

Abstract Submitted
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Complex evolution of the electronic structure from polycrystalline to monocrystalline graphene: generation of a new Dirac point¹
RICARDO NUNES, JOICE ARAÚJO, Depto de Física - UFMG - Brazil — First calculations, employed to address the properties of polycrystalline graphene, indicate that the electronic structure of tilt grain boundaries in this system [1-4] displays a rather complex evolution towards graphene bulk, as the tilt angle decreases, with the generation of a new Dirac point at the Fermi level, and an anisotropic Dirac cone of low energy excitations. Moreover, the usual Dirac point at the \mathbf{K} point falls below the Fermi level, and rises towards it as the tilt angle decreases. Further, our calculations indicate that the grain-boundary formation energy behaves non-monotonically with the tilt angle, due to a change in the the spatial distribution and relative contributions of the bond-stretching and bond-bending deformations associated with the formation of the defect.

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