Abstract Submitted
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Vibrational and thermal properties of ternary semiconductors and their isotopic dependence: chalcopyrite CuGaS2[1] ALDO ROMERO, CINVESTAV, Unidad Queretaro, M. CARDONA, R. KREMER, R. LAUCK, Max Planck Institute, Stuttgart, A. MUÑOZ, ULL, Spain — The availability of *ab initio* electronic calculations and the concomitant techniques for deriving the corresponding lattice dynamics have been profusely used in the past decade for calculating thermodynamic and vibrational properties of semiconductors, as well as their dependence on isotopic masses. The latter have been compared with experimental data for elemental and binary semiconductors with different isotopic compositions [1]. Here we present theoretical and experimental data for several vibronic and thermodynamic properties of a canonical ternary semiconductor of the chalcopyrite family: CuGaS2 [2]. Among these properties are the lattice parameters, the phonon dispersion relations and densities of states (projected on the Cu, Ga, and S constituents), the specific heat and the volume expansion coefficient. The calculations were performed with the ABINIT and VASP codes within the LDA approximation for exchange and correlation.

[1] Cardona *et al.*, PRB81, 075202 (2010)
[2] Gibin *et al.*, Solid State Commun Solid State Commun 133, 569 (2005); Sanati *et al.* S.S. Commun 131 229 (2004).

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Aldo Romero
CINVESTAV, Unidad Queretaro

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