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6b) FIRST-PRINCIPLES CALCULATION OF SOME PEROVSKITE STRUCTURES

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The Perovskites are named after the mineral with the formula CaTiO_3 . Several hundred materials with the formula ABO_3 are known to have this structure. The electronic properties of ABO_3 are calculated by the full potential-linearized augmented plane wave (FP-LAPW) method with the generalized gradient approximation (GGA). The calculated results in comparison with the previous theoretical data are in better agreement with the experimental results.

Keywords: Perovskite Structure, First-principles