Abstract Submitted
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Electronic and geometrical properties of monoatomic and diatomic 2D honeycomb lattices. A DFT study[1] NGELA ROJAS, RAFAEL REY, KAREN FONSECA, Universidad Nacional de Colombia, GRUPO DE PTICA E INFORMACIN CUNTICA TEAM — Since the discovery of graphene by Geim and Novoselov at 2004, several analogous systems have been theoretically and experimentally studied, due to their technological interest. Both monoatomic lattices, such as silicine and germanene, and diatomic lattices (h-GaAs and h-GaN) have been studied. Using Density Functional Theory we obtain and confirm the chemical stability of these hexagonal 2D systems through the total energy curves as a function of interatomic distance. Unlike graphene, silicine and germanene, gapless materials, h-GaAs and h-GaN exhibit electronic gaps, different from that of the bulk, which could be interesting for the industry. On the other hand, the ab initio band structure calculations for graphene, silicene and germanene show a non-circular cross section around K points, at variance with the prediction of usual Tight-binding models. In fact, we have found that Dirac cones display a dihedral group symmetry. This implies that Fermi speed can change up to 30% due to the orientation of the wave vector, for both electrons and holes. Traditional analytic studies use the Dirac equation for the electron dynamics at low energies. However, this equation assumes an isotropic, homogeneous and uniform space.

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