

# Density functional study of the structural and phase transition of silver halides: LDA versus GGA calculations

H. Rekab Djabri

,  
R. Yagoub

,  
S. Bahlouli

,  
S. Amari

and

S. Louhibi Fasla

<https://doi.org/10.1142/S2047684119500064>

[Previous](#)

[Next](#)

- [Tools](#)
- [Share](#)

## Abstract

This paper deals with the theoretical calculation of structural and electronic, properties of AgBr and AgCl compounds using density functional theory within generalized-gradient (GGA) approximation and local density approximation (LDA). We employ the full potential linear muffin-tin orbitals (FP-LMTO) as implemented in the Lmtart code. We have used to examine structure parameter in eight different structures such as in NaCl (B1), CsCl (B2), ZB (B3), NiAs (B8), PbO (B10), Wurtzite (B4), HCP (A3)  $\beta\beta$ Sn (A5) structures. The equilibrium lattice parameter, bulk modulus and its pressure derivative were presented for all calculated phases. The calculated ground state properties are in good agreement with available experimental and theoretical results. A pressure induced structural phase transition from NaCl (B1) to HCP (A3) phases at 37.66 and 18.11 GPa for AgBr and AgCl, respectively, and from NaCl to CsCl phase in AgBr and AgCl

at 90.55 and 24.4GPa, respectively, is also predicted. Furthermore, the band structures are computed. Our results are compared to other theoretical and experimental works, and excellent agreement is obtained.

### Keywords:

- [FP-LMTO](#)
- [structural properties](#)
- [electronic properties](#)
- [AgCl](#)
- [AgBr](#)

## Access content

To read the fulltext, please use one of the options below to sign in or purchase access.

---

- [Personal login](#)
- [Register for access](#)
- **[Purchase](#)**[Save for later](#)

**Article Online Access**GBP35.00

- [Claim](#)
- [Restore content access](#)

This functionality works only for purchases made as a guest