

Abstract Submitted
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Effect of the electric field on buckled and puckered arsenene.
VICTOR HUGO CHAVEZ, HECTOR NOE FERNANDEZ-ESCAMILLA, EDGAR MARTNEZ-GUERRA, UNIVERSIDAD AUTONOMA DE NUEVO LEON — With the emergence of new 2D materials, more recently phosphorene, arsenene appears as a new candidate to be explored for electronic devices. We have studied the stability of arsenene pristine and the effect of a transversal electric field on its electronic properties. The calculations were performed using the SIESTA code, with the GGA exchange-correlation functional in the PBE form. We have used numerical atomic orbitals as the basis set for the valence wavefunctions employing a double ζ -polarized basis. We use the Perdew-Becke pseudopotential for an As atom that includes the scalar-relativistic effect and Troullier-Martins parametrization. We adopt the Monkhorst-Pack scheme for k-point sampling of Brillouin zone integrations with $25 \times 25 \times 1$ and $25 \times 25 \times 1$ for the buckled/planar and puckered systems, respectively. We found that buckled and puckered arsenenes are stable and possess indirect gap. The effect of the electric field on the electronic structure of the buckled arsenene is the modulation of indirect to direct gap, while in puckered arsenene the gap linearly decreases as electric field is increased. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

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