# STRUCTUAL, DYNAMIC AND TERMODYNAMIC PROPERTIES OF $CsPbBr3$ COMPOUND IN CUBIC PEROVSKITES VIA FIRST PRINCIPLES

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## Abstract

The electronic, dynamic and termodynamic properties of $CsPbBr3$ compound in the cubic perovskite phase are systematically investigated using the first principles calculations. The generalized gradient approximation was used for exchanged and correlation interaction. The theoretically calculated lattice constant and band gap are found to be good in agreement with the other theoretical and experimental results. We studied dynamic and termodynamic properties of $CsPbBr3$ in cubic perovskite phase and have not encountered any avaliable data for dynamic and termodynamic properties of $CsPbBr3$ in cubic perovskite phase. We calculated the entropy, constant-volume specific heat, Helmholtz free energy for $CsPbBr3$.

**Keywords:** Electronic properties, dynamic properties, thermodynamic properties

## References

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