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Structural and electronic properties of $Cu_xAg_{1-x}Cl$: First-principles study

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Abstract.

The structural and electronic properties of the ternary $Cu_xAg_{1-x}Cl$CuxAg1−xCl alloy are investigated using a recent version of the full potential linear muffin-tin orbitals method (FPLMTO) based on the density functional theory, within both the local density approximation (LDA) and the generalized gradient approximation (GGA). The lattice constants, bulk modulus and band gap were calculated as a function of copper molar fraction *x* in rock salt ($B1$) and zincblende ($B3$) structures. These parameters were found to depend non-linearly on alloy concentration Cu, except for the lattice parameter which follows Vegard's law. Our results predict the rock salt phase as the ground state for this ternary system.