Computational Materials Science, vol.81, 2014, pages 561–574

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

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 σ, Lamé coefficients λ and Debye temperature ϑ_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 [1 0 0] and [0 0 1] crystalline directions.

Keywords; Cu-based oxides, *Ab initio* calculations, Elastic constants, Electronic properties, Chemical bonding, Pressure effect