AB INITIO CALCULATION OF PHYSICAL PROPERTIES OF RbGeCl3

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Abstract

We have calculated the structural and electronic properties of RbGeCl3 compound using the density functional theory within the generalized gradient approximation and the local density approximation. The calculated results for each physical property are presented and then compared with available experimental and previous theoretical data. To our knowledge, structural properties and energy band structure of RbGeCl3 compound has not been investigated using DFT. Therefore, we investigated the physically properties such as such as structural and volume optimizations, electronic energy band structure and density of states of valance electrons of this crystal.

Keywords: DFT, electronic properties, structural properties

References

[1] Li-Chuan Tang, Li-Qiang Liu, Yia-Chung Chang, Jui-hsien Yao, Jung-Yau Huang and Chen-Shiung Chang, Japanese Jornal of Applied Physics, 48 082001- 082007 (2009).

[2] Dieter Messer, Z. Naturforsch. 33b, 366-369 (1978).

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