Yu-Yang Zhang[1], Yixuan Gao[1], Geng Li[1], Lizhi Zhang[1], Sokrates T. Pantelides[2,1], and Hong-Jun Gao[1]

1. Institute of Physics & University of Chinese Academy of Sciences, CAS, Beijing, China, 100049
2. Vanderbilt University, Nashville, Tennessee, USA, 37240

sxdu@iphy.ac.cn

The epitaxial growth of graphene on transition-metal substrates has proved to be an efficient method to synthesize high-quality large-area graphene. However, due to the interaction between graphene and the transition-metal substrate, the electronic structure of the as-fabricated graphene is distorted. Here, using density functional theory calculations, we investigated the effect of intercalating two-dimensional (2D) silicon and III–V materials, such as double-layer honeycomb AlAs, into the graphene-metal interface. We found that the intercalation of these 2D materials significantly reduces the interaction between graphene and the transition-metal substrate. The Dirac state is largely restored. The doping level of graphene induced by the 2D intercalated material and the metal substrate is proportional to the work function difference between graphene and 2D materials/metal. We carried out a controlled experiment to intercalate silicon into the epitaxial graphene on Ru(0001). By controlling the amount of silicon, ordered arrays of nano flakes as well as single layers and multilayers of silicene can be successfully fabricated between graphene and Ru(0001). Density functional theory calculations show weak interactions between graphene and silicene layers. In addition, the as-fabricated graphene/silicene heterostructures show no observable damage after air exposure for extended periods, indicating good air stability. The I–V characteristics of the vertical graphene/silicene/Ru heterostructures show rectification behavior [1, 2].

References

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