

# Full potential investigations of structural and electronic properties of $\text{ZrSiO}_4$

R. Terki\*, H.I. Feraoun, G. Bertrand, H. Aourag

*LERMPS-UTBM site de Sévénans, 90010 Celfort Cedex, France.*

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The full-potential linearized augmented plane wave (FP-LAPW) method within the density functional theory is used to calculate the structural and electronic properties of  $\text{ZrSiO}_4$  in its low and high pressure phases. In this approach, the generalized gradient approximation was used for the exchange correlation potential. We have firstly optimised the internal parameters and used them to calculate the ground state properties such as lattice constants, bulk modulus and its derivative, inter-atomic distances and angles as well as the structural phase stability. The transition pressure at which  $\text{ZrSiO}_4$  undergoes structural phase transition from zircon to scheelite structure is also determined. The results are compared with previous calculations and with experimental measurements. On the other hand, calculations of the charge densities were performed to describe the nature of chemical bonding; band structure and density of states, which allow us to discuss the features of orbital mixing, are also given. Furthermore, a comparative study between the scheelite and zircon phases of  $\text{ZrSiO}_4$  is presented in this work.

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\* Corresponding author. Tel. 33(0)384583023. FAX 33(0)384583286.  
*Email address:* rachida.terki@utbm.fr (R. Terki).