Electronic and Magnetic Properties of the Low and High Temperature Phases of Gadolinium Orthoborate $GdBO_3$

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Much attention has been recently paid to rare earths orthoborate phosphors ($REBO_3$, RE = Y, La, Gd) due to their high visible light yield as well as chemical and thermal stability (see, e.g., [1-2]). The main aim of the paper is to study electronic and magnetic properties of $GdBO_3$ system crystallizing in the newly discovered phase having triclinic symmetry [3]. Also the high temperature phase having a calcite related structure [4] was investigated. We present results of $ab-initio$ fully relativistic band structure calculations based on the full potential local orbital (FPLO [5]) method. We will present the band structures, local and total densities of electronic states as well as after spin polarized calcualtions the spin and orbitals magnetic moments.

References:

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