

ELECTRON ENERGY BAND STRUCTURE OF GaN
AND InN EVALUATED WITHIN THE MIXED BASIS
APPROACH WITH A NEW EXCHANGE-ENERGY
FUNCTIONAL

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S u m m a r y

The electron energy band spectra of GaN and InN crystals are calculated within the mixed basis (MB) consisting of core Bloch functions and plane waves. The exchange potential is obtained on the basis of a new exchange-energy functional including electron density gradient corrections (*Generalized* Generalized Gradient Approximation, GGGA). The obtained parameters of the energy band structure of crystals are in better agreement with the data calculated using the exact exchange potential than those obtained in the Local Density Approximation (LDA). The calculated energies of semicore *d*-electrons are close to the experimental data.