Electronic structure and exchange interaction in GdB_4 compound

A. E. Baranovskiy

B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Lenin Ave., Kharkov 61103, Ukraine

Ab initio band structure calculations have been carried out using the LDA+U theoretical method with the all-electron Full Potential Linearized Augmented-Plane Wave (FP-LAPW) code for antiferromagnetic GdB_4 compound. The densities of electronic states and ground state energies were calculated for various hypothetic magnetic configurations, including the realistic Shastry-Sutherland lattice. The results obtained were examined and analyzed in the framework of the Heisenberg model in order to shed light on peculiarities of exchange interaction within RB_4 series.