ELECTRONIC PROPERTIES OF (111) SURFACE IN A^3B^5 AND A^2B^6 CRYSTALS

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S u m m a r y

The electronic band structure, the local densities of states (the total and layer-resolved ones), and the distribution of charge density of valence electrons at the (111) polar surface in A^3B^5 and A^2B^6 crystals, such as GaAs and ZnSe, have been studied. The properties of anion- and cation-terminated surfaces have been analyzed separately. The self-consistent "3D" pseudopotential method has been used for numerical calculations in the framework of a model of layered superlattice. The application of an original iterator in the self-consistence procedure allowed difficulties associated with the surface-induced presence of reciprocal-lattice vectors shorter that 1 a.u. to be overcome.