Ab initio study of the optical phonons in one-dimensional antiferromagnet $Ca_2 CuO_3$

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Abstract: We present the cluster-model ab initio study of the optical phonons in the one-dimensional antiferromagnet Ca2 CuO3 based on the Hartree-Fock self-consistent field calculation with the 3-21G basis set. The obtained results showed very good agreement with the observed data. The Cu-O bands generally showed lower shifts in Ca2 CuO3 than in pure CuO and were primarily composed of the vibrations of the oxygen in static host lattice, whereas the Cu movements only happened in the collective lattice vibrations. An almost complete classification of the forbidden phonons is presented. ?? 2008 American Institute of Physics.

Index Keywords: Antiferromagnetic materials; Calcium compounds; Chemical shift; Copper oxides; Lattice vibrations; Optical materials; Cluster model ab initio study; Hartree Fock self-consistent field calculations; Optical phonons; Static host lattices; Phonons

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