CALCULATIONS OF THE TEMPERATURE DEPENDENCES OF THE BAND STRUCTURE AND THE DENSITY OF STATES OF HEXAGONAL ZINC OXIDE

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S u m m a r y

In the framework of the pseudopotential method and making use of phenomenological parameters, the temperature dependences of the energy extrema at highly symmetric points Γ, L, K, M, A, and H of the Brillouin zone in hexagonal zinc oxide, as well as the energies of the main interband transitions between them, have been calculated. The temperature dependence of the density of states has been also studied. The influence of the temperature on the electronic structure of ZnO was studied taking two factors into account: thermal expansion of the lattice and electron-phonon interaction. The temperature dependences of the energy levels, inter- and intraband transitions, and the density of states have been analyzed in detail. The results obtained are in good agreement with experimental data.