CALCULATION OF THE ELECTRON ENERGY STRUCTURE IN AlN, GaN, AND InN CRYSTALS IN THE MIXED BASIS OF SINGLE-PARTICLE STATES

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S u m m a r y

Electron energy bands in crystalline AlN, GaN, and InN have been calculated in the framework of the density functional theory and making use of a mixed basis. In particular, to calculate the Hamiltonian matrix, the wave functions corresponding to the Bloch states of core electrons together with the plane waves were used. The obtained band structure is in better agreement with experiment than that calculated by the method of *a priori* atomic pseudopotentials in the framework of the local density functional theory.