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Ab initio quasiparticle bandstructure of ABA and ABC-stacked graphene trilayers MARCOS MENEZES, RODRIGO CAPAZ, Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil, STEVEN LOUIE, Department of Physics, University of California at Berkeley, Berkeley, California, USA — We obtain the quasiparticle band structure of ABA and ABC-stacked graphene trilayers through ab initio density functional theory (DFT) and many-body quasiparticle calculations within the GW approximation. To interpret our results, we fit the DFT and GW π bands to a low energy tight-binding model, which is found to reproduce very well the observed features near the K point. The values of the extracted hopping parameters are reported and compared with available theoretical and experimental data. For both stackings, the quasiparticle corrections lead to a renormalization of the Fermi velocity, an effect also observed in previous calculations on monolayer graphene. They also increase the separation between the higher energy bands, which is proportional to the nearest neighbor interlayer hopping parameter γ_1. Both features are brought to closer agreement with experiment through the quasiparticle corrections. Finally, other effects, such as trigonal warping, electron-hole assymetry and energy gaps are discussed in terms of the associated parameters. This work was supported by the Brazilian funding agencies: CAPES, CNPq, FAPERJ and INCT-Nanomateriais de Carbono. It was also supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

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