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First-principles studies of the electric-field effect on the band structure of trilayer graphenes[1] YUN-PENG WANG, XIANG-GUO LI, HAI-PING CHENG, University of Florida — Electric-field effects on the electronic structure of trilayer graphene are investigated using the density functional theory in the generalized gradient approximation. Two different stacking orders, namely Bernal and rhombohedral, of trilayer graphene are considered. Our calculations reproduce the experimentally data on band gap opening in Bernal stacking and band overlap in rhombohedral trilayer graphene. In addition, we studied effects of charge doping using dual gate configurations. The size of band gap opening in Bernal trilayer graphene can be tuned by charge doping, and charge doping also causes an electron-hole asymmetry in the density of states. Furthermore, hole-doping can reopen a band gap in the band overlapping region of rhombohedral trilayer grapheme induced by electric fields, which contributes to an extra peak in the optical conductivity spectra.

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