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Fermi-velocity reduction in twisted bilayer graphene: large-scale density-functional calculations KAZUYUKI UCHIDA, JUN-ICHI IWATA, SHINNOSUKE FURUYA, ATSUSHI OSHIYAMA, University of Tokyo — Twisted bilayer graphene (BLG) in which two graphene layers are rotated with a certain angle has been observed experimentally and its electronic structure has been studied using mainly tight-binding models [1]. We here report large-scale electronic-structure calculations with local-density approximation in the density-functional theory that clarify salient nature of the twisted BLG with the small rotation angles. The calculations have been done using the real-space density-functional theory (RSDFT) scheme which we have developed for the next-generation massively parallel computers. Implementation of the ultrasoft pseudopotential scheme in RSDFT allows us to treat thousands -of-carbon-atom systems in moderate-size computers. We have found that the Fermi velocity of the Dirac electron in the twisted BLG is substantially reduced compared with that in single layer graphene when the twist angle is small enough. This corroborates the observed reduction in the tight-binding models. We have also found that the wave functions at the Fermi level is strongly localized at AA-stacked region in the BLGs, opening a possibility of new magnetic functions.

[1] A. Luican et al., PRL 106, 126802 (2011); G. Trambly et al., Nano letters 10, 804 (2010); S. Shallcross et al., PRB 81, 165105 (2010).

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