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Ab initio study of the buckling on silicene and germanene EDGAR MARTINEZ-GUERRA, KARLA HERNÁNDEZ, Universidad Autónoma de Nuevo León, EDUARDO CIFUENTES-QUINTAL, ROMEO DE COSS, CINVESTAV-MERIDA — Recently, a new graphene-like silicon structure was discovered: silicene. Since its discovery, silicene has been more exciting than graphene because this is a semiconductor and it should be compatible with silicon-based electronic. Silicon and germanium atoms have similar electronic configurations as those of carbon and this the reason that the bandstructure of silicene and germacene exhibits the Dirac cones at K point, with a very similar linear dispersion around it, like in graphene. The disvintage is that sp^2 bonded Si is much less stable than for carbon resulting that to be stable in the planar layer their atoms must buckle. In this work, we calculated the sp character on silicene and germacene to correlate its hibridization with the velocity of electrons and holes at Dirac cones. The calculations were performed using the pseudopotential LCAO method with GGA for the exchange-correlation energy functional. The buckling of silicene and germacene layer was 0.50 and 0.69 Å, respectively. In addition, the sp- character of silicene and germacene buckled was 2.33 and 2.64, respectively. Thus, a detailed analysis on the electronic band structure of these system show that as sp character goes from sp2 to sp3 it is correlated with a decrease of velocity of electrons and holes at Dirac cones. This study is primarly important and it could address a new future to modulate carrier velocities on bidimensional systems. This research was supported by Conacyt under Grant No. 133022.

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