

Abstract Submitted
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Dielectric function for doped graphene layer with barium titanate¹ MANUEL MARTINEZ RAMOS, ERIC GARCES GARCIA, FERNANDO MAGANA, GERARDO JORGE VAZQUEZ FONSECA, Univ Nacl Autonoma de Mexico — The aim of our study is to calculate the dielectric function for a system formed with a graphene layer doped with barium titanate. Density functional theory, within the local density approximation, plane-waves and pseudopotentials scheme as implemented in Quantum Espresso suite of programs was used. We considered 128 carbon atoms with a barium titanate cluster of 11 molecules as unit cell with periodic conditions. The geometry optimization is achieved. Optimization of structural configuration is performed by relaxation of all atomic positions to minimize their total energies. Band structure, density of states and linear optical response (the imaginary part of dielectric tensor) were calculated.

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