

Abstract Submitted
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Many body calculations of the optoelectronic properties of h -AlN: from 3D to 2D¹ DENIZ KECIK, National Nanotechnology Research Center, Bilkent University, Ankara 06800, Turkey, CIHAN BACAŞIZ, Department of Physics, Izmir Institute of Technology, 35430 Izmir, Turkey, ENGIN DURGUN, Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey, TUGRUL SENGER, Department of Physics, Izmir Institute of Technology, 35430 Izmir, Turkey — Outstanding electronic and optical properties of graphene, h -BN, MoS₂ etc. motivate the further discovery of novel 2D materials such as AlN, a III-V compound, with remarkable features for potential optoelectronic applications, due to its wide indirect band gap. The layer and strain dependent optoelectronic properties of the recently synthesized monolayer hexagonal AlN (h -AlN) were investigated using density functional and many body perturbation theories, where RPA and BSE were employed on top of the QPG₀W₀ method. The optical spectra of 1-4 layered h -AlN revealed prominent absorption beyond the visible light regime; absorbance within the UV range increasing with the number of layers. In addition, the applied tensile strain (1 – 7%) was observed to gradually redshift the absorption spectra. While the many body corrections induced significant blueshift to the optical spectra, evidence of bound excitons were also found for the layered structures. Hence, the optoelectronic properties of layered h -AlN can be tuned by modifying their structure and applying strain, moreover are greatly altered when electron-hole interactions are considered.

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