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Thermal properties of $CuGaS_2$ from first principles[1]
ALDO H. ROMERO, CINVESTAV, Unidad Queretaro, Mexico, MANUEL CARDONA, REINHARD KREMER, MPI, Stuttgart, ALEXANDER SCHINDLER, NETZSCH-Geratebau GmbH, ALFONSO MUÑOZ, Departamento de Fisica, Universidad de la Laguna, Spain — We have investigated in the past the specific heats of monatomic and binary semiconductors and their dependence on temperature and isotopic mass, both experimentally and theoretically. The theoretical calculations were performed *ab initio* with LDA exchange correlations. We are at present carrying over these investigations to ternary materials, in particular to those with chalcopyrite structure. We present here results involving the dependence of the specific heat and other physical properties (lattice parameters, volume thermal expansion, phonon dispersion) of the chalcopyrite $CuGaS_2$ on temperature and on the isotopic masses of the three constituent atoms. Particular emphasis is paid to the maxima of C_p/T^3 found at low temperatures which correspond to the deviation of Debye's law related to transverse acoustic phonons near the zone boundary. The calculations were performed with the ABINIT and VASP codes within the local density approximation for exchange and correlation. The results are shown to be in excellent agreement with the experimental data. Correlation with similar compounds such as $CuAlS_2$ and $CuInS_2$ is discussed.

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