

# Structural, elastic, electronic, chemical bonding and optical properties of Cu-based oxides ACuO (A = Li, Na, K and Rb): An ab initio study

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**Abstract:** Ab initio total energy calculations were performed to study in details the structural, elastic, electronic, chemical bonding and optical properties of Cu-based ternary oxides ACuO (A = Li, Na, K and Rb). Optimized atomic coordinates and lattice constants agree well with the existing experimental and theoretical data. Numerical estimations of the six independent elastic constants  $C_{ij}$  and their related properties for monocrystalline ACuO were obtained. A set of elastic moduli for polycrystalline ACuO, namely bulk modulus B, shear modulus G, Young's modulus E, Poisson's ratio  $\nu$ , Lamé coefficients  $\lambda$  and  $\mu$  and Debye temperature  $\theta_D$  were evaluated. Band structure, total and site-projected l-decomposed densities of states, charge-carrier effective masses, charge transfers and charge density distribution maps were obtained; analyzed and compared with the available theoretical data. Complex dielectric function, refractive index, extinction coefficient, reflectivity and loss function spectra were calculated with an incident radiation polarized parallel to both [100] and [001] crystalline directions.

**Keywords :** Cu-based oxides Ab initio calculations Elastic constants Electronic properties Chemical bonding