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Tight-binding calculation of single-band and generalized Wannier functions of graphene ALLAN VICTOR RIBEIRO, Instituto Federal de Sao Paulo - IFSP - Birigui/SP - Brazil, ALEXYS BRUNO-ALFONSO, UNESP - Bauru/SP - Brazil — Recent work has shown that a tight-binding approach associated with Wannier functions (WFs) provides an intuitive physical image of the electronic structure of graphene. Regarding the case of graphene, Marzari et al. [1] displayed the calculated WFs and presented a comparison between the Wannier-interpolated bands and the bands generated by using the density-functional code. Jung and MacDonald [2] provided a tight-binding model for the π-bands of graphene that involves maximally localized Wannier functions (MLWFs). The mixing of the bands yields better localized WFs [3]. In the present work, the MLWFs of graphene are calculated by combining the Quantum-ESPRESSO code and tight-binding approach. The MLWFs of graphene are calculated from the Bloch functions obtained through a tight binding approach that includes interactions and overlapping obtained by partially fitting the DFT bands. The phase of the Bloch functions of each band is appropriately chosen to produce MLWFs. The same thing applies to the coefficients of their linear combination in the generalized case. The method allows for an intuitive understanding of the maximally localized WFs of graphene and shows excellent agreement with the literature. Moreover, it provides accurate results at reduced computational cost. [1] N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Rev. Mod. Phys. 84, 1419 (2012). [2] J. Jung and A.H. MacDonald, Phys. Rev. B 87, 195450 (2013). [3] D.R. Nacbar and A. Bruno-Alfonso, Phys. Rev. B 85, 195127 (2012).

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