First-Principles Investigation of the Structural and electronic properties of Ag-Based II–VI and III–V Semiconductor Compounds

Khelil Mohamed [a,b], Ammari Abdelkader [c,d], Ghlamallah Benabdellah [e], Hadji Kouider [c], Abbar Boucif [f], Jaim Lloret Mauri [g]*

[a)] Department of Sciences and Technology, Ibn Khaldoun University, Tiaret (Algeria). [b)] Laboratory of Industrial Technology, Ibn Khaldoun University, Tiaret (Algeria). [c)] Department of Physics, Faculty of Matter Sciences, Ibn Khaldoun University, Tiaret (Algeria). [d)] Laboratory of Micro and Nanophysics, National Polytechnic School (ENPO), Oran (Algeria). [e)] Laboratory of Physical Engineering, Ibn Khaldoun University, Tiaret (Algeria)[f)] Computational Materials Science Laboratory, Djillali Liabès University, Sidi-Bel-Abbes (Algeria). [g)] Department of Communications, Universitat Politècnica de València, Camino de Vera, Valencia (Spain).

m_khelil@univ-tiaret.dz

Silver-based compounds have attracted considerable attention due to their promising applications in optoelectronic, photovoltaic, and thermoelectric devices. In this work, the structural and electronic properties of AgRM (M = S, Se, Te; R = Sb, Bi) compounds in the chalcopyrite, zinc-blende, and rock-salt phases were systematically investigated using density functional theory (DFT) within the full-potential linearized augmented plane wave (FP-LAPW) method. The equilibrium lattice constants and bulk moduli were determined using several exchange-correlation approximations, including the local density approximation (LDA), Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA), and Wu–Cohen generalized gradient approximation (WC-GGA), in order to assess their influence on the structural parameters. The calculated results indicate that the chalcopyrite phase is the energetically most favorable configuration for most of the studied compounds, whereas the zinc-blende and rock-salt phases are found to be metastable under ambient conditions. The calculated equilibrium lattice constants range approximately from 5.3 to 6.1 Å, while the bulk moduli vary between 66 and 102 GPa, depending on the compound and crystal structure, and are in good agreement with available theoretical and experimental data. Furthermore, the electronic properties were investigated through band-structure and density-of-states (DOS) calculations, performed both without and with spin–orbit coupling (SOC). The results show that all the studied compounds exhibit a semimetallic character, while the inclusion of SOC modifies the band dispersion near the Fermi level due to the strong relativistic effects associated with the heavy elements Sb and Bi. These findings provide reliable structural and electronic parameters and offer valuable insights for future investigations of the optical, elastic, and thermoelectric properties of Ag-based compounds.

Keywords:
Density Functional Theory, WIEN2k, FP-LAPW, Silver Chalcogenides, Chalcopyrite, Structural Properties.

References:

[1] Khelil, A. Abdiche, A. Ammari, B. Abbar, M. Guemou, R. Moussa, Bismides ternary alloys GaSb1−xBix: Structural, optoelectronic, and thermodynamic properties under pressure, J. Mater. Res. 37 (2022) 1877–1891. https://doi.org/10.1557/s43578-022-00599-x.
[2] Nozawa, T. Ishiyama, Y. Kiyono, K. Yabuki, T. Suemasu, K. Toko, High-rate capability of III–V anodes enabled by machine-learning-guided compositional design, J. Energy Storage 154 (2026) 121199. https://doi.org/10.1016/j.est.2026.121199.
[3] Mohamed, K., Ammari, A., Benabdellah, G., Hadji, K., & Abbar, B. (2026). First-principles calculations to investigate optoelectronic properties and pressure effect on thermodynamic parameters of the quaternary alloys Ga $_{1-}$ xSb $_{1-}$ yTlxBiy . Applied
Physics A, 132 (8), 753. https://doi.org/10.1007/s00339-026-09896-2.
[4] Benabdellah, K. Benkabou, Structural, elastic, and optoelectronic properties of ternary alloy Bx A l(1 − x) As, Phys. B Condens. Matter 544 (2018) 52–60. https://doi.org/10.1016/j.physb.2018.05.007.
[5] P. Blaha, WIEN 2 k : an augmented plane wave plus local orbital package for the electronic structure of solids, in: 2021: pp. 836–842.https://doi.org/10.1107/S1574870720003171.