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**REACTION OF THE GRAPHENE VALENCE ELECTRONIC SYSTEM TO AN
EXTERNAL ELECTRIC FIELD**

Silkin V.M.

*Donostia International Physics Center, San Sebastián
IKERBASQUE, Basque Foundation for Science, Bilbao*

Various properties of graphene have been intensively investigated in numerous publications after its experimental observation in 2004 [1]. However, a question regarding the way in which the valence charge density is redistributed in the vicinity of a graphene monolayer when an external electric field is applied was not considered in detail.

This topic was touched to some degree by studying the problem of screening of the electric field induced by point charges in bulk graphite [2-5]. Thus, the in-plane distribution of the induced charge has been actively discussed [6-9]. As for the charge distribution in the direction perpendicular to the plane of carbon atoms, it was assumed to be coinciding with it.

The charge distribution in the perpendicular direction was studied by considering two- and multi-layer graphene films [10-11] but, to the best of our knowledge, not for a monolayer graphene. Moreover, regarding the position of its center of mass of the charge induced by an external electric field with respect to the plane of carbon atoms, we are unaware of such work or for a graphene film of any thickness. As a matter of fact, this question is important since, for instance, the position of the centroid of the induced density determines the so-called image-plane position that is a “real position” of a solid surface for many phenomena occurring there. It determines a “physical” position of a metal surface when an external perturbation is applied. A similar problem was widely studied in the case of metal surfaces. In general, this “real” surface position is different from the spatial localization of a geometrical crystal edge, staying towards the vacuum side [12-16].

It is usually assumed for a quasi two-dimensional (2D) system that the excess charge is confined within an infinitesimally thin 2D layer. Certainly, this assumption is reasonable if the relevant distance largely exceeds the atomic scale. However, it is critical to take into consideration what occurs on the atomic scale. Knowledge of the localization of the induced charge density is important in many fields of surface science. For instance, it determines the reference plane for the image-potential felt by an external charge placed in front of a surface. If this charge is an excited electron with energy below the vacuum level, it can be trapped by this image potential in a state belonging to an infinite Rydberg-like series [17]. The members of this series are referred to as image-potential states (IPs).

In our previous work devoted to the IPs in graphene it was assumed [18] that the image plane locates at the carbon atom plane, which seems reasonable owing to the mirror symmetry of the system. Consequently, all the quantum states should be symmetric or anti-symmetric with respect to the carbon atomic plane. As a result, a double Rydberg-like series of IPs was predicted to exist in a free-standing graphene monolayer since two surfaces are separated by a single atomic layer of matter only.

Our goal in this work is to perform the direct density-functional theory (DFT) calculations of redistribution of the valence charge density around a free-standing monolayer graphene upon application of an external electric field. From this, we establish the shape of the induced charge density caused by the electric field. From it we determine the image-plane position. Subsequently, the thus obtained image-plane position is employed for the construction of a new hybrid “DFT+image-tail” potential. With this potential a new set of binding energies for IPs is obtained and compared with the previous ones. Some other applications will be discussed.

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1. K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Electric field effect in atomically thin carbon films, Science 2004. 306, pp. 666-669.

2. P. B. Visscher and L. M. Falicov, Dielectric Screening in a Layered Electron Gas, *Phys. Rev. B* 1971. 3, pp. 2541-2547.
3. L. Pietronero, S. Strässler, H.R. Zeller, M.J. Rice, Charge distribution in c direction in lamellar graphite acceptor intercalation compounds, *Phys. Rev. Lett.* 1978. 41, pp. 763-767.
4. L. Pietronero, S. Strässler, H.R. Zeller, Nonlinear screening in layered semimetals, *Solid State Commun.* 1978. 41, pp. 399-401.
5. S.A. Safran, D.R. Hamann, Electrostatic interactions and staging in graphite intercalation compounds, *Phys. Rev. B* 1980. 22, pp. 606-612.
6. D.P. DiVincenzo, E.J. Mele, Self-consistent effective-mass theory for intralayer screening in graphite intercalation compounds, *Phys. Rev. B* 1984. 29, pp. 1685-1694.
7. S.D. DiCenzo, G.K. Wertheim, S.Basu, J.E. Fischer, Charge distribution in potassium graphite, *Phys. Rev. B* 1981. 24, pp. 2270-2273.
8. N.M.R. Peres, F. Guinea, A.H. Castro Neto, Electronic properties of disordered two-dimensional carbon, *Phys. Rev. B* 2006. 73, 125411.
9. M. Polini, A. Tomadin, R. Asgari, A.H. MacDonald, Density functional theory of graphene sheets, *Phys. Rev. B* 2008. 78, 115426.
10. E.K. Yu, D.A. Stewart, S. Tiwari, Ab initio study of polarizability and induced charge densities in multilayer graphene films, *Phys. Rev. B* 2008. 77, 195406.
11. Y. Gao, S. Okada, Carrier distribution control in bilayer graphene under a perpendicular electric field by interlayer stacking arrangements, *Appl. Phys. Express* 2021. 14, 035001.
12. N.D. Lang, W. Kohn, Theory of Metal Surfaces: Induced Surface Charge and Image Potential, *Phys. Rev. B* 1973. 7, pp. 3541-3550.
13. P.A. Serena, J.M. Soler, N. Garcia, Self-consistent image potential in a metal surface, *Phys. Rev. B* 1986. 34, pp. 6767-6769.
14. J.E. Inglesfield, The screening of an electric field at an Al(001) surface, *Surf. Sci.* 1987. 188, pp. L701-L707.
15. A.G. Eguiluz, W. Hanke, Evaluation of the exchange-correlation potential at a metal surface from many-body perturbation theory, *Phys. Rev. B* 1989. 39, pp. 10433-10436.
16. A. Kiejna, Image plane position at a charged surface of stabilized jellium, *Surf. Sci.* 1993. 287/288, pp. 618-621.
17. P.M. Echenique, J. B. Pendry, Existence and detection of Rydberg states at surfaces, *J. Phys. C: Solid State Phys.* 1978. 11, pp. 2065-2075.
18. V.M. Silkin, J. Zhao, F. Guinea, E.V. Chulkov, P.M. Echenique, H. Petek, Image potential states in graphene, *Phys. Rev. B* 2008. 80, 121408.