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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 Cij 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 r, Lamé coefficients k and Debye temperature hD 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