10.51219./materialsscienceforum.2020.19.NgoufackGuimapi

UNITED RESEARCH FORUM
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International E-Conference on
ADVANCED MATERIALS SCIENCE AND GRAPHENE NANOTECHNOLOGY
November 25-26, 2020 I Webinar

Electronic and Polaronic Properties in Graphene Doped with BN under Weak Coupling

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In this work, we study theoretically the electronic and polaronic properties of graphene doped with boron nitride using the density functional theory with the Generalized Gradient Approximation (GGA), as implemented in the wien2k code, in order to open the band gap energy of the graphene which is known as a zero band gap semiconductor. The modified Becke- Johnson (mBJ) exchange potential is used in the objectif to obtain a better energy band gap value. The properties of the magneto-polaron in monolayer graphene are also studied using the linear combination operator and the conventional Lee–Low–Pine unitary transformation. Numerical calculations indicate that the doping graphene with boron nitride causes a slight opening of the gap at the zero of Fermi level. The results also show that the ground state and the first excited state energy of the polaron in graphene has a linear relationship with the magnetic field strength, the cut- off wave number, the distance between the graphene and the substrates, meanwhile, the ground state energy will split into two branches near the Dirac point.

Keywords: Polaron; Graphene; Lee-Low-Pines-Pekar Variational Method; mBJ Potential

Biography:

Ngoufack Guimapi Cornesse Born January 12, 1991 in Batouri (East of Cameroon). She got bachelor's and master's degrees from Dschang University in physics. PhD student at the same University, Condensed Matter option she is working on the study of the properties of quasi-particles (polaron, bipolaron) in graphene and also semiconductor-based nanostructures. I am currently in Algeria as part of a mobility grant Intra-Africa Academy Project Mobility Scholarship and I recently attended a conference Maghrebian Days of Materials Science- JMSM'2020" in March 2020 of the University of Oran1 Ahmed Ben Bella (Algeria). Oral presentation.

ISBN: 978-1-8382915-1-8