Calculation of the Structural Properties of $GdBO_3$ by the Theoretical Method ab-initio

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Introduction

Actually, the industry demand is still very important inthis field of advanced innovative materials due to their potential applications in many luminescent devises Until now, rare earth ions doped inorganic luminescent nanomaterials with controllable, very clear morphologies has been an important challenge of modern materials physics and chemistry. Actually, it is well established that the properties of such luminescent nano-crystals depend on their structure, phase, shape, dimensionality, and size distribution in addition to their chemical composition,the luminescence quenching due to these defects will be significant. Borate of gadolinium (GdBO3) is an important class of host materials because of their high vacuum ultra- violet (VUV) transparency and exceptional optical damage thresholds. These properties make them good candidates for scintillators, flat displays and mercury-free fluorescent tubes. Primarily, the $GdBO_3$ and YBO_3 orthoborates are isostructural. They own a "YBO_3" type structure derived from the vaterite structure

Theoretical Study

in this work we will calculate the structural properties of $GdBO_3$ after the system relaxation and the optimizationof some parameters such as cut-off energy and the volumeof the elementary cell which corresponds to the mostbasic energy by method ab-initio.

Results and Discussion

Details of structure and calculation of $GdBO_3$

Pure $GdBO_3$ crystal crystallize in the vaterite (Hexagonal structure) space group p63/mmc [1], No 194, In the hexagonal mesh, trivalent rare earth cations (TR3 +) occupy two sites different crystallographic. The first is an octahedral site and the second is coordination twelve.

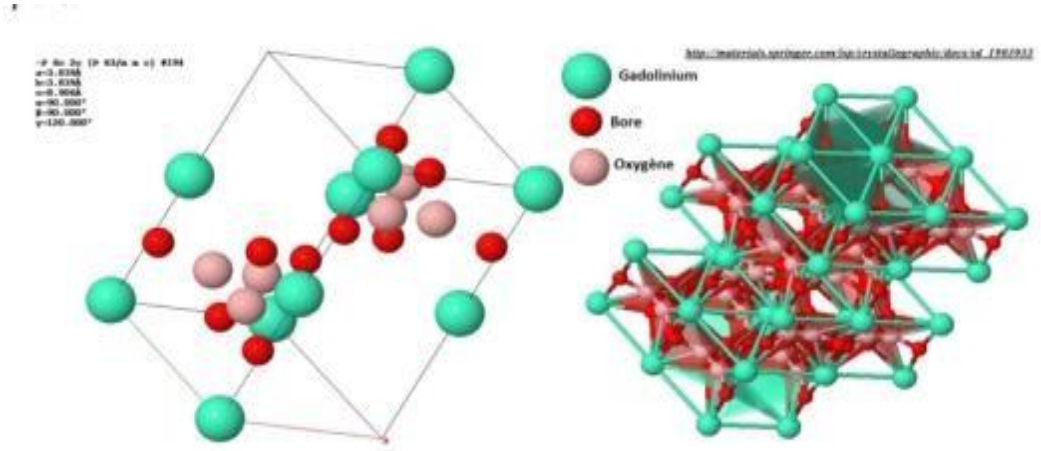

Fig 1 : the structure of $GdBO_3$

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The constant anion model of the GdBO3 structure was firstly considered, $GdBO_3$ has a Hexagonal structure space group p63/mmc, lattice constants a = b = 3.83 Å, c = 8,90 Å, and crystal plane angles α = β = 90°,γ = 120° [2]. As shown in Fig. 1

Relaxation structure

Optimization of Cutt-of energy and volume

After determining the number of points k, we set the latter to the value of 2x2x2 and we vary the breaking energy between 300 and 700 eV, for each of these values, the total energy is calculated and the curve (Figure III.6) of variation of the total energy according to the Ecutvalues. This curve shows us that the energy total converges within the limits of 450 eV. (Fig 2)

We have optimized and relaxed the structure of Y2O3, seeking to minimize energy and canceled out the Hellmann-Feynman forces [3], which act on atoms, we calculated the mesh parameter of the equilibrium statethen the modulus of compression, which gives the lowesttotal energy value (the state fundamental). The mesh parameter values are varied from -10% to 10% of the value of experimental lattice parameter

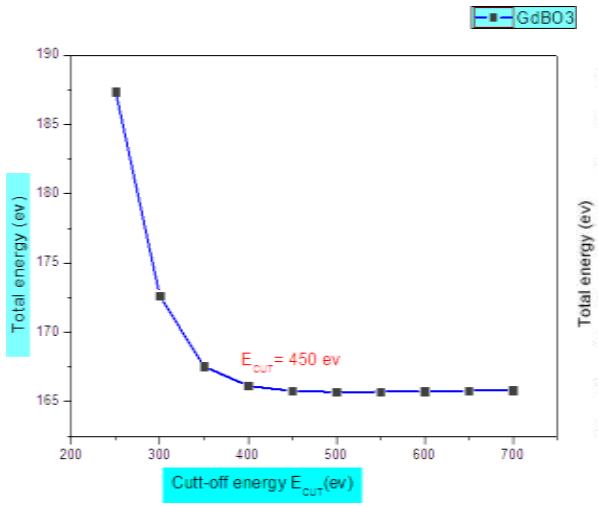

Fig 2 : Optimization of Cutt-of energy

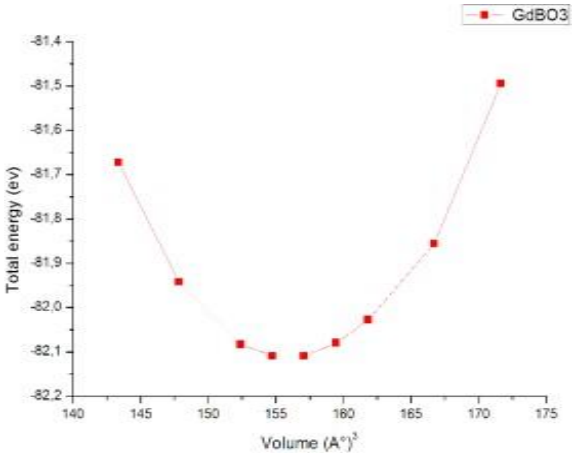

Fig 3 : Optimization of volume

Conclusion

In all cases the calculation of the optimizedstructure and properties were performed until theabove given convergence limits were reached the obtained results are discussed in this work

Acknowledgments

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