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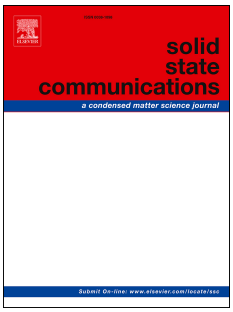

Band alignments of graphene-like III-nitride semiconductors

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Band alignments of graphene-like III-nitride semiconductors

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Abstract

Band alignment in graphene-like III-nitride semiconductors was investigated using first principles calculations and an empirical formula. We estimated the band edge positions using two simple approaches based on the energy of the band gap center (BGC) and electron affinity rules. The energy positions relative to the vacuum level were determined from the BGC and Mulliken electronegativities. These methods provided similar trends in the band lineup. The valence band and conduction band offsets determined by the first principles calculations agreed with the empirical results to within 0.5 eV. The findings suggest that the first principles and empirical methods provide a useful guide for high-throughput device design.

Keywords: DFT calculations, band alignment, layered material, semiconductor
PACS: 71.15.Mb,71.20.Nr,73.40.Kp

1. Introduction

Atomically thin two-dimensional (2D) materials, such as graphene, h-BN, transition-metal dichalcogenides, and 2D oxides have been synthesized [1]. Recently, theoretical studies predicted that conventional II-VI and III-V compound materials can have honeycomb, tetragonal, or armchair monolayer 2D structures [2, 3, 4, 5, 6, 7, 8]. These 2D materials have attracted intense research interest because of their potential applications in electronic and optoelectronic devices. Among them, 2D AlN [9, 10, 11, 12] and GaN [13]

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