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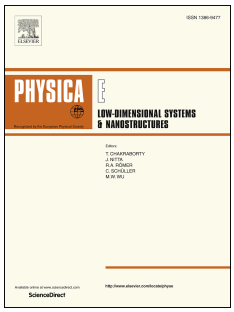

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Anisotropic mechanical properties and strain tuneable band-gap in single-layer SiP, SiAs, GeP and GeAs

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Abstract

Group IV–V-type two-dimensional (2D) materials, such as GeP, GeAs, SiP and SiAs with anisotropic atomic structures, have recently attracted remarkable attention due to their outstanding physics. In this investigation, we conducted density functional theory simulations to explore the mechanical responses of these novel 2D systems. In particular, we explored the possibility of band-gap engineering in these 2D structures through different mechanical loading conditions. First-principles results of uniaxial tensile simulations confirm anisotropic mechanical responses of these novel 2D structures, with considerably higher elastic modulus, tensile strength and stretchability along the zigzag direction as compared with the armchair direction. Notably, the stretchability of considered monolayers along the zigzag direction was found to be slightly higher than that of the single-layer graphene and h-BN. The electronic band-gaps of energy minimized single-layer SiP, SiAs, GeP and GeAs were estimated by HSE06 method to be 2.58 eV, 2.3 eV, 2.24 eV and 1.98 eV, respectively. Our results highlight the strain tuneable band-gap character in single-layer SiP, SiAs, GeP and GeAs and suggest that various mechanical loading conditions can be employed to finely narrow the electronic band-gaps in these structures.

Keywords: 2D materials; first-principles; mechanical; band-gap; simulations;

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