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Electronic structure and electrical conductance properties of two-dimensional arsenin

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Abstract
Arsenene is one of the members of a large group of two-dimensional structures that in the present project, we have investigated the single layer structure and its nanoribbons based on density functional theory. In this study, after calculating the single layer band structure, we discussed the effect of width on the band structure of nanoribbon from the angle of quantum limiting phenomenon. The results show the different effect of quantum limiting phenomenon on different points of each band in the band structure, which is the cause of indirect-direct gap transition due to the reduction of the width of armchair nanoribbon. Also, the electrical conductance properties of arsenene single layer have been obtained by calculating the mobility of load carriers and the effect of uniaxial strain of crystalline structure on them has been investigated. In order to investigate the mobility, crystalline structure defects have been neglected and only phonon dispersion is considered based on Takagi relationship. In this process, the focus is not on the quantitative accuracy of the obtained values for the mobility of load carriers and the existing anisotropy between mobility in the two directions of armchair and zigzag has been the focus of the discussion. The results of the calculations show a significant anisotropy of mobility in the two directions of armchair and zigzag and the effect of uniaxial strain of crystal structure on it. Also, a significant difference between the mobility of electrons and holes in the direction of armchair is one of the key results.

Keywords: nanoribbon, bandstructure, mobility, anisotropy

For full article, refer to the Persian section