FIRST PRINCIPLE CALCULATION OF ELECTROINIC BAND STRUCTURE OF LuRhO3 COMPOUND

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MSC 2000: 34C10

Abstract

The structural and volume optimization, electronic band structure density of states of valance electrons of crystal LuRhO3 have been investigated using the density functional methods, local density approximation and generalized gradient approximation, in Abinit package program. The obtained band structure and calculated density of states of valance electrons for LuRhO3 compound shows that the electronic structure of crystal has a semiconductor state. Besides, the structural and volume optimization has been performed. To our knowledge in literature, the structural and volume optimization, energy band structure and density of states of valance electrons LuRhO3 crystal have not been investigated as either experimentally or theoretically. Therefore, in present work, using density functional theory, we investigated the physical properties such as the structural and volume optimization, energy band structure and density of states of valance of this compound.

Keywords: Structural properties, electronic band structure, density of states

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