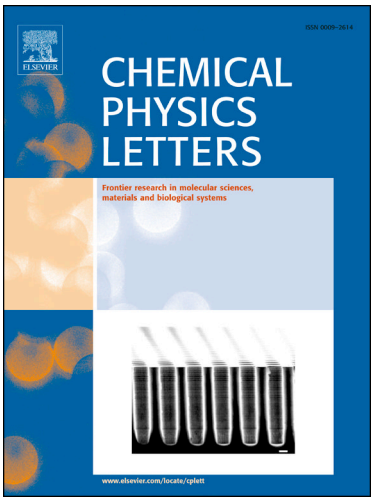

Research paper

Investigation on the stability and electronic properties of Penta-XP_5 (X=Al, Ga, In) monolayer semiconductors by using first principles calculations

Mosayeb Naseri

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Investigation on the stability and electronic properties of Penta-XP_5 (X=Al, Ga, In) monolayer semiconductors by using first principles calculations

Mosayeb Naseri[1*]

[1] Department of Physics, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

Abstract

In this paper, based on the density functional theory, three new two-dimensional pentagonal monolayer semiconductors namely penta-XP_5 monolayer (X= Al, Ga, In) are reported. The cohesive energy calculation confirms that the predicted structures are energetically stable. Furthermore, the dynamic and thermal stabilities of the structures are testified by phonon dispersion curves analysis and first principles molecular dynamic simulations respectively. Our calculations show that two-dimensional penta-AlP5, penta-GaP5, and penta-InP5 are indirect semiconductors with tunable wide band gaps (2.69 and 2.71, 2.70 eV respectively). The obtained results suggest these materials as promising candidates for application in new electronic devices in nano scale.

Key Words: First principles prediction, Monolayer, Penta-XP_5, Electronic properties

To whom correspondence should be addressed. Email: m.naseri@iauksh.ac.ir .

Introduction