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Electronic structure of beta-Si₃N₄ crystals with substitutional icosagen group impurities

By: Kutlu, E (Kutlu, E.)^[1]; Narin, P (Narin, P.)^[1]; Atmaca, G (Atmaca, G.)^[1]; Sarikavak-Lisesivdin, B (Sarikavak-Lisesivdin, B.)^[1]; Lisesivdin, SB (Lisesivdin, S. Bora)^[1]; Ozbay, E (Ozbay, E.)^[2,3,4]

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Abstract

The beta-Si₃N₄ crystals are widely used in industrial and electronics areas. Therefore, beta-Si₃N₄ has drawn the attention of researchers for many years. In this study, effects of icosagen group impurity atoms in the IIIA group on the electronic properties of the beta-Si₃N₄ crystal were analyzed by using the density functional theory. As a result of these analyses, it was determined that the electronic properties of the crystal change significantly. Basic electronic characteristics for pure beta-Si₃N₄ crystal and icosagen group impurity beta-Si₃N₄ crystals, such as band structures, densities of states, binding energies, and formation energies were investigated. We identified that the band gap of the beta-Si₃N₄ crystal was affected significantly by the impurity, and this change was varying linearly in line with the formation energy for the impurity cases. As a result of calculations, the Al-impurity was found to be the lowest-energy impurity state.

Keywords

Author Keywords: DFT; beta-Si₃N₄; Electronic structure; Formation energy; Impurity

KeyWords Plus: SILICON-NITRIDE; OPTICAL-PROPERTIES; 1ST-PRINCIPLES CALCULATIONS; MECHANICAL-PROPERTIES; GAMMA-SI₃N₄; BETA-C₃N₄; FIELD

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By: Kutlu, E (Kutlu, E.)^[1]; Narin, P (Narin, P.)^[1]; Atmaca, G (Atmaca, G.)^[1]; Sarikavak-Lisesivdin, B (Sarikavak-Lisesivdin, B.)^[1]; Lisesivdin, SB (Lisesivdin, S. Bora)^[1]; Ozbay, E (Ozbay, E.)^[2,3,4]

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