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Ab-Initio Study of Structural, Electronic, and Elastic Properties of Graphene

© M. Guemou[1], M. Khelil[1], R. Moussa[2], A. Abdiche[3]

[1] Departement of Sciences and Technologies, University of Tiaret,
14000 Algeria
[2] Department of Physic, University of Djelfa,
17000 Algeria
[3] Electrical engineering department, University of Tiaret,
14000 Algeria

E-mail: guemoumhamed7@gmail.com

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Since its discovery in 2004, graphene has attracted the intention of several researchers in the world because of its fascinating electronic and mechanical properties. Various theoretical and experimental works have been devoted to this material. In this paper, we used a full-potential linearized augmented plane-wave (FP-LAPW) method to investigate the structural, electronic, and mechanical properties of graphene in hexagonal structure within local density and generalized gradient approximations (LDA and GGA). Our results are found in good agreement with other theoretical and experimental contributions. Using a modified Becke–Johnsone GGA approximation, we have also confirmed that graphene is a zero-gap semiconductor with the presence of a Dirac cone.

In our contribution, we have also calculated the elastic constants, the Young's modulus and Poisson's ratio of graphene that are found in good agreement with the results published in the literature.

Keywords: graphene, Dirac cone, Wien2k, mBJ-GGA approximation, elastic constants.