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Influence of different exchange correlation potentials on band structure and optical constant calculations of $ZrGa_2$ and $ZrGe_2$ single crystals

Abstract

The all-electron full potential linearized augmented plane wave method was used to solve the Kohn Sham DFT equations. We have employed different approximations for the exchange correlation potentials, namely: LDA, GGA and EVGGA, and insignificant effect on the band structure and the density of states were found. Calculations show that there is a significant difference in the band dispersion with replacement of Ga by Ge that is attributed to the fact that in the $ZrGe_2$ compound Zr atom is situated at 4c site and two Ge atoms are situated at 4c site. Whereas for $ZrGa_2$ compound Zr is located at 4g site and the three Ga atoms are situated at 4h, 2c and 2a sites, respectively. There exists strong hybridization between the states. Moving from $ZrGa_2$ to $ZrGe_2$ has significant influence on the magnitudes and the peak positions of states. The optical properties of the two compounds were studied and analyzed.

Keywords — Crystal growth, electronic band structure, inorganic materials