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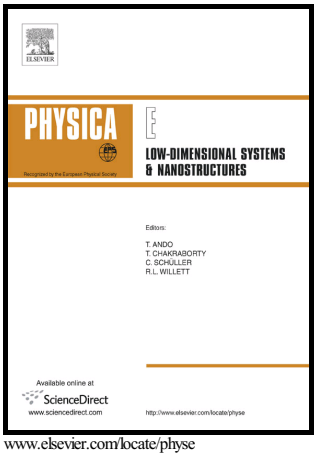

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Study of electronic and optical properties of two-layered hydrogenated aluminum nitrate nanosheet

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Abstract

First principle calculations based on density functional theory using GW approximation and two particle Bethe–Salpeter equation with electron-hole effect were performed to investigate electronic structure and optical properties of two-layered hydrogenated AlN. According to many body green function due to decrease in dimension and considering electron-electron effect, direct (indirect) band gap change from 2 (1.01) eV to 4.83 (3.62) eV. The first peak in imaginary part of dielectric function was observed in parallel direction to a plane obtaining 3.4 was achieved by bound exciton states possess 1.39 eV. The first absorption peak was seen in two parallel and perpendicular directions to a plane which are in UV region.

Graphical Abstract

The electronic structure and optical properties of the two-layered hydrogenated aluminum nitrate nanosheet based on first principle many body Green's function and Bethe Salpeter equation formalism are investigated.