First-principles studies of the electric-field effect on the electronic structure of trilayer graphenes

Yun-Peng Wang, Xiang-Guo Li, and Hai-Ping Cheng
Quantum Theory Project and Department of Physics, University of Florida, Gainesville, Florida 32611, USA

Electric-field effects on the electronic structure of trilayer graphene were investigated using the density functional theory in conjunction with the effective screen medium method. Two different stacking orders, Bernal (ABC) and rhombohedral (ABA) were considered. Our calculations reproduced the experimentally observed band gap opening in ABC-stacked and band overlap in ABA-stacked trilayer graphene. In addition, we studied effects of charge doping using the dual-gate configurations. The electric field induced band gap in ABC-stacked trilayer graphene can be tuned by charge doping. Electron- and hole-dopings induce distinct changes to the electronic structure of ABA-stacked trilayer graphene; hole-doping can reopen a band gap in the band overlapping region induced by electric fields.